

**NINTH ANNUAL CONFERENCE OF THE YUGOSLAV MATERIALS  
RESEARCH SOCIETY**

# **YUCOMAT 2007**

Hotel "Plaža", Herceg Novi, Montenegro, September 10–14, 2007  
<http://www.yu-mrs.org.yu>



## **Programme and The Book of Abstracts**

Organised by:

**Yugoslav Materials Research Society,  
Faculty of Metallurgy and Technology, Podgorica  
and**

**Institute of Technical Sciences of the  
Serbian Academy of Sciences and Arts, Belgrade**

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**Title:** THE NINTH YUGOSLAV MATERIALS RESEARCH SOCIETY CONFERENCE  
“YUCOMAT 2007”  
Programme  
and  
The Book of Abstracts

**Publisher:** Institute of Technical Sciences of SASA  
Knez Mihailova 35/IV; P.O. Box 377, 11000 Belgrade, Serbia  
Phone: +381 11 2185-437; Fax: + 381 11 2185-263  
<http://www.itn.sanu.ac.yu>

**Editor:** Prof. Dr. Dragan P. Uskoković

**Technical editor:** Aleksandra Stojičić

**Cover page:** Aleksandra Stojičić

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**Acknowledgment:** The editor of the book of abstracts is grateful to the Ministry of Science of the Republic of Serbia for its financial support of this book and The Ninth Yugoslav Materials Research Society Conference “YUCOMAT 2007” held in Herceg Novi.



**Printed in:** Printing office “Čigoja”  
Studentski trg 15, 11000 Belgrade  
Phones: + 381 11 2186-725; + 381 11 625-954  
Circulation: 300 copies. The end of printing: July 2007.

## **Yu-MRS**

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## **HISTORY:**

Materials science and engineering incorporate acquiring of knowledge on synthesis and processing of materials, their composition and structure, properties and behaviour, functions and potentialities as well as application of that knowledge to various final products. Economic prosperity, life quality, and healthy environment are tightly connected with the improvements in the existing and the development of new materials and processing technologies. These improvements and development can contribute greatly to the national priorities: energy saving, environment and health protection, information and communication, infrastructure, transportation, etc.

The Yugoslav Materials Research Society (Yu-MRS), a non-government and non-profit scientific association, was founded in 1997 to promote multidisciplinary goal-oriented research in materials science and engineering. Main task and objective of the Society is to encourage creativity in materials research and engineering to reach a harmonic coordination between achievements in this field in our country and analogous activities in the world with an aim to include our country into the global international projects.

The First Conference on materials science and engineering, including physics, physical chemistry, condensed matter chemistry, and technology in general, was held in September 1995, in Herceg Novi. An initiative to establish Yugoslav Materials Research Society was born at the conference. Similar to other MR societies in the world, the programme was made and objectives determined. Until 2003 Conferences were held every second year and then they grew into Annual Conference that will be traditionally held in Herceg Novi in September of every year.

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# Programme

### **CONFERENCE PROGRAMME**

**SYMPOSIUM A** Advanced Methods in Synthesis and Processing of Materials  
**SYMPOSIUM B** Advanced Materials for High-Technology Application  
**SYMPOSIUM C** Nanostructured Materials  
**SYMPOSIUM D** Composites  
**SYMPOSIUM E** Biomaterials  
**WORKSHOP:** Serbia-Slovenia Bilateral Cooperation  
**TECHNOLOGICAL FORUM**

### **GENERAL INFORMATION**

**DATE AND VENUE:** The conference will be held on September 10-14, 2007, at the PLAŽA Hotel, in Herceg Novi, Montenegro. Participants will be accommodated at the Plaža Hotel. The conference will begin on Monday, September 10<sup>th</sup>, at 09.00 and end on Friday, September 14<sup>th</sup>, 2007 at 12.30.

**REGISTRATION:** Registration, registration fee payment, conference materials distribution, etc. will take place at the conference desk (Conference Secretariat) open on Sunday, September 9, and Monday, September 10, from 8.00 to 19.00, on Tuesday to Thursday 8.00-10.00, 14.00-16.00 and 18.00-20.00, and on Friday from 8.00 to 12.30. At registration, the participants are requested to submit proof of their advance registration fee payment.

**INSTRUCTION FOR AUTHORS:** The conference will feature plenary sessions, poster sessions, Workshop on Slovenia-Serbia Bilateral Cooperation and Technological Forum.

Oral presentations of papers to be given in **PLENARY SESSIONS** are limited. Time available for delivery is 30 min for invited and 15 min for other papers including discussion (5-10 min). Video-beam is available. PowerPoint presentations, recorded on CD only, should be given at registration.

In **POSTER SESSIONS**, the authors are requested to display their papers minimum two hours before the session and to be present beside their posters during the session. Poster sessions are held in Business Club (next to the National Restaurant, looking at the beach) and it is open Tuesday to Thursday 8.00-10.00, 14.00-16.00 and 18.00-22.00.

During Technological Forum, leading experts from business, industry, research laboratories and universities from Europe and United States will be discussing topics related to the current status of various aspects in the field of advanced materials (education, research, technological aspects), the significance of transferring technologies and outsourcing to the developing countries, the significance of innovations and spin off companies in the modern production network, clean production, environment recognition, the necessities of industries in specialized engineering staff, etc.

**PUBLICATION OF PAPERS:** Abstracts will be included in a book of abstracts and distributed to each participant at registration.

The Proceedings will be published, as those from the previous conferences, by Trans Tech Publications Ltd., Switzerland, in Materials Science Forum Edition. The papers will be refereed and those selected will be included in the Proceedings Volume. Certain number of papers will be published as special thematic issue in "Materials and Manufacturing Processes" and "Surface Engineering", invited by the publishers "Taylor and Francis" and "Maney Publishing".

**CONFERENCE AWARDS:** The Yugoslav Materials Research Society will award the authors (preferable young members under 35) of the best oral and poster presentation at the conference, and also the authors of highly rated PhD and MSc theses defended between two conferences. The benefits include free registration and YUCOMAT 2007 Conference Proceedings.

**EXCURSIONS:** Excursions will be organised on Wednesday afternoon (bus trip to Dubrovnik) and Friday after the close of the Conference (boat trip around Boka Kotorska Bay).

## GENERAL CONFERENCE PROGRAMME

### Sunday, September 9, 2007

08<sup>00</sup>-19<sup>00</sup> Registration  
16<sup>00</sup>-18<sup>00</sup> **Technological Forum**  
(Press-Hall)

### Monday, September 10, 2007

07<sup>30</sup>-09<sup>00</sup> Registration

09<sup>00</sup> **OPENING CEREMONY**  
- Introduction and Welcome

10<sup>00</sup>-13<sup>30</sup> **First Plenary Session**  
(Chairpersons: R. Sinclair, M. Vukčević and V. Radmilović)

13<sup>30</sup> **Photo Session**

15<sup>00</sup>-19<sup>15</sup> **Symposium A** (Chairpersons: J. Varela, V. Dondur and M. Drogenik)

19<sup>30</sup>-20<sup>30</sup> **Cocktail Party**

### Tuesday, September 11, 2007

09<sup>00</sup>-12<sup>30</sup> **Second Plenary Session**(Chairpersons: F. Ross, D. Suvorov and S. Milonjić)

15<sup>00</sup>-19<sup>15</sup> **Symposium B** (Chairmen: N. Kallay, S. Mentus and M. Davidović)

15<sup>00</sup>-16<sup>45</sup> **Workshop Serbian-Slovenian Bilateral Cooperation** (Press-Hall)  
(Chairpersons: M. Remškar, Z.Lj. Petrović and N. Rajić)

20<sup>30</sup>-22<sup>00</sup> **Poster Session I** (Symposium A)

### Wednesday, September 12, 2007

09<sup>00</sup>-12<sup>30</sup> **Third Plenary Session**  
(Chairpersons: A. Auroux, A.Ye. Yermakov and D. Raković)

14<sup>00</sup>-19<sup>00</sup> **Excursion to Dubrovnik**

20<sup>30</sup>-22<sup>00</sup> **Poster Session II** (Symposium B)

### Thursday, September 13, 2007

09<sup>00</sup>-12<sup>30</sup> **Fourth Plenary Session** (Chairmen: E. Traversa, J. Czernuszka and M. Plavšić)

15<sup>00</sup>-19<sup>00</sup> **Symposium C** (Chairmen: X. Batlle, M. Zlatanović and J. Nedeljković)

20<sup>30</sup>-22<sup>00</sup> **Poster Session III** (Symposiums C, D and E)

### Friday, September 14, 2007

09<sup>00</sup>-12<sup>00</sup> **Symposium E** (Chairpersons: I. Ćosić, Dj. Koruga and J.P. Šetrajić)

12<sup>00</sup>-12<sup>30</sup> **Awards and Closing of the Conference**

14<sup>00</sup> **Excursion around Boka Kotorska Bay**

<b>SYMPOSIUM A:</b> Advanced Methods in Synthesis and Processing of Materials
<b>SYMPOSIUM B:</b> Advanced Materials for High- Technology Application
<b>SYMPOSIUM C:</b> Nanostructured Materials
<b>SYMPOSIUM D:</b> Composites
<b>SYMPOSIUM E:</b> Biomaterials



## **FIRST PLENARY SESSION**

*Monday, September 10, 2007*

**Session I:** 10<sup>00</sup>-13<sup>30</sup>

Chairpersons: R. Sinclair, M. Vukčević and V. Radmilović

10<sup>00</sup>-10<sup>30</sup> **CHARACTERIZATION AND MANIPULATION OF FUNCTIONAL NANOSTRUCTURES USING HIGH RESOLUTION ANALYTICAL TEM AND COMBINED SPM-TEM**

E. Olsson

*Department of Applied Physics, Chalmers University of Technology, Göteborg, Sweden*

10<sup>30</sup>-11<sup>00</sup> **CONTROLLED ASSEMBLY OF EPITAXIAL NANOSTRUCTURES FOR NANO-ELECTRONIC APPLICATIONS**

R. Hull<sup>1</sup>, J. Gray<sup>1,2</sup>, J. Graham<sup>1</sup>, M. Kammler<sup>1,3</sup>, A. Portavoce<sup>1,4</sup>, M. Gherasimova<sup>1</sup>, S. Wolf<sup>1</sup>, J. Floro<sup>1</sup>, F. Ross<sup>5</sup>

*<sup>1</sup>Department of MSE, University of Virginia, Charlottesville, Virginia, USA, <sup>2</sup>Now at U. Pittsburgh, PA, USA, <sup>3</sup>Now at Infineon, Dresden, Germany; <sup>4</sup>Now at CNRS, Marseilles, France; <sup>5</sup>IBM TJ Watson Research Center, Yorktown Heights New York, USA*

11<sup>00</sup>-11<sup>30</sup> **SEMICONDUCTOR NANOWIRE NUCLEATION AND GROWTH KINETICS**

F.M. Ross

*IBM T.J. Watson Research Center, Yorktown Heights, New York, USA*

**Break:** 11<sup>30</sup>-12<sup>00</sup>

12<sup>00</sup>-12<sup>30</sup> **SOME RECENT DEVELOPMENTS IN NANO-MATERIALS**

R. Sinclair

*Department of Materials Science and Engineering, Stanford University, Stanford, California, USA*

12<sup>30</sup>-13<sup>00</sup> **FINITE SIZE EFFECTS ON DISTRIBUTION AND SHAPE OF SMALL PARTICLES**

D. Chatain

*CRM-CNRS, Marseille, France*

13<sup>00</sup>-13<sup>30</sup> **NOVEL METALLIC THIN FILMS FOR NEMS APPLICATION**

V. Radmilović<sup>1</sup>, D. Mitlin<sup>2</sup>

<sup>1</sup>National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, University of California, Berkeley, California, <sup>2</sup>Chemical and Materials Engineering, University of Alberta and National Institute for Nanotechnology, Edmonton, Alberta, Canada

**Break: 13<sup>30</sup>-15<sup>00</sup>**

**SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS**

**Session I: 15<sup>00</sup>-19<sup>15</sup>**

Chairpersons: J.A. Varela, V. Dondur and M. Drogenik

15<sup>00</sup>-15<sup>15</sup> **PREPARATION AND STUDY OF ZINC – DOPED MAGHEMITE NANOPARTICLES**

M. Drogenik<sup>1,2</sup>, M. Kristl<sup>2</sup>, D. Makovec<sup>1</sup>, Z. Jagličič<sup>3</sup>, D. Hanžel<sup>1</sup>

<sup>1</sup>Jožef Stefan Institute, Ljubljana, Slovenia, <sup>2</sup>Faculty of Chemistry and Chemical Engineering, University of Maribor, Slovenia, <sup>3</sup>Institute of Mathematics, Physics and Mechanics and Faculty of Civil and Geodetic Engineering, University of Ljubljana, Slovenia

15<sup>15</sup>-15<sup>30</sup> **PREPARATION AND MULTILAYERED AGGREGATION OF UNIFORM COLLOIDAL CHOLESTEROL PARTICLES**

V. Uskoković, E. Matijević

Center for Advanced Materials Processing, Clarkson University, Potsdam, NY, USA

15<sup>30</sup>-15<sup>45</sup> **DESIGN OF 3D FUNCTIONAL ARTICLES BY USING COMBINED SHS-SLS**

M.V. Kuznetsov<sup>1</sup>, Yu.G. Morozov<sup>1</sup>, I.V. Shishkovsky<sup>2</sup>, I.P. Parkin<sup>3</sup>

<sup>1</sup>Institute of Structural Macrokineics and Materials Science Russian Academy of Sciences, Chernogolovka, Moscow region, Russia, <sup>2</sup>Lebedev Physics Institute, Samara Branch, Russian Academy of Sciences, Samara, Russia, <sup>3</sup>Department of Chemistry, Christopher Ingold Labs, University College London, London, UK

15<sup>45</sup>-16<sup>00</sup> **SYNTHESIS AND CHARACTERIZATION OF POLYANILINE-ZEOLITE NANOCOMPOSITE**

V. Dondur<sup>1</sup>, G. Ćirić-Marjanović<sup>1</sup>, A. Radulović<sup>2</sup>, Z. Vuković<sup>3</sup>, M. Milojević<sup>1</sup>

<sup>1</sup>Faculty of Physical Chemistry, Belgrade, Serbia

<sup>2</sup>Institute of General and Physical Chemistry, Belgrade, Serbia

<sup>3</sup>Department of Catalysis and Chemical Engineering, ICTM, Belgrade, Serbia

16<sup>00</sup>-16<sup>15</sup> **HARD MAGNETIC Co-Pt FILMS PREPARED BY ELECTRODEPOSITION**  
K. Žužek Rožman<sup>1,2</sup>, A. Krause<sup>2</sup>, K. Leistner<sup>2</sup>, H. Schlörb<sup>2</sup>, S. Fähler<sup>2</sup>, S. Baunack<sup>2</sup>,  
L. Schultz<sup>2</sup>  
<sup>1</sup>*Jozef Stefan Institute, Ljubljana, Slovenia*, <sup>2</sup>*IFW Dresden, Dresden, Germany*

16<sup>15</sup>-16<sup>30</sup> **SYNTHESIS OF Bi<sub>3</sub>Nb<sub>1-x</sub>Ta<sub>x</sub>O<sub>7</sub> FLURITE - TYPE DIELECTRICS BY POLYMERIC PRECURSOR METHOD**  
U. Pirnat<sup>1</sup>, S.D. Škapin<sup>1</sup>, D. Suvorov<sup>1</sup>, M.A. Zaghete<sup>2</sup>, J.A. Varela<sup>2</sup>  
<sup>1</sup>*Advanced Materials Department, Jozef Stefan Institute, Ljubljana, Slovenia*,  
<sup>2</sup>*Instituto de Química, UNESP, Araraquara, Brasil*

16<sup>30</sup>-16<sup>45</sup> **RHOMBOHEDRAL CALCITE PRECIPITATION FROM CO<sub>2</sub>-H<sub>2</sub>O-Ca(OH)<sub>2</sub> SLURRY AT 90 °C AND 90 bar**  
G. Montes-Hernandez, F. Renard, L. Charlet  
*LGIT, Maison de Géosciences, BP 53 X, Grenoble, France*

16<sup>45</sup>-17<sup>00</sup> **HYDROTHERMAL PROCESSING OF 1D -NANOMATERIALS FROM MINERAL SANDS**  
L. Mančić<sup>1</sup>, B. Marinković<sup>2</sup>, P. Jardim<sup>2</sup>, F. Rizzo<sup>2</sup>, O. Milošević<sup>1</sup>  
<sup>1</sup>*Institute of Technical Science of SASA, Belgrade, Serbia*,  
<sup>2</sup>*Pontificia Universidade Catolica do Rio de Janeiro, Rio de Janeiro, Brasil*

**Break: 17<sup>00</sup>-17<sup>30</sup>**

17<sup>30</sup>-17<sup>45</sup> **FRACTAL ASPECTS OF DISCRETE FRACTURE MECHANICS**  
M.P. Wnuk  
*College of Engineering and Mathematical Science, University of Wisconsin – Milwaukee, Milwaukee, USA*

17<sup>45</sup>-18<sup>00</sup> **SOLVENT-FREE MECHANOCHEMICAL SYNTHESIS OF SOME PHYSIOLOGICALLY ACTIVE SUBSTANCES**  
N. Pankrushina<sup>1,2</sup>, I. Nikitina<sup>1,2</sup>, E. Chernjak<sup>1</sup>, C. Myz<sup>2,3</sup>, T. Shakhtshneider<sup>2,3</sup>, V. Boldyrev<sup>2,3</sup>  
<sup>1</sup>*Institute of Organic Chemistry, Novosibirsk, Russia*, <sup>2</sup>*Research and Education Centre "Molecular Design and Ecologically Safe Technologies" at Novosibirsk State University, Russia*, <sup>3</sup>*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*

18<sup>00</sup>-18<sup>15</sup> **MECHANICAL MILLING: EVOLUTION OF CRYSTAL PARAMETER OF IRON POWDER**  
I. Taut<sup>1</sup>, G. Arghir<sup>1</sup>, C. Popa<sup>1</sup>, S.-D. Bolboacă<sup>2</sup>, L. Jäntschi<sup>1</sup>  
<sup>1</sup>*Technical University of Cluj-Napoca, Romania*, <sup>2</sup>*"Iuliu Hatieganu" University of Medicine and Pharmacy Cluj-Napoca, Romania*

- 18<sup>15</sup>-18<sup>30</sup> **SUPERFICIAL DISTORTION INFLUENCE ON CHARACTERISTICS OF THE IRON-BASED MATERIALS**  
L. Brândușan, L. Jäntschi  
*Technical University of Cluj-Napoca, Romania*
- 18<sup>30</sup>-18<sup>45</sup> **PLASMA POST-PROCESSING IN OXYGEN AND CARBON CONTAINING ATMOSPHERES FOR WIND TURBINE COMPONENTS TREATMENT**  
M. Zlatanović<sup>1</sup>, N. Popović<sup>2</sup>  
<sup>1</sup>*Faculty of Electrical Engineering, Belgrade, Serbia,*  
<sup>2</sup>*Nuclear Science Institute Vinča, Belgrade, Serbia*
- 18<sup>45</sup>-19<sup>00</sup> **SYNTHESIS OF OLIVINE-TYPE LiFePO<sub>4</sub> BY SONOCHEMICAL METHOD**  
D. Jugović<sup>1</sup>, M. Mitrić<sup>2</sup>, N. Cvjetičanin<sup>3</sup>, S. Mentus<sup>3</sup>, D. Uskoković<sup>1</sup>  
<sup>1</sup>*Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia,* <sup>2</sup>*The Vinča Institute of Nuclear Sciences, Belgrade, Serbia,*  
<sup>3</sup>*Faculty of Physical Chemistry, University of Belgrade, Serbia*
- 19<sup>00</sup>-19<sup>15</sup> **SYNTHESIS AND CHARACTERIZATION OF IRON CONTAINING MCM-41 POROUS SILICA – APPLICATION TO ADSORPTION OF ARSENATES**  
E.A. Deliyanni, K.S. Triantafyllidis, E.N. Peleka, K.A. Matis  
*Section of Chemical Technology & Industrial Chemistry, Department of Chemistry, Aristotle University, Thessaloniki, Greece*

## SECOND PLENARY SESSION

*Tuesday, September 11, 2007*

**Session II:** 09<sup>00</sup>-13<sup>00</sup>

Chairpersons: F. Ross, D. Suvorov and S. Milonjić

09<sup>00</sup>-09<sup>30</sup> **NEW DEVELOPMENTS IN QUANTITATIVE 3D STRUCTURE ANALYSIS OF THIN SOLID FILMS BY TRANSMISSION ELECTRON MICROSCOPY**  
E. Spiecker  
*Microanalysis of Materials, Faculty of Engineering, Kiel University, Kiel, Germany*

09<sup>30</sup>-10<sup>00</sup> **USING REAL TIME MICROSCOPY TO QUANTITATIVELY DETERMINE NUCLEATION MECHANISMS AND KINETICS DURING THE GROWTH OF Si NANOWIRES AND CARBON NANOTUBES**  
E. A. Stach<sup>1</sup>, B.-J. Kim<sup>1</sup>, S.M. Kim<sup>1</sup>, S. Kodambaka<sup>2</sup>, J. Tersoff<sup>2</sup>, M.C. Reuter<sup>2</sup>, K. Reuter<sup>2</sup>, F.M. Ross<sup>2</sup>, B. Maruyama<sup>3</sup>, M. Pender<sup>3</sup>  
<sup>1</sup>*School of Materials Engineering & Birck Nanotechnology Center, Purdue Univ., West-Lafayette, IN, USA*, <sup>2</sup>*Research Division, IBM T.J. Watson Research Center, Yorktown Heights, NY, USA*, <sup>3</sup>*Materials and Manufacturing Directorate, Air Force Research Laboratory, Dayton, OH, USA*

10<sup>00</sup>-10<sup>30</sup> **BULK NANOCRYSTALLINE ALLOYS STUDIED BY TEM**  
H.P. Karnthaler, Ch. Rentenberger, Th. Waitz  
*Materials Physics, University of Vienna, Vienna, Austria*

10<sup>30</sup>-11<sup>00</sup> **APPLICATION OF HIGH SPATIAL AND HIGH ENERGY RESOLUTION ANALYTICAL TOOLS FOR THE CHARACTERIZATION OF ADVANCED MATERIALS**  
Ch.A. Evans  
*Evans Analytical Group (EAG), Sunnyvale, CA, USA*

**Break:** 11<sup>00</sup>-11<sup>30</sup>

11<sup>30</sup>-12<sup>00</sup> **BIOLOGICALLY ENABLED ASSEMBLY OF NANOSTRUCTURED MATERIALS WITH COMPLEX THREE-DIMENSIONAL MORPHOLOGIES AND CHEMISTRIES**  
K.H. Sandhage, M.R. Weatherspoon, S. Shian, Zh. Bao, E. Ernst, Ph. Graham, M.B. Dickerson, G. Ahmad  
*School of Materials Science & Engineering, Georgia Institute of Technology, Atlanta, GA, USA*

12<sup>00</sup>-12<sup>30</sup> **CHARACTERIZATION OF SOLID/LIQUID INTERFACES BY SURFACE POTENTIAL MEASUREMENTS**

N. Kallay, T. Preočanin, F. Šupljika  
*Laboratory of Physical Chemistry, Department of Chemistry, Faculty of Science,  
University of Zagreb, Zagreb, Croatia*

12<sup>30</sup>-13<sup>00</sup> **BI-BASED MATERIALS FOR GLASS-FREE LTCC MODULES**

D. Suvorov  
*Advanced Materials Department, »Jozef Stefan« Institute, Ljubljana, Slovenia*

**Break: 13<sup>00</sup>-15<sup>00</sup>**

**SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION**

**Session I: 15<sup>00</sup>-19<sup>15</sup>**

Chairmen: N. Kallay, S. Mentus and M. Davidović

15<sup>00</sup>-15<sup>15</sup> **LITHIUM CONDUCTING PEROVSKITES**

A. Belous  
*V.I.Vernadskii Institute of General and Inorganic Chemistry NAS of Ukraine, Kyiv,  
Ukraine*

15<sup>15</sup>-15<sup>30</sup> **LOW-LOSS MICROWAVE DIELECTRICS BASED ON THE COLUMBITES A<sup>2+</sup>Nb<sub>2</sub>O<sub>6</sub> AND PEROVSKITES Ba(A<sup>2+</sup><sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>: THE EFFECT OF COMPOSITIONAL VARIATION**

A. Belous<sup>1</sup>, O. Ovchar<sup>1</sup>, B. Jančar<sup>2</sup>  
*<sup>1</sup>V.I.Vernadskii Institute of General and Inorganic Chemistry NAS of Ukraine, Kyiv,  
Ukraine, <sup>2</sup>Jozef Stefan Institute, Ljubljana, Slovenia*

15<sup>30</sup>-15<sup>45</sup> **MOLDING FLUORESCENCE EMISSION BY PHOTONIC BAND GAP ENGINEERING**

B. Kolarić, K. Baert, R.A.L. Vallée, M. Van der Auweraer, K. Clays  
*Department of Chemistry, K.U. Leuven and the Institute of Nanoscale Physics and  
Chemistry (INPAC), Heverlee, Belgium*

15<sup>45</sup>-16<sup>00</sup> **PROPERTIES OF NdCr<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> BORATE: SPECTROSCOPIC STUDY**

M.N. Popova<sup>1</sup>, E.P. Chukalina<sup>1</sup>, K.N. Boldyrev<sup>1</sup>, N.I. Leonyuk<sup>2</sup>  
*<sup>1</sup>Institute of Spectroscopy of RAS, Troitsk, Moscow region, Russia, <sup>2</sup>Moscow State  
University, Moscow, Russia*

- 16<sup>00</sup>-16<sup>15</sup> **EXITON-IMPURITY ENERGY TRANSFER DYNAMICS IN NEW LOW PHONON ENERGY LASER MATERIALS**  
A.M. Tkachuk<sup>1,2</sup>, S.E. Ivanova<sup>2</sup>, M.-F. Joubert<sup>3</sup>, Y. Guyot<sup>3</sup>  
<sup>1</sup>*Scientific Production Corporation "S.I. Vavilov State Optical Institute", St. Petersburg, Russia,* <sup>2</sup>*University of Information Technology, Mechanics and Optics, St. Petersburg, Russia,* <sup>3</sup>*LPCML, UMR 5620 du CNRS, Universite Lyon 1, Villeurbanne, France*
- 16<sup>15</sup>-16<sup>30</sup> **NEW RE DOPED FLUORIDE AND CHLORIDE CRYSTALS FOR EFFICIENT OPTICAL CONVERTERS**  
S.E. Ivanova<sup>1</sup>, A.M. Tkachuk<sup>1,2</sup>, M.-F. Joubert<sup>3</sup>, Y. Guyot<sup>3</sup>, V.P. Gapontzev<sup>4</sup>  
<sup>1</sup>*University of Information Technology, Mechanics and Optics, St. Petersburg, Russia,* <sup>2</sup>*Scientific Production Corporation "S.I. Vavilov State Optical Institute", St. Petersburg, Russia,* <sup>3</sup>*LPCML, UMR 5620 du CNRS, Universite Lyon 1, Villeurbanne, France,* <sup>4</sup>*IPG Laser GmbH, Burbach, Germany*
- 16<sup>30</sup>-16<sup>45</sup> **MAGNETIC PHENOMENA IN THE 4F-ELECTRON INTERMETALLIC COMPOUNDS**  
A. Szytuła  
*M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland*
- 16<sup>45</sup>-17<sup>00</sup> **THE DISPROPORTIONATION PROCESS IN RARE-EARTH-TRANSITION-METAL-BASED MATERIALS: AN EXPERIMENTAL AND MODELING APPROACH**  
P.J. McGuinness, K. Žužek-Rožman, M. Komelj, S. Kobe  
*Department for Nanostructured Materials, Jozef Stefan Institute, Ljubljana, Slovenia*
- Break: 17<sup>00</sup>-17<sup>30</sup>**
- 17<sup>30</sup>-17<sup>45</sup> **MESOPOROUS TITANIUM DIOXIDE: SYNTHESIS AND PHOTOCATALYTIC ACTIVITY**  
I.V. Kolesnik, M.V. Kharlamova, A.V. Garshev, A.A. Eliseev, A.V. Lukashin, Yu.D. Tretyakov  
*Department of Material Science, Moscow State University, Moscow, Russia*
- 17<sup>45</sup>-18<sup>00</sup> **INCOMMENSURATE-COMMENSURATE PHASE TRANSFORMATION IN THE Bi<sub>2</sub>O<sub>3</sub>-Nb<sub>2</sub>O<sub>5</sub> SOLID SOLUTION**  
B. Jančar, U. Pirnat, S. Šturm, D. Suvorov  
*Jozef Stefan Institute, Ljubljana, Slovenia*

- 18<sup>00</sup>-18<sup>15</sup> **SOL-GEL SYNTHESIS AND CHARACTERIZATION OF A NEW BISMUTH TITANATE PYROCHLORE CERAMIC**  
Š. Kunej, D. Suvorov  
*Jožef Stefan Institute, Ljubljana, Slovenia*
- 18<sup>15</sup>-18<sup>30</sup> **INFLUENCE OF CRYSTAL SYMMETRY ON THE VOLTAGE-TUNABILITY OF Na<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub>-BASED SYSTEMS**  
M. Spreitzer, B. Jančar, D. Suvorov  
*Advanced Materials Department, Jozef Stefan Institute, Ljubljana, Slovenia*
- 18<sup>30</sup>-18<sup>45</sup> **PHYSICOCHEMICAL CHARACTERISTICS OF Rb<sup>+</sup> AND Cs<sup>+</sup> SALTS OF 12-TUNGSTOPHOSPHORIC ACID**  
I. Holclajtner-Antunović<sup>1</sup>, Ž. Čupić<sup>2</sup>, M. Davidović<sup>3</sup>, U.B. Mioč<sup>1</sup>, M. Todorović<sup>4</sup>, D. Jovanović<sup>2</sup>, P. Banković<sup>2</sup>  
<sup>1</sup>*Faculty of Physical Chemistry University of Belgrade, Belgrade, Serbia,* <sup>2</sup>*IHTM, Center of Catalysis and Chemical Engineering, Belgrade, Serbia,* <sup>3</sup>*Goša Institute, Belgrade, Serbia,* <sup>4</sup>*Faculty of Chemistry, Belgrade, Serbia*
- 18<sup>45</sup>-19<sup>00</sup> **CARBON/CARBON-SILICON-CARBIDE DUAL-MATRIX COMPOSITES FOR BRAKE DISCS**  
K. Krnel<sup>1</sup>, T. Kosmač<sup>1</sup>, Z. Stadler<sup>2</sup>  
<sup>1</sup>*Jožef Stefan Institute, Ljubljana, Slovenia,* <sup>2</sup>*MS Production, Bled, Slovenia*
- 19<sup>00</sup>-19<sup>15</sup> **DETECTION OF THE DEGREE OF BRANCHING IN HYPERBRANCHED POLYMERS**  
F. Schallausky<sup>1</sup>, S. Reichelt<sup>1</sup>, A. Lederer<sup>1</sup>, M. Netopilík<sup>2</sup>  
<sup>1</sup>*Leibniz-Institute of Polymer Research Dresden, Dresden, Germany,* <sup>2</sup>*Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, v.v.i., Prague, Czech Republic*

## WORKSHOP: SERBIA – SLOVENIA BILATERAL COOPERATION

Press-Hall

### Session I: 15<sup>00</sup>-16<sup>45</sup>

Chairpersons: M. Remškar, Z.Lj. Petrović and N. Rajić

- 15<sup>00</sup>-15<sup>15</sup> **PHONONS IN MoS<sub>2</sub> AND W S<sub>2</sub> NANOTUBES**  
M. Damjanović<sup>1</sup>, M. Remškar<sup>2</sup>, E. Dobardžić<sup>1</sup>, B. Dakić<sup>1</sup>, M. Viršek<sup>2</sup>, I. Milošević<sup>1</sup>  
<sup>1</sup>*Faculty of Physics, Belgrade, Serbia,* <sup>2</sup>*Jožef Stefan Institute, Ljubljana, Slovenia*
- 15<sup>15</sup>-15<sup>30</sup> **STUDIES OF APPLICATION AND CHARACTERIZATION OF PLASMAS USED IN TREATMENT OF POLYMERS AND ORGANIC MATERIALS**



A. Jesih<sup>1</sup>, N. Puač<sup>2</sup>, M. Radetič<sup>3</sup>, Z.Lj. Petrovič<sup>2</sup>, G. Malović<sup>2</sup>, S. Lazović<sup>2</sup>  
<sup>1</sup>*Institute "Jožef Stefan", Ljubljana, Slovenia,* <sup>2</sup>*Institute of Physics, Belgrade, Serbia,*  
<sup>3</sup>*Textile Engineering Department, Faculty of Technology and Metallurgy, Belgrade, Serbia*

15<sup>30</sup>-15<sup>45</sup> **PULSED LASER ABLATION OF PVD MULTI-LAYERED COATINGS:  
PROFILOMETRIC ANALYSIS**

B. Gaković<sup>1</sup>, M. Trtica<sup>1</sup>, S. Petrovič<sup>1</sup>, P. Panjan<sup>2</sup>, M. Čekada<sup>2</sup>, M. Panjan<sup>2</sup>  
<sup>1</sup>*Institute of Nuclear Sciences "Vinča", Belgrade, Serbia*  
<sup>2</sup>*Jožef Stefan Institute, Ljubljana, Slovenia*

15<sup>45</sup>-16<sup>00</sup> **TEM STUDY OF TiAlN/CrN NANOLAYER COATINGS**

M. Panjan, S. Šturm, P. Panjan, M. Čekada  
*Jožef Stefan Institute, Ljubljana, Slovenia*

16<sup>00</sup>-16<sup>15</sup> **SYNTHESIS AND MAGNETIC PROPERTIES OF Fe<sub>2</sub>O<sub>3</sub> NANOPARTICLES  
IN A SILICA MATRIX**

M. Tadić<sup>1</sup>, D. Marković<sup>1</sup>, V. Spasojević<sup>1</sup>, V. Kusigerski<sup>1</sup>, J. Pirnat<sup>2</sup>, Z. Jagličić<sup>2</sup>, Z. Trontelj<sup>2</sup>, M. Remškar<sup>3</sup>  
<sup>1</sup>*Condensed Matter Physics Laboratory, Institute of Nuclear Sciences Vinca, Belgrade, Serbia,* <sup>2</sup>*Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia,* <sup>3</sup>*Jozef Stefan Institute, Ljubljana, Slovenia*

16<sup>15</sup>-16<sup>30</sup> **SOL-GEL PRODUCED THIN FILMS FOR PHOTOCATALYSIS**

U. Lavrenčič Štangar, U. Černigoj, K. Maver, D. Mahne, S. Patil, P. Trebše  
*Laboratory for Environmental Research, University of Nova Gorica, Nova Gorica, Slovenia*

16<sup>30</sup>-16<sup>45</sup> **ON THE PREPARATION OF METAL-ORGANIC FRAMEWORKS (MOF)  
AS POTENTIAL MATERIALS FOR HYDROGEN STORAGE**

N. Rajič<sup>1</sup>, Dj. Stojaković<sup>1</sup>, N. Zabukovec Logar<sup>2</sup>, V. Kaučič<sup>2</sup>  
<sup>1</sup>*Faculty of Technology and Metallurgy, Belgrade, Serbia*  
<sup>2</sup>*National Institute of Slovenia, Ljubljana, Slovenia*

## THIRD PLENARY SESSION

*Wednesday, September 12, 2007*

### Session III: 09<sup>00</sup>-12<sup>00</sup>

Chairpersons: A. Auroux, A.Ye. Yermakov and D. Raković

09<sup>00</sup>-9<sup>30</sup> **NANOSTRUCTURED MATERIALS FOR INTERMEDIATE TEMPERATURE SOLID OXIDE FUEL CELLS (IT-SOFCs)**

E. Traversa

*Department of Chemical Science and Technology, University of Rome Tor Vergata, Rome, Italy*

9<sup>30</sup>-10<sup>00</sup> **TRANSPORT PROPERTIES OF NANOSTRUCTURED ANTIMONY-DOPED TIN OXIDE FILMS**

J.A. Varela, T.R. Giraldi, E. Longo

*Universidade Estadual Paulista – UNESP, Araraquara, SP, Brazil*

10<sup>00</sup>-10<sup>30</sup> **NO<sub>x</sub> ABATEMENT OVER SUPPORTED BINARY OXIDE CATALYSTS CONTAINING CuO COUPLED WITH Ga<sub>2</sub>O<sub>3</sub> AND SnO<sub>2</sub>**

S. Bennici<sup>1,2</sup>, A. Gervasini<sup>1</sup>, A. Auroux<sup>2</sup>

*<sup>1</sup>Dip. Chimica Fisica ed Elettrochimica, Università degli Studi di Milano, Milano, Italy, <sup>2</sup>IRCELYON, UMR5256 CNRS-Université Lyon 1, Villeurbanne, France*

### Break: 10<sup>30</sup>-11<sup>00</sup>

11<sup>00</sup>-11<sup>30</sup> **ELECTRICAL RELAXATIONS DUE TO ELECTRONS IN OXIDES**

J.-C. Badot

*Laboratoire de Chimie de la Matière Condensée de Paris, UMR CNRS 7574, ENSCP, Paris, France*

11<sup>30</sup>-12<sup>00</sup> **SURFACE REACTIVITY OF METAL OXIDES: SORPTION AND ADHESION PROCESSES**

G. Lefèvre, Lj. Čerović, M. Fédoroff

*Laboratory of Electrochemistry and Analytical Chemistry UMR7575, ENSCP-CNRS-Paris6, Paris, France*

## FOURTH PLENARY SESSION

*Thursday, September 13, 2007*

### Session IV: 09<sup>00</sup>-12<sup>30</sup>

Chairmen: E. Traversa, J. Czernuszka and M. Plavšić

09<sup>00</sup>-9<sup>30</sup> **THE FIRST INORGANIC NANOBUDS AND PEA-PODS: WS<sub>2</sub> AND MoS<sub>2</sub> FULLERENES GROWN BY DIFFUSION PROCESS**

M. Remškar, M. Viršek, A. Mrzel, A. Jesih  
*Jozef Stefan Institute, Ljubljana, Slovenia*

09<sup>30</sup>-10<sup>00</sup> **PROCESSING AND CHARACTERIZATION OF MAGNETIC NANOSTRUCTURED MATERIALS**

J. Wittig  
*Vanderbilt University, Nashville, Tennessee USA*

10<sup>00</sup>-10<sup>30</sup> **SYNTHESIS AND PROPERTIES OF METAL-CARBON NANOCOMPOSITES. SOME PERSPECTIVE APPLICATIONS IN CATALYSTS CHEMISTRY AND MEDICINE (PHOTO-THERMAL THERAPY OF TUMORS)**

A.Ye.Yermakov<sup>1</sup>, M.A.Uimin<sup>1</sup>, A.A.Mysik<sup>1</sup>, E.S.Lokteva<sup>2</sup>, A.A. Stratonnikov<sup>3</sup>  
<sup>1</sup>*Institute of Metal Physics, Ural Branch of RAS, Ekaterinburg, Russia*  
<sup>2</sup>*M.V. Lomonosov Moscow State University, Moscow, Russia*  
<sup>3</sup>*Natural Science Center of General Physics Institute of RAS, Moscow, Russia*

### Break: 10<sup>30</sup>-11<sup>00</sup>

11<sup>00</sup>-11<sup>30</sup> **Fe<sub>3</sub>O<sub>4</sub> NANOPARTICLES FOR BIOMEDICAL APPLICATIONS: THE ROLE OF THE SURFACTANT**

P. Guardia<sup>1</sup>, N. Pérez<sup>1</sup>, A. G. Roca<sup>2</sup>, O. Iglesias<sup>1</sup>, M. P. Morales<sup>2</sup>, C. J. Serna<sup>2</sup>, A. Labarta<sup>1</sup>, X. Batlle<sup>1</sup>  
<sup>1</sup>*Departament de Física Fonamental and Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, Martí i Franqués 1, Barcelona, Catalonia, Spain*, <sup>2</sup>*Instituto de Ciencia de Materiales de Madrid, CSIC, Sor Juana Inés de la Cruz, Madrid, Spain*

11<sup>30</sup>-12<sup>00</sup> **3-D SCAFFOLDS FOR 3-D TISSUE ENGINEERING**

J. Czernuszka  
*Department of Materials Sciences, Oxford University, Oxford, United Kingdom*

**12<sup>00</sup>-12<sup>30</sup> BIOACTIVE PEPTIDE DESIGN USING THE RESONANT RECOGNITION MODEL**

I. Čosić, E. Pirogova, J. Fang, V. Vojisavljević  
*School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia, Australian Centre for Radiofrequency Bioeffects Research (ACRBR)*

**Break: 12<sup>30</sup>-15<sup>00</sup>**

**SYMPOSIUM C: NANOSTRUCTURED MATERIALS**

**Session I: 15<sup>00</sup>-19<sup>00</sup>**

Chairmen: X. Battle, M. Zlatanović and J. Nedeljković

**15<sup>00</sup>-15<sup>15</sup> ATOMIC RESOLUTION HAADF-STEM: APPLICATIONS IN MATERIALS SCIENCE**

M. Čeh<sup>1</sup>, S. Šturm<sup>1</sup>, M. Shiojiri<sup>2</sup>  
<sup>1</sup>*Institute Jožef Stefan, Ljubljana, Slovenia,* <sup>2</sup>*Kyoto Institute of Technology, Kyoto, Japan*

**15<sup>15</sup>-15<sup>30</sup> NANOCATALYST ENGINEERING ON EXTENDED AND NANOSCALE SURFACES**

V. Stamenković, D. Strmcnik, D. Tripković, D. van der Vliet, H. You, N.M. Marković  
*Argonne National Laboratory, Materials Science Division, Argonne, IL, USA*

**15<sup>30</sup>-15<sup>45</sup> PREPARATION OF AMINE-FREE SILICA-COATED AgI NANOPARTICLES WITH A MODIFIED STÖBER METHOD**

Y. Kobayashi<sup>1,2</sup>, N. Shimizu<sup>1</sup>, M. Takeda<sup>3</sup>, N. Ohuchi<sup>3</sup>, A. Kasuya<sup>4</sup>, M. Konno<sup>1</sup>  
<sup>1</sup>*Department of Chemical Engineering, Graduate School of Engineering, Tohoku University, Aoba, Aramaki-aza, Aoba-ku, Sendai, Japan,* <sup>2</sup>*Present address: Department of Biomolecular Functional Engineering, College of Engineering, Ibaraki University, Naka-narusawa-cho, Hitachi, Ibaraki, Japan,* <sup>3</sup>*Division of Surgical Oncology, Graduate School of Medicine, Tohoku University, Seiryomachi, Aoba-ku, Sendai, Japan,* <sup>4</sup>*Center for Interdisciplinary Research, Tohoku University, Aoba, Aramaki-aza, Aoba-ku, Sendai, Japan*

**15<sup>45</sup>-16<sup>00</sup> CHARACTERIZATION OF NANOPARTICLES BY FLUORESCENCE CORRELATION SPECTROSCOPY**

M. Štěpánek<sup>1</sup>, J. Humpolíčková<sup>2</sup>, T. Kral<sup>2</sup>  
<sup>1</sup>*Department of Physical and Macromolecular Chemistry, Charles University, Prague, Czech Republic,* <sup>2</sup>*Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic*

- 16<sup>00</sup>-16<sup>15</sup> **MULTILAYER POLYMERIC NANOPARTICLES BASED ON SPECIFIC INTERACTIONS IN SOLUTION: LIGHT SCATTERING AND ATOMIC FORCE MICROSCOPY STUDY**  
P. Matějček<sup>1</sup>, M. Uchman<sup>1</sup>, J. Lokajová<sup>1</sup>, M. Špírková<sup>2</sup>, K. Procházka<sup>1</sup>  
<sup>1</sup>*Department of Physical and Macromolecular Chemistry, Charles University, Prague, Czech Republic,* <sup>2</sup>*Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic*
- 16<sup>15</sup>-16<sup>30</sup> **POLYURETHANE NETWORKS WITH INORGANIC NANO-BUILDING BLOCKS**  
A. Strachota<sup>1</sup>, B. Strachotová<sup>1</sup>, M. Špírková<sup>1</sup>, F. Ribot<sup>2</sup>  
<sup>1</sup>*Department of Polymer Networks and Mechanical Properties, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Praha, Czech Republic,* <sup>2</sup>*Institute Laboratoire de Chimie de la Matière Condensée, UMR CNRS 7574, Université Pierre et Marie Curie, Paris, France*
- 16<sup>30</sup>-16<sup>45</sup> **EPITAXIAL GROWTH BY MONOLAYER RESTRICTED GALVANIC DISPLACEMENT**  
R. Vasilic<sup>1</sup>, N. Dimitrov<sup>2</sup>  
<sup>1</sup>*Laboratory for Atomic Physics, Institute of Nuclear Sciences Vinca, Belgrade, Serbia,* <sup>2</sup>*Materials Science and Engineering Program, SUNY Binghamton, Binghamton, NY, USA*
- 16<sup>45</sup>-17<sup>00</sup> **THIN SEMI-CONDUCTOR FILMS FORMED BY PULSED ION DEPOSITION**  
M.S. Saltymakov<sup>1</sup>, G.E. Remnev<sup>1</sup>, I.V. Ivonin<sup>2</sup>, V.I. Yurchenko<sup>3</sup>, E.P. Nayden<sup>4</sup>, V.A. Novikov<sup>2</sup>  
<sup>1</sup>*High Voltage Research Institute, Tomsk, Russia,* <sup>2</sup>*Tomsk State University, Tomsk, Russia,* <sup>3</sup>*Federal Researches Institute of Semiconductor Devices, Tomsk, Russia,* <sup>4</sup>*Siberian Physical-Technical Institute, Tomsk, Russia*
- Break:** 17<sup>00</sup>-17<sup>30</sup>
- 17<sup>30</sup>-17<sup>45</sup> **LASER-INDUCED CHANGE IN THE REFRACTIVE INDEX IN THE ORGANIC SYSTEMS DOPED WITH NANOOBJECTS**  
N.V. Kamanina<sup>1</sup>, D.P. Uskokovic<sup>2</sup>  
<sup>1</sup>*Vavilov State Optical Institute, St. Petersburg, Russia;* <sup>2</sup>*Institute of Technical Sciences of the SASA, Belgrade, Serbia*
- 17<sup>45</sup>-18<sup>00</sup> **RAMAN SPECTROSCOPY METHOD FOR DETERMINATION OF PARTICLE SIZE DISTRIBUTION IN ANATASE TiO<sub>2</sub> NANOPOWDERS**

M.J. Šćepanović, M.U. Grujić-Brojčin, Z.D. Dohčević-Mitrović, S. Aškračić, R. Kostić, Z.V. Popović  
*Center for Solid State Physics and New Materials, Institute of Physics, Belgrade, Serbia*

18<sup>00</sup>-18<sup>15</sup> **LUMINESCENT PROPERTIES OF EUROPIUM DOPED YTTRIUM AND GADOLINIUM SESQUIOXIDE PREPARED USING POLYETHYLENE GLYCOL ASSISTED COMBUSTION METHOD**

R. Krsmanović, Ž. Andrić, M.D. Dramićanin  
*Institute of Nuclear Sciences "Vinca", Belgrade, Serbia*

18<sup>15</sup>-18<sup>30</sup> **SYNTHESIS AND CHARACTERIZATION OF HIGH-QUALITY ORGANIC BASED MAGNETIC FLUIDS**

A. Drmota<sup>1</sup>, A. Košak<sup>2</sup>, A. Žnidaršič<sup>1,2</sup>  
<sup>1</sup>*Nanotesla Institute, KOLEKTOR GROUP, Ljubljana, Slovenia*  
<sup>2</sup>*Iskra-Feriti d.o.o., KOLEKTOR GROUP, Ljubljana, Slovenia*

18<sup>30</sup>-18<sup>45</sup> **HIGH PRESSURE SINTERING OF NANOCRYSTALLINE TITANIUM CARBONITRIDE**

V.S. Urbanovich<sup>1</sup>, G.P. Okatova<sup>2</sup>, K.I. Yanushkevich<sup>1</sup>, G.K. Zubovich<sup>1</sup>, L.P. Stafetski<sup>3</sup>  
<sup>1</sup>*Joint Institute of Solid State and Semiconductor Physics, National Academy of Sciences of Belarus, Minsk, Belarus*, <sup>2</sup>*Belarusian State Technological University, Minsk, Belarus*, <sup>3</sup>*Joint-stock Neomat Co, Salaspils, Latvia*

18<sup>45</sup>-19<sup>00</sup> **Fe-C BULK NANOCOMPOSITES PREPARED BY MECHANICAL ALLOYING AND MAGNETIC PULSE COMPACTION**

E. Yelsukov<sup>1</sup>, V. Ivanov<sup>2</sup>, S. Zayatz<sup>2</sup>, S. Lomayeva<sup>1</sup>  
<sup>1</sup>*Physical - Technical Institute UrB RAS, Izhevsk, Russia*  
<sup>2</sup>*Institute of Electrophysics UrB RAS, Ekaterinburg, Russia*

## SYMPOSIUM E: BIOMATERIALS

*Friday, September 14, 2007*

**Session I:** 09<sup>00</sup>-12<sup>00</sup>

Chairpersons: I. Ćosić, Dj. Koruga and J.P. Šetrajić

- 09<sup>00</sup>-09<sup>15</sup> **POTENTIALITIES OF MAGNETOLIPOSOMES AS INTRACELLULAR THERANOSTICS**  
S.J.H. Soenen<sup>1</sup>, J. Cocquyt<sup>2</sup>, L. DeFour<sup>1</sup>, P. Saveyn<sup>2</sup>, P. Van der Meeren<sup>2</sup>, M. De Cuyper<sup>1</sup>  
<sup>1</sup>*Interdisciplinary Research Centre, Katholieke Universiteit Leuven – Campus Kortrijk, Kortrijk, Belgium;* <sup>2</sup>*Particle and Interfacial Technology Group, Faculty of Bioscience Engineering, Ghent University, Ghent, Belgium*
- 09<sup>15</sup>-09<sup>30</sup> **CHEMICAL AND PHYSICAL CHARACTERIZATION OF REGULAR AND ULTRA THIN CHITOSAN FILMS STORED AT VARIOUS TEMPERATURES**  
S. Živanović, J. Li, T. Wu, G. Rajpal  
*University of Tennessee, Knoxville, TN, USA*
- 09<sup>30</sup>-09<sup>45</sup> **NANOBIOLOGICAL ATOMIC FORCE MICROSCOPY STUDY OF THE SPORULATION OF *BACILLUS SUBTILIS***  
O. Hekele<sup>1</sup>, C.G. Goesselsberger<sup>1</sup>, M. Brandstetter<sup>1</sup>, R. Sommer<sup>2</sup>, I.C. Gebeshuber<sup>1</sup>  
<sup>1</sup>*Institut fuer Allgemeine Physik, Vienna University of Technology, Vienna, Austria*  
<sup>2</sup>*Hygiene-Institute, Medical University of Vienna, Wien, Austria*
- 09<sup>45</sup>-10<sup>00</sup> **NANOMEDICINE PERFORMED WITH THE ATOMIC FORCE MICROSCOPE ON HUMAN RED BLOOD CELLS**  
O. Hekele, C.G. Goesselsberger, I.C. Gebeshuber  
*Institut fuer Allgemeine Physik, Vienna University of Technology, Vienna, Austria*
- 10<sup>00</sup>-10<sup>15</sup> **SYNTHESIS AND CHARACTERIZATION OF DLPLG NANOPARTICLES FOR CONTROLLED DELIVERY OF WATER-SOLUBLE VITAMINS**  
M. Stevanović<sup>1</sup>, A. Radulović<sup>2</sup>, D. Uskoković<sup>1</sup>  
<sup>1</sup>*Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia;* <sup>2</sup>*Institute of General and Physical Chemistry, Belgrade, Serbia*
- 10<sup>15</sup>-10<sup>30</sup> **GENOTOXICITY OF THE POLY-D,L-LACTIDE MICROPARTICLES ON THE HUMAN LYMPHOCYTES**  
I. Jovanović, M. Petković<sup>1</sup>, G. Joksić<sup>2</sup>, D. Uskoković<sup>1</sup>  
<sup>1</sup>*Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia;* <sup>2</sup>*Laboratory of Physical Chemistry, Institute of Nuclear Sciences „Vinča“, Belgrade, Serbia*

**Break: 10<sup>30</sup>-11<sup>00</sup>**

- 11<sup>00</sup>-11<sup>15</sup> **NONLINEAR EXCITATIONS IN Q1D STRUCTURAL POLYMER TRANSITIONS**  
G. Keković<sup>1</sup>, D. Raković<sup>1</sup>, D. Davidović<sup>2,3</sup>  
<sup>1</sup>*Faculty of Electrical Engineering, Belgrade, Serbia,* <sup>2</sup>*Vinca Institute of Nuclear Sciences, Belgrade, Serbia,* <sup>3</sup>*School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia*
- 11<sup>15</sup>-11<sup>30</sup> **PARAMAGNETIC/DIAMAGNETIC DYNAMICS OF BIOMOLECULES-WATER COMPLEXES ON NANOTESLA SCALE**  
Dj. Koruga  
*Department of Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia*
- 11<sup>30</sup>-11<sup>45</sup> **OBTAINING NANO CALCIUM PHOSPHATE/POLY(DL-LACTIDE-CO-GLYCOLIDE) COMPOSITE BIOMATERIAL BY SONOCHEMICAL PROCESSING**  
N. Ignjatović<sup>1</sup>, M. Dramićanin<sup>2</sup>, D. Vasiljević-Radović<sup>3</sup>, D. Uskoković<sup>1</sup>  
<sup>1</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia,* <sup>2</sup>*Institute of Nuclear Sciences Vinca, Belgrade, Serbia,* <sup>3</sup>*Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia*
- 11<sup>45</sup>-12<sup>00</sup> **SIMILARITIES ANALYSIS ON HYDROXYAPATITE-ZIRCONIA COMPOSITES**  
S.D. Bolboacă<sup>1</sup>, L. Jäntschi<sup>2</sup>  
<sup>1</sup>*"Iuliu Hațieganu" University of Medicine and Pharmacy, Cluj-Napoca, Romania,* <sup>2</sup>*Technical University of Cluj-Napoca, Romania*



## POSTER SESSION I

Tuesday, September 11, 2007, 20<sup>30</sup>-22<sup>00</sup>

### SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

**P.S.A.1. THE SYNTHESIS IN COMBUSTION MODE OF COMPLEX OXIDE FOR GAS SENSING MATERIALS**

M.L. Chernega, M.V. Kuznetsov, Yu.G. Morozov

*Institute of Structural Macrokinetics and Materials Science RAS, Chernogolovka, Moscow Region, Russia*

**P.S.A.2. THE EFFECT OF AN APPLIED ELECTRIC FIELD ON SELF-PROPAGATING HIGH-TEMPERATURE SYNTHESIS OF FERRITES**

S.M. Busurin, Yu.G. Morozov, M.V. Kuznetsov

*Institute of Structural Macrokinetics and Materials Science RAS, Chernogolovka, Moscow region, Russia*

**P.S.A.3. TiO<sub>2</sub> COATINGS PREPARED BY SOL-GEL METHOD FOR POTENTIAL USE FOR AIR DEODORIZING**

W. Mielcarek<sup>1</sup>, I.Zareba-Głodź<sup>2</sup>, K. Prociow<sup>1</sup>, J. Warycha<sup>1</sup>

<sup>1</sup>*Electrotechnical Institute, Wrocław, Poland*, <sup>2</sup>*Wrocław University of Technology, Wrocław, Poland*

**P.S.A.4. BIOMETIC METHOD SUITABILITY FOR PROCESSING OF TiO<sub>2</sub> COATINGS APPLICABLE FOR AIR DEODORIZING**

W. Mielcarek, K. Prociow, J. Warycha

*Electrotechnical Institute, Wrocław, Poland*

**P.S.A.5. ELECTRICAL PROPERTIES OF TiO<sub>2</sub> THIN FILMS WITH Eu AND Pd DOPANTS PREPARED BY MAGNETRON SPUTTERING ON SILICON**

E.L. Prociow, J. Domaradzki, D. Kaczmarek, T. Berlicki

*Faculty of Microsystem Electronics and Photonics, Wrocław University of Technology, Wrocław, Poland*

**P.S.A.6. A STUDY OF MICROSTRUCTURAL CHANGES IN TiN THIN FILMS INDUCED BY ION IMPLANTATION**

M. Popović, M. Novaković, D. Peruško, I. Radović, V. Milinović, M. Mitrić, M. Milosavljević

*VINČA Institute of Nuclear Sciences, Belgrade, Serbia*

- P.S.A.7. INFLUENCE OF NITROGEN ION IMPLANTATION ON THE MECHANICAL PROPERTIES OF C1045 STEEL**  
D. Peruško, S. Petrović, M. Mitrić, M. Novaković, M. Popović, M. Milosavljević  
*Institute of Nuclear Sciences Vinca, Belgrade, Serbia*
- P.S.A.8. SURFACE MODIFICATION WTi SYSTEM INDUCED BY TEA CO<sub>2</sub> LASER BEAM**  
S. Petrović<sup>1</sup>, B. Gaković<sup>1</sup>, M. Trtica<sup>1</sup>, D. Peruško<sup>1</sup>, Š. Miljanić<sup>2</sup>  
<sup>1</sup>*Institute of Nuclear Science Vinča, Belgrade, Serbia*  
<sup>2</sup>*Faculty of Physical Chemistry, Belgrade, Serbia*
- P.S.A.9. STUDY OF SUBSTRATE PRETREATMENT ON TOPOGRAPHY AND DEFECTS IN DEFECTS IN PVD-HARD COATINGS**  
P. Panjan<sup>1</sup>, M. Čekada<sup>1</sup>, B. Gaković<sup>2</sup>, M. Panjan<sup>1</sup>, D. Kek-Merl<sup>1</sup>, S. Paskvale<sup>1</sup>  
<sup>1</sup>*Jožef Stefan Institute, Ljubljana, Slovenia,* <sup>2</sup>*Vinca Institute of Nuclear Sciences, Belgrade, Serbia*
- P.S.A.10. THEORETICAL CALCULATION OF PARTITION AND THERMODYNAMIC FUNCTIONS OF B<sub>2</sub>C AND BC<sub>2</sub> GAS PHASE MOLECULES**  
J. Radić-Perić  
*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia*
- P.S.A.11. THE INFLUENCE OF THE GAS DISCHARGE ELECTRICAL PROPERTIES ON UNIPOLAR PULSE PLASMA SYSTEM RESPONSE**  
I. Popović, M. Zlatanović  
*Faculty of Electrical Engineering, Belgrade, Serbia*
- P.S.A.12. SILICON SURFACE PROCESSING BY QUASISTATIONARY PLASMA FLOW**  
I.P. Dojčinović<sup>1,2</sup>, M.M. Kuraica<sup>1,2</sup>, J. Purić<sup>1,2</sup>  
<sup>1</sup>*Faculty of Physics, University of Belgrade, Belgrade, Serbia*  
<sup>2</sup>*Center for Science and Technology Development, Belgrade, Serbia*
- P.S.A.13. INFLUENCE OF THE LASER PROCESSING PARAMETERS ON STRUCTURAL CHANGES OF SUPER ALLOY HASTELLOY**  
K. Kovačević<sup>1</sup>, A. Milosavljević<sup>2</sup>, M. Srećković<sup>3</sup>, E. Počuča<sup>4</sup>, I. Nešić<sup>2</sup>  
<sup>1</sup>*Institute for Metallurgy, Nikšić, Montenegro,* <sup>2</sup>*Faculty of Mechanical Engineering, Belgrade University, Serbia,* <sup>3</sup>*Faculty of Electrical Engineering, Belgrade University, Serbia,* <sup>4</sup>*“Nicola Tesla” Airport, Belgrade, Serbia*

- P.S.A.14 **THE INFLUENCE OF LASER BORONIZING ON THE SURFACE LAYERS STRUCTURE OF 500-7 NODULAR IRON**  
M. Paczkowska, W. Waligóra  
*Institute of Machines and Motor Vehicles, Poznan University of Technology, Poznan, Poland*
- P.S.A.15. **THE EFFECT OF TEMPERATURE AND ZINC CONCENTRATION ON ZINC COATINGS DEPOSITED WITH PACK CEMENTATION**  
D. Chaliampalias, N. Pistofidis, G. Vourlias  
*Physics Department, Aristotle University of Thessaloniki, Thessaloniki, Greece*
- P.S.A.16. **STUDY OF THE GROWTH MECHANISM OF ZINC HOT-DIP GALVANIZING COATINGS**  
N. Pistofidis, G. Vourlias, D. Chaliampalias  
*Physics Department, Aristotle University of Thessaloniki, Thessaloniki, Greece*
- P.S.A.17. **EXAMINATION OF THE MICROSTRUCTURAL FEATURES OF ZINC PROTECTIVE COATINGS ON LOW CARBON STEEL FORMED IN A FLUIDIZED BED REACTOR**  
D. Chaliampalias, G. Vourlias, N. Pistofidis  
*Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece*
- P.S.A.18. **FORMATION AND GROWTH OF COPPER DEPOSITS UNDER HYDROGEN CODEPOSITION**  
N.D. Nikolić, Lj.J. Pavlović  
*ICTM – Institute of Electrochemistry, University of Belgrade, Belgrade, Serbia*
- P.S.A.19. **CHARACTERIZATION OF CARBON FIBROUS MATERIALS MODIFIED BY RUBY LASER RADIATION**  
J. Stašić<sup>1</sup>, M. Srećković<sup>2</sup>, B. Kaludjerović<sup>1</sup>, S. Ristić<sup>3</sup>  
*<sup>1</sup>Institute of Nuclear Sciences "Vinča", Laboratory for materials science, Belgrade, Serbia, <sup>2</sup>Faculty of Electrical Engineering, Belgrade, Serbia, <sup>3</sup>Military Technical Institute, Belgrade, Serbia*
- P.S.A.20. **RAPID QUENCHED METAL FIBRES AND POROUS FIBROUS MATERIALS**  
V.N. Antsiferov, A.A. Smetkin  
*Centre of Powder Materials Science of PSTU, Perm, Russia*
- P.S.A.21. **PREPARATION OF Al(OH)<sub>3</sub> POWDER BY FIB FOR TEM INVESTIGATION**  
I. Nikolić<sup>1</sup>, V. Radmilović<sup>2</sup>, T.Z. Sholklapper<sup>3</sup>, D. Blečić<sup>1</sup>

<sup>1</sup>University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro, <sup>2</sup>LBNL, NCEM, MS-72, University of California, Berkeley, CA, USA, <sup>3</sup>T.Z. Sholklapper, LBNL, MSSM, University of California, Berkeley, CA, USA

- P.S.A.22. **MASS-SPECTROMETRIC DIFFERENTIATION OF SULFUR CONTAINING, ELECTRON-RICH HETEROCYCLES**  
J. Hadži-Djordjević<sup>1</sup>, I. Cekić-Lasković<sup>1</sup>, R. Marković<sup>2,3</sup>, A. Rašović<sup>3</sup>, D. Minić<sup>1,3</sup>  
<sup>1</sup>Faculty of Physical Chemistry, University of Belgrade, Serbia, <sup>2</sup>Faculty of Chemistry, University of Belgrade, Serbia, <sup>3</sup>Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia
- P.S.A.23. **POINT OF ZERO CHARGE AND ISOELECTRIC POINT OF ALUMINA**  
J.J. Gulicovski, L.J.S. Čerović, S.K. Milonjić  
The Vinča Institute of Nuclear Sciences, Belgrade, Serbia
- P.S.A.24. **STABILITY OF ZIRCONIA SOL IN THE PRESENCE OF VARIOUS INORGANIC ELECTROLYTES**  
J.M. Marković<sup>1</sup>, S.K. Milonjić<sup>1</sup>, V. Leovac<sup>2</sup>  
<sup>1</sup>The Vinča Institute of Nuclear Sciences, Belgrade, Serbia, <sup>2</sup>Chemistry Department, Faculty of Sciences, Novi Sad, Serbia
- P.S.A.25. **SYNTHESIS OF  $\text{Li}_{1-x}\text{Mn}_{2-x}\text{O}_4$  CATHODE MATERIAL USING GEL-COMBUSTION METHOD**  
I. Stojković<sup>1</sup>, D. Jugović<sup>2</sup>, M. Mitrić<sup>3</sup>, N. Cvjetičanin<sup>1</sup>, S. Mentus<sup>1</sup>  
<sup>1</sup>Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>Institute of Technical Sciences, Serbian Academy of Sciences, Belgrade, Serbia, <sup>3</sup>The Vinča Institute of Nuclear Sciences, Laboratory for Theoretical and Condensed Matter Physics, Belgrade, Serbia
- P.S.A.26. **HYDROTHERMAL SYNTHESIS OF CATHODE MATERIALS FOR LITHIUM-ION BATTERIES**  
Z. Stojanović, D. Jugović, D. Uskoković  
Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia
- P.S.A.27. **MODELING OF EMULSION PROCESS GENERATION USING REAL TIME MEASUREMENTS**  
S. Petrušić<sup>2</sup>, S. Pašalić<sup>1</sup>, P. Jovanić<sup>3</sup>  
<sup>1</sup>Ministry for Science, Belgrade, Serbia, <sup>2</sup>Faculty for Technology and Metalurgy, Belgrade, Serbia, <sup>3</sup>Institute for Plant Protection and Environment, Belgrade, Serbia
- P.S.A.28. **INNOVATIVE MATERIALS FOR H<sub>2</sub> STORAGE**  
D. Swierczynski, S. Bennici, A. Auroux  
IRCELYON, Institut de recherches sur la catalyse et l'environnement de Lyon, UMR5256, CNRS – Université Lyon 1, Villeurbanne, France

- P.S.A.29. **THE INFLUENCE OF EXCESS SODIUM CATIONS FROM LTA ZEOLITE ON HIGH TEMPERATURE CRYSTALLIZATION AND STABILITY OF LOW-CARNEGIEITE**  
A. Radulović<sup>1</sup>, D. Arandjelović<sup>1</sup>, R. Dimitrijević<sup>2</sup>, P. Vulić<sup>2</sup>, V. Dondur<sup>3</sup>  
<sup>1</sup>*Institute of General and Physical Chemistry, Belgrade, Serbia*, <sup>2</sup>*Faculty of Mining and Geology, Belgrade, Serbia*, <sup>3</sup>*Faculty of Physical Chemistry, Belgrade, Serbia*
- P.S.A.30. **PREPARATION AND CHARACTERIZATION OF ZEOLITE ENCAGED ENZYME-MIMETIC COPPER HISTIDINE COMPLEXES**  
Lj. Damjanović<sup>1</sup>, V. Rac<sup>2</sup>, V. Dondur<sup>1</sup>, R. Hercigonja<sup>1</sup>, V. Rakić<sup>2</sup>  
<sup>1</sup>*University of Belgrade, Faculty of Physical Chemistry, Beograd, Serbia*  
<sup>2</sup>*University of Belgrade, Faculty of Agriculture, Zemun, Serbia*
- P.S.A.31. **STRUCTURAL DESTABILIZATION IN MAGNESIUM HYDRIDE**  
S. Milovanović<sup>1</sup>, N. Novaković<sup>1</sup>, M. Šiljegović<sup>1</sup>, J. Grbović Novaković<sup>1</sup>, N. Ivanović<sup>1</sup>  
<sup>1</sup>*Institute of Nuclear Sciences Vinca, Belgrad, Serbia*, <sup>a</sup>*Laboratory of material sciences*, <sup>b</sup>*Laboratory of nuclear and plasma physics*, <sup>c</sup>*Laboratory of physics*
- P.S.A.32. **EFFECTS OF ORGANIC SURFACTANTS ON MECHANOCHEMICALLY SYNTHESIZED ZnO PARTICLES**  
A. Stanković, Z. Stojanović, D. Uskoković  
*Institute of Technical Science of the Serbian Academy of Sciences and Arts, Belgrade, Serbia*
- P.S.A.33. **THEORETICAL APPROACH FOR DEVELOPMENT OF ANTIMICROBIAL MATERIALS BASED ON Ag-APATITES**  
S. Raičević, V. Stanić  
*Vinča Institute of Nuclear Sciences, Radiation and Environmental Protection Laboratory, Belgrade, Serbia*
- P.S.A.34. **INFLUENCE OF MgO ADDITION ON THE SYNTHESIS OF ZINC-TITANATE CERAMICS**  
N. Obradović<sup>1</sup>, N. Labus<sup>1</sup>, M. Mitrić<sup>2</sup>, M.V. Nikolić<sup>3</sup>, M.M. Ristić<sup>4</sup>  
<sup>1</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia*, <sup>2</sup>*The Vinca Institute of Nuclear Sciences, Belgrade, Serbia*, <sup>3</sup>*Center for Multidisciplinary Studies, University of Belgrade, Belgrade, Serbia*, <sup>4</sup>*Serbian Academy of Sciences and Arts, Belgrade, Serbia*
- P.S.A.35. **ARSENIC (V) SORPTION BY IRON MODIFIED NATURAL ZEOLITE TUFF**  
T. Stanić<sup>1</sup>, M. Tomašević-Čanović<sup>1</sup>, A. Živanović<sup>2</sup>, A. Radosavljević-Mihajlović<sup>3</sup>, S. Milićević<sup>1</sup>

*<sup>1</sup>Institute for Technology of Nuclear and Other Raw Mineral Materials, Belgrade, Serbia, <sup>2</sup>VMA, Institute for Hygiene, Belgrade, Serbia, <sup>3</sup>VINČA Institute of Nuclear Science, Material Science Lab., Beograd, Serbia*

**P.S.A.36. ORIENTATION-INDUCED CHANGES IN MICROSTRUCTURE AND CRYSTALLINITY OF DIFFERENT PEs**

D. Miličević, A. Leskovac, M. Mitrić, E. Suljovrujić  
*Vinča Institute of Nuclear Sciences, Belgrade, Serbia*

**P.S.A.37. THE STUDY OF NUCLEATION OF SECONDARY PHASE IN GLASS WITH PRIMARY CRYSTALLIZATION**

M.B. Tošić<sup>1</sup>, V.D. Živanović<sup>1</sup>, N.S. Blagojević<sup>2</sup>, S.R. Grujić<sup>2</sup>, J.D. Nikolić<sup>1</sup>  
*<sup>1</sup>Institute for Technology of Nuclear and other Mineral Raw Materials, Belgrade, Serbia, <sup>2</sup>Faculty of Technology and Metallurgy, Belgrade, Serbia*

**P.S.A.38. CONJUGATED POLYMER CHARACTERISATION USING LASER BEAM SCATTERING TECHNIQUES**

V. Arsoski, R. Ramović, M. Srećković  
*School of Electrical Engineering, University of Belgrade, Serbia*

**P.S.A.39. COMPARISON OF SELECTIVE CATALYSTS FOR POLYURETHANE FOAMS**

B. Strachotová, A. Strachota, M. Špírková  
*<sup>1</sup>Department of Polymer Networks and Mechanical Properties, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Praha, Czech Republic*

**P.S.A.40. CURING REACTIONS OF SEMI-DRYING OILS ALKYDS WITH MELAMINE RESIN**

M.C. Jovičić, R.Ž. Radičević, J.K. Budinski-Simendić  
*University of Novi Sad, Faculty of Technology, Novi Sad, Serbia*

**P.S.A.41. DEGRADATION OF SOLAR CELLS DUE TO DIFFERENT WORKING ENVIRONMENTS**

A. Vasić-Milovanović<sup>1</sup>, P.Osmokrović<sup>2</sup>, B.Lončar<sup>3</sup>, S.Stanković<sup>4</sup>  
*<sup>1</sup>Faculty of Mechanical Engineering, Belgrade, Serbia, <sup>2</sup>Faculty of Electrical Engineering, Belgrade, Serbia, <sup>3</sup>Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>4</sup>The Vinča Institute of Nuclear Sciences, Belgrade, Serbia*

**P.S.A.42. INFLUENCE OF COMPOSITION OF BORONISING MIXTURE ON THE DEPTH OF BORIDE LAYERS PRESSED AND BORIDED SAMPLES FROM IRON POWDER**

E. Požega<sup>1</sup>, S. Ivanov<sup>2</sup>

<sup>1</sup>Copper Institute, Bor, Serbia, <sup>2</sup>University of Belgrade, Technical Faculty in Bor, Bor, Serbia

**P.S.A.43. SYNTHESIS OF OLIGOADDUCTS OF MALONIC ACID C<sub>60</sub>**

A. Djordjević, I. Ičević

*Department of Chemistry, Faculty of Science, University of Novi Sad, Novi Sad, Serbia*

**P.S.A.44. CHEMICAL SYNTHESIS AND CHARACTERIZATION OF LITHIUM ORTHOSILICATE (Li<sub>2</sub>SiO<sub>4</sub>). CO<sub>2</sub> ABSORPTION CAPACITIES**

V.V. Kovačević<sup>1</sup>, B.P. Dojčinović<sup>2</sup>, B.M. Obradović<sup>1,5</sup>, M.M. Kuraica<sup>1,5</sup>, D.D. Manojlović<sup>3</sup>, V.M. Rakić<sup>4</sup>

*<sup>1</sup>University of Belgrade, Faculty of Physics, Belgrade, Serbia, <sup>2</sup>Centre of Chemistry, Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Faculty of Chemistry, Belgrade, Serbia, <sup>4</sup>University of Belgrade, Faculty of Agriculture, Zemun, Serbia, <sup>5</sup>Center for Science and Technology Development, Belgrade, Serbia*

**P.S.A.45. SIMILARITY AND DIFFERENCE BETWEEN EXPLOSION WELDING AND LASER HYBRID ON STRUCTURAL LEVEL**

M. Kutin<sup>1</sup>, S. Bunić<sup>2</sup>, M. Davidović<sup>1</sup>

*<sup>1</sup>Institute Goša, Research and Development, Belgrade, Serbia*

*<sup>2</sup>Faculty of Technology, Banja Luka, Republic of Srpska, BiH*

**P.S.A.46. EXPERIMENTAL RESEARCH OF EFFECTS OF AIR PRESSURE TO THE WALLS OF BYPASSING HIGH SPEED TRAINS**

M. Puharić, M. Kutin, J. Tanasković

*GOŠA Institute, Belgrade, Serbia*

**P.S.A.47. THERMAL STABILITY AND FRAGILITY PARAMETERS OF Fe-M-Al-Ga-P-C-B (M=Nb) AMORPHOUS ALLOYS**

N. Mitrović<sup>1</sup>, A. Kalezić-Glišović<sup>1</sup>, S. Roth<sup>2</sup>, J. Eckert<sup>3</sup>

*<sup>1</sup>Joint Laboratory for Advanced Materials of SASA, Section for Amorphous Systems, Technical Faculty Čačak, Čačak, Serbia, <sup>2</sup>IFW Dresden, Institute for Metallic Materials, Dresden, Germany, <sup>3</sup>IFW Dresden, Institute for Complex Materials, Dresden, Germany*

**P.S.A.48. XRD ANALYSIS OF HIGH-COPPER AlCuMg ALLOYS**

B. Zlatičanin<sup>1</sup>, B. Radonjić<sup>1</sup>, M. Filipović<sup>2</sup>

*<sup>1</sup>University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro, <sup>2</sup>Faculty of Technology and Metallurgy, Belgrade, Serbia*

- P.S.A.49. **TRICALCIUM ALUMINATE HEXAHYDRATE (TCA) FILTER AID IN THE BAYER INDUSTRY**  
P. Tomić<sup>1</sup>, M. Davidović<sup>2</sup>, S. Batinić<sup>1</sup>, V. Petković<sup>1</sup>  
<sup>1</sup>Fabrika glinice "Birac" AD, Zvornik, Republika Srpska, BiH  
<sup>2</sup>Institute Goša, Belgrade, Serbia
- P.S.A.50. **AN INFLUENCE OF MICROSTRUCTURE OF SCREEN FORMED BY LASER EXPOSURE OF LIGHT-SENSITIVE FILM ON TON VALUE INCREASE IN PRINTING**  
P.M. Živković, P.S. Uskoković, A. Krstić, N. Borna  
Faculty of Technology and Metallurgy, University of Belgrade, Serbia
- P.S.A.51. **EXPERIMENTAL ANALYSIS OF CRACK INITIATION AND GROWTH IN WELDED JOINT OF STEEL FOR OPERATION AT ELEVATED TEMPERATURES**  
M. Burzić, M. Kutin, M. Puharić  
Institute GOŠA d.o.o., Belgrade, Serbia
- P.S.A.52. **THE POSSIBILITIES OF USING ELECTRO FILTER ASH OF STEAM POWER PLANT „PLJEVLJA“ AS RAW MATERIALS MIXTURE COMPONENT FOR OBTAINING SINTERED PRODUCT**  
M. Krgović<sup>1</sup>, S. Djurković<sup>1</sup>, N. Marstijepović<sup>1</sup>, M. Ivanović<sup>1</sup>, R. Zejak<sup>2</sup>, M. Knežević<sup>2</sup>  
<sup>1</sup>Faculty of Metallurgy and Technology, Podgorica, Montenegro,  
<sup>2</sup>Faculty of Civil Engineering, Podgorica, Montenegro,
- P.S.A.53. **INFLUENCE OF BASICITY OF ELECTRODES COVERING AND WIRE COMPOSITION OF ELECTRODES KERNEL ON THE STRUCTURE AND PROPERTIES OF WELD OF LOW ALLOY STEELS**  
Ž. Blečić<sup>1</sup>, D. Blečić<sup>1</sup>, D. Bajić<sup>2</sup>, D. Čabarkapa<sup>3</sup>  
<sup>1</sup>University of Montenegro, Faculty of Metallurgy and Tehnology, Podgorica, Montenegro, <sup>2</sup>University of Montenegro, Faculty of Mechanical Engineering, Podgorica, Montenegro, <sup>3</sup>Elektrodes Plant Piva – Pluzine, Montenegro
- P.S.A.54. **NEW DIRECTION IN SOLID STATE SCIENCE**  
Yu.I. Vesnin  
Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia
- P.S.A.55. **PREPARATION OF BORON CARBIDE NANOWIRES VIA EPITAXIAL VLS GROWTH**  
M. Jazirehpur, A. Alizadeh  
MUT University of Tehran, Iran



- P.S.A.56. **SYNTHESIS OF BORON CARBIDE NANOWIRES AND NANORODS VIA CARBOTHERMAL-VLS ROUTE**  
M. Jazirehpur, A. Alizadeh  
*MUT University of Tehran, Iran*
- P.S.A.57. **STRAIGHT BORON CARBID NANORODS VIA A CARBOTHERMAL TEMPLATE ASSISTED METHOD**  
M. Jazirehpur, A. Alizadeh  
*MUT University of Tehran, Iran*
- P.S.A.58. **SYNTHESIS OF TITANIUM DIBORIDE NANOWIRES AND NANORODS VIA CARBOTHERMAL-VLS ROUTE**  
M. Jazirehpur, A. Alizadeh  
*MUT University of Tehran, Iran*
- P.S.A.59. **PREPARATION OF BORON CARBIDE NANOWIRES VIA A TEMPLATE ASSISTED POLYMERIC PRECURSOR**  
M. Jazirehpur, A. Alizadeh  
*MUT University of Tehran, Iran*
- P.S.A.60. **PREPARATION OF BORON CARBIDE NANOFIBERS VIA A THREE STEP METHOD FROM PAN NANOFIBERS**  
M. Jazirehpur, A. Alizadeh  
*MUT University of Tehran, Iran*
- P.S.A.61. **TIME-DOMAIN PHOTOTHERMAL RESPONSE OF MEDIA WITH THERMAL MEMORY FOR VARIOUS SHAPES OF INCIDENT PULSES**  
S. Galović, D. Čevizović, M. Popović, Z. Stojanović  
*The Vinca Institute of Nuclear Sciences, Belgrade, Serbia*
- P.S.A.62. **SMALL POLARON ELECTRICAL CONDUCTIVITY IN MACROMOLECULAR CHAINS**  
D. Čevizović, S. Galović, Z. Ivić  
*The Vinca Institute of Nuclear Sciences, Belgrade, Serbia*
- P.S.A.63. **CHARACTERIZATION OF ORGANIC/METAL INTERFACES USING QUANTUM THEORY OF ATOMS IN MOLECULES: CORRELATION WITH EXPERIMENT**  
P.M. Mitrašinović, M.L. Mihajlović  
*Center for Multidisciplinary Studies, University of Belgrade, Belgrade, Serbia*
- P.S.A.64. **URANIUM (VI) ADSORPTION ON ACIDS MODIFIED ZEOLITIC TUFF**  
S. Matijašević<sup>1</sup>, A. Daković<sup>1</sup>, A. Stojanović<sup>1</sup>, D. Ileš<sup>1</sup>, G. Vitorović<sup>2</sup>, B. Mitrović<sup>2</sup>  
<sup>1</sup>*Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade,*

*Serbia, <sup>2</sup>Faculty of Veterinary Medicine, Belgrade, Serbia*

**P.S.A.65. BASIC OPTICAL MATERIALS OF FERRULE AND THEIR PERFORMANCE**

S. Pantelić<sup>1</sup>, M. Srečković<sup>2</sup>

<sup>1</sup>*Institute of Security, Belgrade, Serbia*

<sup>2</sup>*Faculty of Electrical Engineering, Belgrade, Serbia*

**P.S.A.66. CORRELATION BETWEEN ISOTHERMAL ANNEALING AND MAGNETIC SUSCEPTIBILITY RELATIVE CHANGE OF THE  $\text{Fe}_{89.8}\text{Ni}_{1.5}\text{Si}_{5.2}\text{B}_3\text{C}_{0.5}$  AMORPHOUS ALLOY**

A. Maričić, A. Kalezić-Glišović, N. Mitrović, R. Simeunović, S. Djukić

*Joint Laboratory for Advanced Materials of SASA, Section for Amorphous Systems, Technical Faculty Čačak, Čačak, Serbia*

## POSTER SESSION II

*Wednesday, September 12, 2007, 20<sup>30</sup>-22<sup>00</sup>*

### SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATIONS

- P.S.B.1. EXCITON STATES IN IRREGULAR TYPE-II QUANTUM-DOT SUPERLATTICES IN A MAGNETIC FIELD**  
D. Veljković<sup>1</sup>, M. Tadić<sup>1,2</sup>, F.M. Peeters<sup>2</sup>  
<sup>1</sup>*Faculty of Electrical Engineering, University of Belgrade, Belgrade, Serbia*  
<sup>2</sup>*Department of Physics, University of Antwerp, Groenenborgerlaan, Belgium*
- P.S.B.2. CORE-LEVEL AND VALENCE BAND STUDIES OF (GaMn)As WHISKERS**  
L. Ulfat<sup>1,2</sup>, J. Adell<sup>1</sup>, J. Sadowski<sup>3</sup>, L. Ilver<sup>1</sup>, J. Kanski<sup>1</sup>  
<sup>1</sup>*Department of Applied Physics, Chalmers University of Technology, Göteborg, Sweden,* <sup>2</sup>*Department of Physics University of Karachi, Karachi, Pakistan,*  
<sup>3</sup>*Institute of Physics, Polish Academy of Sciences, Warszawa, Poland*
- P.S.B.3. MODELLING THE INFLUENCE OF DIFFERENT PACKAGING ON RADFET RESPONSE TO PROTON IRRADIATION**  
S.J. Stanković, R.D. Ilić, D. Davidović, M. Kovačević  
*Vinča Institute of Nuclear Sciences, Belgrade, Serbia*
- P.S.B.4. COMPOSITION DEPENDENCE OF THE DC AND AC CONDUCTIVITY OF NON-CRYSTALLINE SEMICONDUCTORS OF  $\text{Cu}_x[(\text{As}_2\text{Se}_3)_{0.9}(\text{AsI}_3)_{0.1}]_{100-x}$  TYPE**  
F. Skuban<sup>1</sup>, S.R. Lukić<sup>1</sup>, M. Slankamenac<sup>2</sup>, D.M. Petrović<sup>1</sup>  
<sup>1</sup>*Department of Physics, Faculty of Sciences, University of Novi Sad, Novi Sad, Serbia,* <sup>2</sup>*Faculty of Electrical Engineering, University of Novi Sad, Novi Sad, Serbia*
- P.S.B.5. DEVELOPMENT OF FINE-GRAINED OXIDE CERAMICS USING PULSED COMPACTION OF LOW AGGLOMERATED NANOPOWDERS**  
V.V. Ivanov  
*Institute of Electrophysics, UD RAS, Ekaterinburg, Russia*
- P.S.B.6. SINGLE CRYSTAL ALLOYS. THERMAL FATIGUE AND CREEP.**  
L.B. Getsov, E.R. Golubovskii, A.I. Rybnikov  
*NPO Central Boiler and Turbine Institute, St. Petersburg, Russia*

- P.S.B.7. **OPTICAL AND MAGNETIC PROPERTIES OF PbTe(Ni) SINGLE CRYSTALS**  
N. Romčević<sup>1</sup>, M. Romčević<sup>1</sup>, J. Trajić<sup>1</sup>, W. Dobrowolski<sup>2</sup>, T.A. Kuznetsova<sup>3</sup>, D.R. Khokhlov<sup>3</sup>  
<sup>1</sup>*Institute of Physics, Belgrade, Serbia*  
<sup>2</sup>*Institute of Physics, Polish Academy of Sciences, Warsaw, Poland*  
<sup>3</sup>*Department of Physics, Moscow State University, Moscow, Russia*
- P.S.B.8. **ELECTRON STRUCTURE AND LUMINESCENCE PROPERTIES OF Ca<sub>3</sub>Ga<sub>2</sub>Ge<sub>3</sub>O<sub>12</sub> GARNET CRYSTALS**  
I.D. Shcherba<sup>1</sup>, D. Uskoković<sup>2</sup>, L.V. Kostyk<sup>3</sup>, L.O. Dobrjanska<sup>3</sup>, V.M. Uvarov<sup>4</sup>, A.J. Senkivich<sup>4</sup>, B.M. Jatcyk<sup>5</sup>  
<sup>1</sup>*Institute of Techniques, Academy of Pedagogy, Podchorazych, Krakow, Poland*  
<sup>2</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia*, <sup>3</sup>*Lviv National University by Ivan Franko, Lviv, Ukraine*, <sup>4</sup>*Institute of Metals Physics NAN Ukraine, Kyi, Ukraine*, <sup>5</sup>*University of Forestry and Wood Technology, Lviv, Ukraine*
- P.S.B.9. **REFRACTION IN 2D HEXAGONAL-LIKE PHOTONIC CRYSTALS**  
Dj. Jovanović<sup>1</sup>, R. Gajić<sup>1</sup>, K. Hingerl<sup>2</sup>  
<sup>1</sup>*Institute of Physics, Belgrade, Serbia*, <sup>2</sup>*Christian Doppler Laboratory, Institute for Semiconductors and Solid State Physics, University of Linz, Linz, Austria*
- P.S.B.10. **SYNTHESIS AND XRD STUDY OF POROUS ANODIC TiO<sub>2</sub> FILMS**  
D.I. Petukhov, I.V. Kolesnik, A.A. Eliseev, A.V. Lukashin, Yu.D. Tretyakov  
*Department of Material Science Moscow State University, Moscow, Russia*
- P.S.B.11. **DYNAMIC OF THE PROFILE CHARGING IN TWO FREQUENCY PLASMA ETCHING OF SiO<sub>2</sub>**  
B. Radjenović<sup>1</sup>, M. Radmilović-Radjenović<sup>2</sup>, Z.Lj. Petrović<sup>2</sup>, Ž. Nikitović<sup>2</sup>  
<sup>1</sup>*Vinča Institute of Nuclear Sciences, Belgrade, Serbia*, <sup>2</sup>*Institute of Physics, Belgrade, Serbia*
- P.S.B.12. **CRYSTAL STRUCTURE OF A AND B SITE Ce DOPED CaMnO<sub>3</sub> PEROVSKITE**  
J. Dukić<sup>1</sup>, S. Bošković<sup>1</sup>, B. Matović<sup>1</sup>, V. Kahlenberg<sup>2</sup>  
<sup>1</sup>*Institute of Nuclear Sciences „Vinča”, Materials Science Laboratory, Belgrade, Serbia*, <sup>2</sup>*Institute of Mineralogy and Petrography, University of Innsbruck, Innsbruck, Austria*

- P.S.B.13. PHONON CONTRIBUTION IN THERMODYNAMICS OF CRYSTALLINE QUANTUM WIRES**  
D.I. Ilić<sup>1</sup>, J.P. Šetrajić<sup>2</sup>, D.Lj. Mirjanić<sup>3</sup>, S.M. Vučenović<sup>3</sup>, S.K. Jaćimovski<sup>4</sup>, V.D. Sajfert<sup>5</sup>, V.M. Zorić<sup>2</sup>  
<sup>1</sup>*Faculty of Technical Sciences, University of Novi Sad, Vojvodina, Serbia,*  
<sup>2</sup>*Department of Physics, Faculty of Sciences, University of Novi Sad, Vojvodina, Serbia,* <sup>3</sup>*Faculty of Medicine, University of Banja Luka, Banja Luka, Republic of Srpska, Bosnia and Herzegovina,* <sup>4</sup>*Faculty of Electrical Engineering, University of Belgrade, Serbia,* <sup>5</sup>*Technical Faculty “M.Pupin” – Zrenjanin, University of Novi Sad, Vojvodina, Serbia*
- P.S.B.14. STRUCTURAL DEFORMATION IN Hf<sub>2</sub>Ni OBSERVED BY TDPAC METHOD**  
B. Cekić, A. Umićević, V. Ivanovski, V. Koteski, J. Belošević-Čavor, S. Pavlović, M. Šiljegović  
*Institute of Nuclear Sciences Vinča, Belgrade, Serbia*
- P.S.B.15. THE EFFECTS OF POLARIZATIONAL BREMSSTRAHLUNG IN ELECTRON COLLISIONS WITH CLUSTERS**  
A.R. Tančić<sup>1</sup>, M. Davidović<sup>2</sup>  
<sup>1</sup>*VINČA Institute for Nuclear Sciences, Beograd, Serbia*  
<sup>2</sup>*GOŠA Institute, Belgrade, Serbia*
- P.S.B.16. PREPARATION AND IR-SPECTROSCOPIC CHARACTERIZATION OF AURIVILIUS BI-LAYERED PEROVSKITE**  
Z.Ž. Lazarević<sup>1</sup>, B.D. Stojanović<sup>2</sup>, M.J. Romčević<sup>1</sup>, N.Ž. Romčević<sup>1</sup>  
<sup>1</sup>*Institute of Physics, Belgrade, Serbia*  
<sup>2</sup>*Center for Multidisciplinary Studies University of Belgrade, Belgrade, Serbia*
- P.S.B.17. EVOLUTION OF STRUCTURE AND PROPERTIES OF Ti-Si-C COMPOSITES AT MECHANICAL SYNTHESIS AND HOT PRESSING**  
M.N. Kachenjuk, A.A. Smetkin  
*Centre of Powder Materials Science of PSTU, Perm, Russia*
- P.S.B.18. ANALYTICAL MODEL OF DRIFT REGION VOLTAGE IMPACT ON SiC DIMOSFET STRUCTURE CHARACTERISTICS**  
R.M. Ramović<sup>1</sup>, S.M. Ostojić<sup>2</sup>, P.M. Lukić<sup>3</sup>, R.M. Šašić<sup>2</sup>  
<sup>1</sup>*Faculty of Electrical Engineering, University of Belgrade, Serbia,*  
<sup>2</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Serbia,*  
<sup>3</sup>*Faculty of Mechanical Engineering, University of Belgrade, Serbia*

- P.S.B.19. ENERGY LOSS AND DEFLECTION OF FAST IONS MOVING PARALLEL TO THE GRAPHENE SHEET**  
I. Radović<sup>1</sup>, Lj. Hadžievski<sup>1</sup>, N. Bibić<sup>1</sup>, Z.L. Mišković<sup>2</sup>  
<sup>1</sup>*VINČA Institute of Nuclear Sciences, Belgrade, Serbia,* <sup>2</sup>*Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, Canada*
- P.S.B.20. INVESTIGATION OF GAMMA-RAY INDUCED CHARGE IN SILICON DIOXIDE FILMS BASED ON A STOCHASTIC MODEL**  
M. Odalović, D. Petković  
*Faculty of Science and Mathematics, University of Pristina, Kosovska Mitrovica, Serbia*
- P.S.B.21. MATHEMATICAL MODELLING AND MULTICRITERIA DESIGN OPTIMIZATION OF A THIN-WALLED BEAM**  
N. Andjelić, B. Rosić, V. Milošević Mitić  
*Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia*
- P.S.B.22. PARALLEL ANALYSIS OF HF MEASUREMENTS AND METHOD-OF-MOMENTS BASED ELECTROMAGNETIC SIMULATION OF LC EMI CHIP FILTERS**  
M. Luković<sup>1</sup>, O. Aleksić<sup>2</sup>, V. Marić<sup>3</sup>, Lj. Živanov<sup>3</sup>  
<sup>1</sup>*Institute of Security, Belgrade, Serbia,* <sup>2</sup>*Centre for Multidisciplinary Studies, Belgrade University, Serbia,* <sup>3</sup>*Faculty of Technical Sciences, University of Novi Sad, Serbia*
- P.S.B.23. MOLECULAR STRUCTURE IN CORRELATION WITH ELECTROCHEMICAL PROPERTIES OF MIXED-LIGAND COBALT COMPLEXES**  
V.M. Jovanović<sup>1</sup>, K. Babić Samardžija<sup>2,3</sup>, S.P. Sovilj<sup>4</sup>  
<sup>1</sup>*University of Belgrade, ICTM-Institute of Electrochemistry, Belgrade, Serbia,* <sup>2</sup>*Rice University, Chemistry Department, Houston, TX, USA,* <sup>3</sup>*Baker Petrolite, Sugar Land, TX, USA,* <sup>4</sup>*University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*
- P.S.B.24. ANTIFERROMAGNETIC COUPLING OF COPPER(II) IONS VIA HYDROGEN BONDING IN Cu(II) COMPLEX WITH AN ARYLPIRAZOLE LIGAND**  
V. Leovac<sup>1</sup>, V. Spasojević<sup>2</sup>, V. Kusigerski<sup>2</sup>, M. Joksović<sup>3</sup>, N. Lazarov<sup>2</sup>, S. Novaković<sup>2</sup>  
<sup>1</sup>*Faculty of Sciences, University of Novi Sad, Serbia,* <sup>2</sup>*The Vinca Institute of Nuclear Sciences, Condensed Matter Physics Laboratory, Belgrade, Serbia* <sup>3</sup>*Faculty of Sciences, University of Kragujevac, Kragujevac, Serbia*
- P.S.B.25. UPWARD PENETRATION OF GRAINS THROUGH A GRANULAR MEDIUM**

Z.M. Jakšić, S.B. Vrhovac, B. Panić, B.M. Jelenković  
*Institute of Physics, Zemun, Belgrade, Serbia*

**P.S.B.26. ON THE PREPARATION OF OPEN-FRAMEWORK MANGANESE(II)-SUBSTITUTED ALUMINOPHOSPHATE**

S. Jevtić<sup>1</sup>, N. Rajić<sup>1</sup>, Dj. Stojaković<sup>1</sup>, M. Mazaj<sup>2</sup>, V. Kaučić<sup>2</sup>  
<sup>1</sup>*Faculty of Technology and Metallurgy, Beograd, Serbia*  
<sup>2</sup>*National Institute of Chemistry, Ljubljana, Slovenia*

**P.S.B.27. SYNTHESIS AND PROPERTIES OF NANO-SPINELS**

M. Pošarac<sup>1</sup>, B. Matović<sup>1</sup>, T. Volkov-Husović<sup>2</sup>, M. Logar<sup>3</sup>, M. Ninić<sup>1</sup>  
<sup>1</sup>*INN Vinca, Materials Science Laboratory, Belgrade, Serbia*  
<sup>2</sup>*Faculty of Technology and Metallurgy, Belgrade, Serbia*,  
<sup>3</sup>*Faculty of Mining and Geology, Belgrade, Serbia*

**P.S.B.28. MODIFICATION OF PILLARED CLAYS WITH COBALT FUNCTIONALITY. THEIR CATALYTIC PROPERTIES**

S. Sredić<sup>1</sup>, Ž. Čupić<sup>2</sup>, M. Davidović<sup>3</sup>, V. Malbašić<sup>1</sup>, D. Jovanović<sup>2</sup>, U.B. Mioč<sup>4</sup>, D. Lončarević<sup>2</sup>  
<sup>1</sup>*Institute of Mining, Prijedor, Republic of Srpska, Bosnia and Herzegovina*, <sup>2</sup>*IHTM, Center of Catalysis and Chemical Engineering, Belgrade, Serbia*, <sup>3</sup>*Goša Institute, Belgrade, Serbia*, <sup>4</sup>*Faculty of Physical Chemistry University of Belgrade, Belgrade, Serbia*

**P.S.B.29. SELF-ORGANIZING PROCESSES IN CONDENSED NANO-SYSTEMS**

O.V. Sobol<sup>1</sup>, L. Ribić<sup>2</sup>, L.Yu. Kunitskaya<sup>1</sup>  
<sup>1</sup>*Technical Centre of National Academy of Science of Ukraine*,  
<sup>2</sup>*Technical Faculty of Agronomy, Cacak, University of Kragujevac, Serbia*

**P.S.B.30. CHANGES IN THE MICROSTRUCTURE OF Fe-DOPPED Gd<sub>5</sub>Si<sub>2</sub>Ge<sub>2</sub>**

I. Škulj<sup>1</sup>, P.J. McGuinness<sup>2</sup>, B. Podmiljšak<sup>2</sup>, B. Šuštaršič<sup>1</sup>, M. Jenko<sup>1</sup>  
<sup>1</sup>*Institute of Metals and Technology, Ljubljana, Slovenia*  
<sup>2</sup>*Jožef Stefan Institute, Ljubljana, Slovenia*

**P.S.B.31. INVESTIGATION OF THE BEHAVIOUR OF NANOSIZED FERROMAGNETIC SOLUTIONS IN THE ELECTROMAGNETIC FIELD**

D. Dimitrov<sup>1</sup>, N. Piperov<sup>2</sup>, S. Vasileva<sup>3</sup>, M. Natov<sup>3</sup>  
<sup>1</sup>*Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria*  
<sup>2</sup>*Institute of Metal Science, Bulgarian Academy of Sciences, Sofia, Bulgaria*  
<sup>3</sup>*University of Chemical Technology and Metallurgy, Sofia, Bulgaria*

**P.S.B.32. IN-SITU INORGANIC NANOPARTICLE FORMATION IN SELF-ASSEMBLED POLYELECTROLYTE MULTILAYER FILMS**

M. Logar, B. Jančar, D. Suvorov  
*Jožef Stefan Institute, Advanced Materials Department, Ljubljana, Slovenia*

- P.S.B.33. **MODELING AND SIMULATION OF THICK FILM NTC THERMISTORS BASED ON NANO-STRUCTURED MANGANITE -NiMn<sub>2</sub>O<sub>4</sub>**  
B. Radojčić<sup>1</sup>, O. Aleksić<sup>2</sup>, R. Ramović<sup>3</sup>, S. Savić<sup>4</sup>  
<sup>1</sup>*Institute of Security, Belgrade, Serbia,* <sup>2</sup>*Centre for Multidisciplinary Studies, Belgrade University, Serbia,* <sup>3</sup>*Faculty of Electrical Engineering, Belgrade University, Serbia,* <sup>4</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia*
- P.S.B.34. **CHARACTERIZATION OF BARIUM TITANATE CERAMICS BY IMPEDANCE SPECTROSCOPY**  
S. Marković<sup>1</sup>, S. Mentus<sup>2</sup>, Č. Jovalekić<sup>3</sup>, D. Uskoković<sup>1</sup>  
<sup>1</sup>*Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia,* <sup>2</sup>*Faculty of Physical Chemistry, Belgrade, Serbia,* <sup>3</sup>*Center for Multidisciplinary Studies, University of Belgrade, Belgrade, Serbia*
- P.S.B.35. **ELECTROCHEMICALLY DEPOSITED CUPROUS OXIDE AND ZINC OXIDE FILMS FOR SOLAR APPLICATION**  
V. Georgieva, M. Georgieva  
*Faculty of Electrical Engineering and Information Technology, The "St. Cyril & Methodius" University, Skopje, Macedonia*
- P.S.B.36. **ELECTROCHEMICALLY DEPOSITED ZnO THIN FILMS AND THE INFLUENCE OF HYDROGEN PLASMA ON THEIR TRANSMITTANCE**  
V. Georgieva<sup>1</sup>, J. Wienke-Ullrich<sup>2</sup>, A. Tanuševski<sup>3</sup>  
<sup>1</sup>*Faculty of Electrical Engineering, The "St. Cyril & Methodius" University, Skopje, Macedonia,* <sup>2</sup>*ECN, Petten, The Netherlands,* <sup>3</sup>*Institute of Physics, Faculty of Natural Sciences and Mathematics, The "St. Cyril and Methodius" University, Skopje, Macedonia*
- P.S.B.37. **ELECTRICAL RESISTANCE AND TERMOPHYSICAL PROPERTIES OF Sc AND Ca AT SHOCK-WAVE COMPRESSION**  
D.V. Shakh-ray, V.V. Avdonin, A.A. Golyshev  
*Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia*
- P.S.B.38. **CONDUCTIVITY OF C<sub>60</sub> AND C<sub>70</sub> FULLERENES UNDER DYNAMIC SHOCK COMPRESSION**  
V. Avdonin<sup>1</sup>, D. Shakh-ray<sup>1</sup>, A. Golyshev<sup>1</sup>, N. Sidorov<sup>2</sup>  
<sup>1</sup>*Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia*  
<sup>2</sup>*Institute of Solid State Physics RAS, Chernogolovka, Russia*
- P.S.B.39. **INTRINSIC BULK CARRIER CONCENTRATION AND MOBILITY IN NANOSTRUCTURED MANGANITE AFTER POWDER ACTIVATION**  
S.M. Savić<sup>1</sup>, O.S. Aleksić<sup>2</sup>, G.M. Stojanović<sup>3</sup>, M.V. Nikolić<sup>2</sup>, D.T. Luković<sup>1</sup>  
<sup>1</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia*



<sup>2</sup>Center for multidisciplinary studies of the University of Belgrade, Belgrade, Serbia  
<sup>3</sup>Faculty of Technical Sciences of University of Novi Sad, Novi Sad, Serbia

**P.S.B.40. REMOVAL OF ANTIBIOTIC DOXYCYCLINE FROM WASTE WATERS BY SURFACTANT-MODIFIED ZEOLITES**

Lj. Damjanović<sup>1</sup>, M. Petković<sup>1</sup>, V. Jovanović<sup>2</sup>, D. Čebzan<sup>2</sup>, V. Dondur<sup>1</sup>  
<sup>1</sup>University of Belgrade, Faculty of Physical Chemistry, Beograd, Serbia  
<sup>2</sup>Hemofarm Institute, Vršac, Serbia

**P.S.B.41. SYNTHESIS AND CHARACTERIZATION OF MESOPOROUS MATERIALS OBTAINED USING FAU ZEOLITE IN THE PRESENCE OF CITRIC ACID**

V. Dondur<sup>1</sup>, M. Milojević<sup>1</sup>, Lj. Damjanović<sup>1</sup>, O. Cvetković<sup>2</sup>, Z. Vuković<sup>3</sup>  
<sup>1</sup>Faculty of Physical Chemistry, Belgrade, Serbia; <sup>2</sup>Department of Chemistry, ICTM, Belgrade, Serbia; <sup>3</sup>Department of Catalysis and Chemical Engineering, ICTM, Belgrade, Serbia

**P.S.B.42. CRYSTAL STRUCTURES OF RARE-EARTH DOPED HEXACELSIANS**

B. Nedić<sup>1</sup>, V. Dondur<sup>1</sup>, A. Kremenović<sup>2,3</sup>, R. Dimitrijević<sup>2</sup>, B. Antić<sup>3</sup>, J. Blanuša<sup>3</sup>  
<sup>1</sup>Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>Faculty of Mining and Geology, Belgrade, Serbia, <sup>3</sup>Institute of Nuclear Sciences "Vinca", Condensed Matter Physics Laboratory, Belgrade, Serbia

**P.S.B.43. CONDUCTING NANOSTRUCTURES OF POLYANILINE DOPED WITH SULFURIC ACID**

M. Savić<sup>1</sup>, A. Radulović<sup>2</sup>, G. Ćirić-Marjanović<sup>1</sup>  
<sup>1</sup>Faculty of Physical Chemistry, Belgrade, Serbia  
<sup>2</sup>Institute of General and Physical Chemistry, Belgrade, Serbia

**P.S.B.44. SYNTHESIS OF NANOSTRUCTURED CONDUCTING POLYANILINE IN THE PRESENCE OF 3,5-DINITROSALICYLIC ACID**

A. Janošević<sup>1</sup>, G. Ćirić-Marjanović<sup>1</sup>, B. Simonović<sup>2</sup>, M. Trchová<sup>3</sup>, P. Holler<sup>3</sup>, J. Stejskal<sup>3</sup>  
<sup>1</sup>Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>Institute of General and Physical Chemistry, Belgrade, Serbia, <sup>3</sup>Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic

**P.S.B.45. SYNTHESIS AND CHARACTERIZATION OF THE BENZOCAINE OLIGOMERS**

D. Kosić<sup>1</sup>, B. Marjanović<sup>2</sup>, M. Trchová<sup>3</sup>, P. Holler<sup>3</sup>, G. Ćirić-Marjanović<sup>4</sup>  
<sup>1</sup>Ministry of Health of the Republic of Serbia, Belgrade, Serbia, <sup>2</sup>Centrohlem, Stara Pazova, Serbia, <sup>3</sup>Institute of Macromolecular Chemistry, Academy of Sciences of the

*Czech Republic, Prague, Czech Republic, <sup>4</sup>Faculty of Physical Chemistry, Belgrade, Serbia*

**P.S.B.46. CHEMICAL OXIDATIVE OLIGOMERIZATION OF THE ETHACRIDINE LACTATE**

B. Marjanović<sup>1</sup>, I. Juranić<sup>2</sup>, M. Trchová<sup>3</sup>, P. Holler<sup>3</sup>, G. Ćirić-Marjanović<sup>4</sup>  
<sup>1</sup>*Centrohem, Stara Pazova, Serbia, <sup>2</sup>Faculty of Chemistry, Belgrade, Serbia,*  
<sup>3</sup>*Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic, <sup>4</sup>Faculty of Physical Chemistry, Belgrade, Serbia*

**P.S.B.47. RADICAL POLYMERISATION OF MONO-n-BUTYL ITACONATE**

Lj. Milovanović<sup>1</sup>, B. Mazalica<sup>2</sup>, L. Katsikas<sup>2</sup>, I.G. Popović<sup>2</sup>  
<sup>1</sup>*Institute of Nuclear Sciences VINČA, Belgrade, Serbia*  
<sup>2</sup>*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*

**P.S.B.48. THE INFLUENCE OF RADIATION ON THERMAL STABILITY OF POLYIMIDES BASED ON N-[4-BENZOYL-2-(2,5-DIOXO-2,5-DIHYDRO-PYRROL-1-YL)-PHENYL]-ACETAMIDE**

M. Marinović-Cincović<sup>1</sup>, D. Babić<sup>1</sup>, E. Džunuzović<sup>2</sup>, K. Popov-Pergal<sup>3</sup>, M. Rančić<sup>3</sup>  
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<sup>2</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia*  
<sup>3</sup>*Faculty of Forestry Science, University of Belgrade, Belgrade, Serbia*

**P.S.B.49. CALCULATIONS OF STRUCTURE, ELECTRONIC AND VIBRATIONAL SPECTRA OF DISILOXANE BISBENZOCYCLOBUTEN**

N. Ivanović, I. Radisavljević, D. Marjanović, N. Novaković  
*Institute for Nuclear Sciences "VINČA", Belgrade, Serbia*

**P.S.B.50. EVALUATION OF MOLECULAR DYNAMICS IN ELASTOMER BLENDS BY MDSC MEASUREMENTS**

M.B. Plavšić<sup>1</sup>, N. Lazić<sup>2</sup>, S. Ostojić<sup>2</sup>, M. Kićanović<sup>2</sup>  
<sup>1</sup>*Faculty of Technology and Metallurgy, Belgrade University, Belgrade, Serbia*  
<sup>2</sup>*Institute of General and Physical Chemistry, Belgrade, Serbia*

**P.S.B.51. ORGANO Bentonite-SYNTHESIS AND CHARACTERIZATION**

N. Jović<sup>1</sup>, A. Milutinović-Nikolić<sup>1</sup>, I. Gržetić<sup>2</sup>, D. Jovanović<sup>1</sup>  
<sup>1</sup>*Institute of Chemistry, Technology and Metallurgy-Department of Catalysis and Chemical Engineering, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*

- P.S.B.52. **SINTERING OF SILICON NITRIDE WITH Mg-EXCHANGE ZEOLITE ADDITIVE**  
B. Matović, A. Šaponjić, M. Pošarac, A. Radosavljević Mihajlović, E. Volceanov, S. Bošković  
*Institute of Nuclear Sciences "Vinca", Materials Department, Belgrade, Serbia*
- P.S.B.53. **PREPARATION OF SiALON POWDER USING DIATOMACIOUS EARTH**  
A. Šaponjić, B. Matović, S. Bosković, A. Radosavljević Mihajlović  
*Institute of Nuclear Sciences Vinca, Materials Science laboratory, Belgrade, Serbia*
- P.S.B.54. **PREPARATION OF HIGHLY POROUS SiC CERAMICS**  
A. Egelja<sup>1</sup>, A. Devečerski<sup>1</sup>, M. Miljković<sup>2</sup>, I. Pongrac<sup>1</sup>, B. Matović<sup>1</sup>  
<sup>1</sup>*Institute of Nuclear Sciences "Vinca", Materials Department, Belgrade, Serbia*  
<sup>2</sup>*Faculty of Medicine, University of Nis, Serbia*
- P.S.B.55. **COMPUTER SIMULATION OF SiO<sub>2</sub> DISSOLUTION IN NaOH AQUEOUS SOLUTION**  
M. Stanković, L. Pezo, B. Kovačević<sup>1</sup>, M. Jovanović<sup>2</sup>, D. Debeljković<sup>3</sup>  
<sup>1</sup>*Eng. Dept. Holding Institute of General and Physical Chemistry, Belgrade, Serbia*  
<sup>2</sup>*Faculty of Technology and Metallurgy, Belgrade, Serbia*  
<sup>3</sup>*Faculty of Mechanical Engineering, Belgrade, Serbia*
- P.S.B.56. **NEW OPTIMAL TECHNOLOGY FOR SMALL SECTIONS OF HSS AND SOFTWARE FOR DOCUMENTATION PROCESSING**  
J. Rodić<sup>2</sup>, W. Holzgruber<sup>1</sup>, H. Holzgruber<sup>1</sup>, A. Scheriau<sup>1</sup>, R. Tarmann<sup>1</sup>, R. Hartner<sup>1</sup>  
<sup>1</sup>*INTECO – Special Melting Technologies, Bruck a.d.Mur, Austria*  
<sup>2</sup>*INTECO / MINDOC C&S, Grosuplje, Slovenia*
- P.S.B.57. **AGEING EFFECT ON THE PSEUDOELASTICITY CHARACTERISTICS OF Ti-RICH TiNi SHAPE MEMORY ALLOY**  
S. Narendranath S<sup>1</sup>, G. Das<sup>3</sup>, S. Ghosh<sup>2</sup>, M. Chakraborty<sup>2</sup>  
<sup>1</sup>*Dept of Mechanical Engineering, National Institute of Technology Karnataka, India,* <sup>2</sup>*Dept of Metallurgical and Materials engineering, Indian Institute of Technology Kharagpur, India,* <sup>3</sup>*National Metallurgical Laboratory, Jamshedpur, India*
- P.S.B.58. **HIGH TEMPERATURE LOW CYCLE FATIGUE OF SUPERALLOY INCONEL 738LC**  
K. Obrtlík, A. Chlupová, M. Petre nec, J. Polák  
*Institute of Physics of Materials AS CR, v.v.i., Brno, Czech Republic*

- P.S.B.59. **DESTRUCTIVE AND NON-DESTRUCTIVE TECHNIQUES APPLIED TO THE CHARACTERIZATION OF AS-CAST MODEL STEELS WITH PARAMETRIC VARIATION OF Ni, Mn, Si AND Cr CONTENT**  
J. Degmová<sup>1,2</sup>, L. Debarberis<sup>1</sup>  
<sup>1</sup>JRC-IE, Joint Research Centre, Institute for Energy, Petten, The Netherlands,  
<sup>2</sup>Department of Nuclear Physics and Technology, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology, Bratislava, Slovakia
- P.S.B.60. **NUMERICAL MODELLING OF DUCTILE FRACTURE INITIATION IN PRESSURE VESSEL STEEL**  
D. Veljić<sup>1</sup>, M. Rakin<sup>2</sup>, Z. Cvijović<sup>2</sup>, M. Zrilić<sup>2</sup>, V. Grabulov<sup>3</sup>, A. Sedmak<sup>4</sup>  
<sup>1</sup>Montaža Ad", Belgrade, Serbia, <sup>2</sup>Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>3</sup>Military Technical Institute, Belgrade, Serbia, <sup>4</sup>Faculty of Mechanical Engineering, Belgrade, Serbia
- P.S.B.61. **THE ANALYSIS OF MICROSTRUCTURE AND MECHANICAL PROPERTIES OF WELDED JOINTS OBTAINED WITH TWO TYPES OF CORED FILLER WIRES**  
N. Bajić<sup>1</sup>, V. Šijački-Žeravčić<sup>2</sup>, M. Rakin<sup>3</sup>, D. Čikara<sup>4</sup>  
<sup>1</sup>Chemical Power Sources ReseArch Institute, Serbia, <sup>2</sup>Faculty of Mechanical Engineering, Belgrade, Serbia, <sup>3</sup>Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>4</sup>Faculty of Technical Sciences, Kosovska Mitrovica, Serbia
- P.S.B.62. **MECHANICAL AND MICROSTRUCTURAL PROPERTIES OF HIGH-CARBON STEEL SURFACE WELDED LAYER**  
O. Popović<sup>1</sup>, R. Prokić-Cvetković<sup>1</sup>, A. Sedmak<sup>1</sup>, V. Grabulov<sup>2</sup>, Z. Burzić<sup>2</sup>, M. Rakin<sup>3</sup>  
<sup>1</sup>Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia,  
<sup>2</sup>Military Technical Institute, Belgrade, Serbia, <sup>3</sup>Faculty of Technology and Metallurgy, Belgrade, Serbia
- P.S.B.63. **THE APPLICATION OF MODERN TECHNIQUES IN SUPER ALLOYS INVESTIGATION**  
A. Milosavljević<sup>1</sup>, S. Petronić<sup>1</sup>, V. Negovanović<sup>2</sup>  
<sup>1</sup>Faculty of Mechanical Engineering, Serbia  
<sup>2</sup>Faculty of Business studies, University of Belgrade, Belgrade, Serbia
- P.S.B.64. **STUDY OF THE SIMULATED HAZ OF CREEP RESISTANT 9-12% ADVANCED CHROMIUM STEEL**  
Lj. Milović<sup>1</sup>, T. Vuherer<sup>2</sup>, M. Zrilić<sup>1</sup>, S. Putić<sup>1</sup>  
<sup>1</sup>Faculty of Technology and Metallurgy, Beograd, Serbia  
<sup>2</sup>Faculty of Mechanical Engineering, Maribor, Slovenia
- P.S.B.65. **USE OF IN-SITU SEM OBSERVATIONS FOR THE CHARACTERISATION OF FRACTURE PROCESS IN Al-Zn-Mg-Cu ALLOYS**

M. Vratnica<sup>1</sup>, Z. Cvijović<sup>2</sup>

<sup>1</sup>*Faculty of Metallurgy and Technology, Podgorica, Montenegro*

<sup>2</sup>*Faculty of Technology and Metallurgy, Belgrade, Serbia*

P.S.B.66. **PERFORMANCE OF ALUMINOTHERMIC RAILS WELDING  
TECHNOLOGY**

B. Sladojević, T. Brdarić

*Institut „Kirilo Savić“, Beograd, Srbija*

## POSTER SESSION III

*Thursday, September 13, 2007, 20<sup>30</sup>-22<sup>00</sup>*

### SYMPOSIUM C: NANOSTRUCTURED MATERIALS

**P.S.C.1. SIZE DEPENDENT INTRABAND ABSORPTION IN P-TYPE DOPED SELF-ASSEMBLED NANODOTS**

M. Ćosić<sup>1</sup>, M. Tadić<sup>1,2</sup>, F.M. Peeters<sup>1</sup>

<sup>1</sup>*Department of Physics, University of Antwerp, Belgium*

<sup>2</sup>*Faculty of Electrical Engineering, University of Belgrade, Belgrade, Serbia*

**P.S.C.2. VIBRATIONAL SPECTROSCOPY OF CdTe/ZnTe QUANTUM DOT SUPERLATTICES**

M. Romčević<sup>1</sup>, N. Romčević<sup>1</sup>, A. Milutinović<sup>1</sup>, R. Kostić<sup>1</sup>, G. Karczewski<sup>2</sup>, R. Galazka<sup>2</sup>, A. Boukenter<sup>3</sup>, F. Goutaland<sup>3</sup>

<sup>1</sup>*Institute of Physics, Belgrade, Serbia*, <sup>2</sup>*Institute of Physics, Polish Academy of Sciences, Warsaw, Poland*, <sup>3</sup>*Saint-Etienne University, Saint-Etienne, France*

**P.S.C.3. ELECTRON -ELECTRON SCATTERING IN THE ACTIVE REGION OF GaAs/AlGaAs QUANTUM CASCADE LASER IN MAGNETIC FIELD**

B. Novaković<sup>1</sup>, J. Radovanović<sup>2</sup>, A. Mirčetić<sup>2</sup>, V. Milanović<sup>2</sup>, Z. Ikonić<sup>3</sup>, D. Indjin<sup>3</sup>

<sup>1</sup>*Institute of Physics, Belgrade, Serbia*, <sup>2</sup>*Faculty of Electrical Engineering, Belgrade, Serbia*, <sup>3</sup>*Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds, Leeds, UK*

**P.S.C.4. EELS/HRTEM CHARACTERIZATION OF PHASES OBTAINED DURING THE HYDROTHERMAL SYNTHESIS OF CaTiO<sub>3</sub>**

S. Šturm, B. Jančar, I. Bračko

*Jozef Stefan Institute, Ljubljana, Slovenia*

**P.S.C.5. SYNTHESIS OF CdSe/MESOPOROUS SiO<sub>2</sub> COMPOSITES WITH NARROW PARTICLE SIZE DISTRIBUTION**

I.V. Kolesnik, D.I. Petukhov, A.A. Eliseev, A.V. Lukashin, Yu.D. Tretyakov

*Department of Material Science, Moscow State University, Moscow, Russia*

**P.S.C.6. SYNTHESIS AND CHARACTERIZATION OF BaTiO<sub>3</sub> NANORODS**

K. Žagar, S. Šturm, M. Čeh

*Jozef Stefan Institute, Ljubljana, Slovenia*

- P.S.C.7. **THE  $W_{18}O_{49}$  NANOWIRES USED FOR SYNTHESIS OF THE  $WS_2$  NANOTUBES**  
M. Viršek<sup>1</sup>, M. Remškar<sup>1</sup>, A. Jesih<sup>1</sup>, J. Jelenc<sup>2</sup>  
<sup>1</sup>Jozef Stefan Institute, Ljubljana, Slovenia, <sup>2</sup>Faculty of Mathematics and Physics, Department of Physics, University in Ljubljana, Slovenia
- P.S.C.8. **SCANNING PROBE MICROSCOPY OF ATOMIC AND NANO STRUCTURES**  
A. Beltaos<sup>1</sup>, R. Gajić<sup>1</sup>, G. Isić<sup>1</sup>, Dj. Jovanović<sup>1</sup>, B. Novaković<sup>1</sup>, N. Paunović<sup>1</sup>, Z.V. Popović<sup>1</sup>, M. Radović<sup>1</sup>, K. Winkler<sup>2</sup>  
<sup>1</sup>Institute of Physics, Belgrade, Serbia, <sup>2</sup>Omicron Nanotechnology GmbH, Taunusstein, Germany
- P.S.C.9. **SYNTHESIS AND CHARACTERIZATION OF SHAPED ZnS NANOCRYSTALS IN WATER IN OIL MICROEMULSIONS**  
D.J. Jovanović, I.Lj. Validžić, I.A. Janković, N. Bibić, J.M. Nedeljković  
Vinča Institute of Nuclear Sciences, Belgrade, Serbia
- P.S.C.10. **LOW TEMPERATURE SYNTHESIS OF DISODIUM DIMOLYBDATE**  
D.J. Jovanović, I.Lj. Validžić, I.A. Janković, M. Mitrić, J.M. Nedeljković  
Vinča Institute of Nuclear Sciences, Belgrade, Serbia
- P.S.C.11. **RADIOLYTIC SYNTHESIS AND CHARACTERIZATION OF PVA HIDROGEL –Au NANOCOMPOSITES**  
A. Krklješ, M. Marinović-Cincović, Z. Kačarević-Popović, J.M. Nedeljković  
Vinča Institute of Nuclear Science, Belgrade, Serbia
- P.S.C.12. **CHARACTERIZATION OF Au NANOPARTICLES DISPERSED IN WATER AND POLYMER MATRIX**  
V.V. Vodnik, Z.V. Šaponjić, N.D. Abazović, M.I. Čomor, J.M. Nedeljković  
Vinča Institute of Nuclear Sciences, Belgrade, Serbia
- P.S.C.13. **NANOSIZED SILICALITE-1 CRYSTALLIZATION – INFLUENCE OF TPA<sup>+</sup>**  
O.A. Kovačević<sup>1</sup>, B.T. Kovačević<sup>1</sup>, D. Arandjelović<sup>1</sup>, K. Andjelković<sup>3</sup>, V. Dondur<sup>2</sup>, Ž.Lj. Tešić<sup>3</sup>  
<sup>1</sup>Institute of General and Physical Chemistry, Belgrade, Serbia  
<sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Serbia  
<sup>3</sup>Faculty of Chemistry, University of Belgrade, Serbia
- P.S.C.14. **INVESTIGATION OF NANOSIZED SILICALITE-1 BY FTIR**

## SPECTROSCOPY

B.T. Kovačević<sup>1</sup>, O.A. Kovačević<sup>1</sup>, D. Arandjelović<sup>1</sup>, L. Pezo<sup>1</sup>, V. Dondur<sup>2</sup>, Ž.Lj. Tešić<sup>3</sup>

<sup>1</sup>*Institute of General and Physical Chemistry, Belgrade, Serbia*

<sup>2</sup>*Faculty of Physical Chemistry, University of Belgrade, Serbia*

<sup>3</sup>*Faculty of Chemistry, University of Belgrade, Serbia*

P.S.C.15. **SYNTHESIS AND CHARACTERIZATION OF SILVER NANOPARTICLES AND COMPLEX IT'S WITH LYSINE AND ANTIBODY OF PSA AND THEIR APPLICATION IN PRODUCING DIAGNOSTIC PROSTATE CANCER KIT**

D. Zare<sup>3</sup>, A. Akbarzadeh<sup>1</sup>, B. Mohajerani<sup>2</sup>, D. Norouzian<sup>1</sup>, M. Atyabi<sup>1</sup>, M.R. Mehrabi<sup>1</sup>, A. Farhangi<sup>1</sup>, H. Ansari<sup>1</sup>, M. Mortazavi<sup>1</sup>, Z. Saffari<sup>1</sup>, M. Shafiei<sup>1</sup>

<sup>1</sup>*Department of Pilot of Bio Technology, Institute Pasteur of Iran, Tehran, Iran,*

<sup>2</sup>*Chemistry & Petrochemical Research Institute, Research Institute of Petroleum Industry (RIPI), Tehran, Iran,* <sup>3</sup>*Department of Chemistry, University of Isfahan, Isfahan, Iran*

P.S.C.16. **CHARACTERIZATION OF Eu-DOPED Zn<sub>2</sub>SiO<sub>4</sub> POWDERS OBTAINED BY POLYMER INDUCED SOL-GEL SYNTHESIS**

Ž. Andrić<sup>1</sup>, R. Krsmanović<sup>1</sup>, M. Mitrić<sup>1</sup>, I. Zeković<sup>1</sup>, Lj. Djačanin<sup>2</sup>, M.D. Dramićanin<sup>1</sup>

<sup>1</sup>*Institute of nuclear sciences "Vinča", Belgrade, Serbia*

<sup>2</sup>*Department of Physics, University of Novi Sad, Novi Sad, Serbia*

P.S.C.17. **SYNTHESIS AND STRUCTURE OF FERRITE POLYMER NANOCOMPOSITES**

B. Pilić, M. Maletin, V. Srdić

*Faculty of Technology, Novi Sad, Srbija*

P.S.C.18. **STUDY OF STRUCTURAL AND OPTICAL BEHAVIORS OF TiO<sub>2</sub>:Eu, Pd THIN FILMS**

D. Kaczmarek, J. Domaradzki, E.L. Prociow, A. Borkowska

*Faculty of Microsystem Electronics and Photonics, Wrocław University of Technology, Wrocław, Poland*

P.S.C.19. **TEMPERATURE DEPENDENCE OF OXYGEN REDUCTION KINETICS ON CARBON SUPPORTED Pt NANOPARTICLES**

N.R. Elezović<sup>1</sup>, B.M. Babić<sup>2</sup>, N.V. Krstajić<sup>3</sup>, S.Lj. Gojković<sup>3</sup>, Lj.M. Vračar<sup>3</sup>

<sup>1</sup>*Center for Multidisciplinary Studies, University of Belgrade, Belgrade, Serbia*

<sup>2</sup>*Vinča Institute of Nuclear Sciences, Belgrade, Serbia*

<sup>3</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia*

P.S.C.20. **SYNTHESIS AND PROPERTIES OF POLYSTYRENE-CO-MALEIC ACID/Cd<sub>1-x</sub>Mn<sub>x</sub>S NANOCOMPOSITES**



D. Milivojević, B. Babić-Stojić, V. Djoković, J. Blanuša  
*Vinca Institute of Nuclear Sciences, Belgrade, Serbia*

- P.S.C.21. **STRUCTURAL PROPERTIES OF EUROPIUM-DOPED YTTRIA OBTAINED VIA AEROSOL SYNTHESIS**  
K. Marinković<sup>1</sup>, M.E. Rabanal<sup>2</sup>, L.S. Gomez<sup>2</sup>, I. Martin<sup>2</sup>, L. Mančić<sup>1</sup>, O. Milošević<sup>1</sup>  
<sup>1</sup>*Institute of Technical Sciences of Serbian Academy of Sciences and Arts, Belgrade, Serbia*, <sup>2</sup>*Universidad Carlos III de Madrid, Leganes, Madrid, Spain*
- P.S.C.22. **OPTICAL AND ELECTRICAL PROPERTIES OF INDIUM DOPED NANOCRYSTAL ZINC OXIDE PREPARED BY SPRAY PYROLYSIS METHOD**  
A. Tanuševski<sup>1</sup>, M. Ristova<sup>1</sup>, V. Georgieva<sup>2</sup>  
<sup>1</sup>*Institute of Physics, Faculty of Natural Sciences and Mathematics, University "Sts. Cyril and Methodius", Skopje, Macedonia*, <sup>2</sup>*Faculty of Electrical Engineering, The "Sts. Cyril & Methodius" University, Skopje, Macedonia*
- P.S.C.23. **THE INFLUENCE OF THE CONCENTRATION AND KIND OF MODIFICATION OF MONTMORILLONITE ON PROPERTIES OF NANOCOMPOSITE COATINGS**  
M. Špírková, A. Strachota, J. Brus, B. Strachotová, M. Urbanová  
*Institute of Macromolecular Chemistry ASCR, v.v.i., Prague, Czech Republic*
- P.S.C.24. **STRUCTURE PARTICULATES OF NANOSTRUCTURED CONDENSATES OF QUASIBINARY**  
O. Sobol<sup>1</sup>, L. Ribic<sup>2</sup>, L. Kuniytska<sup>3</sup>  
<sup>1</sup>*National Technical University «Kharkov Polytechnical Institute», Kharkov, Ukraine*, <sup>2</sup>*Technical Faculty, Cacak, Serbia*, <sup>3</sup>*Institute of Surface Chemistry of NAS of Ukraine, Kiev, Ukraine*
- P.S.C.25. **CORRELATION BETWEEN THE CHANGE OF ELECTRON DENSITY STATES ON THE FERMI LEVEL AND THE RELATIVE CHANGE OF THE MAGNETIC PERMEABILITY OF THE Fe<sub>81</sub>B<sub>13</sub>Si<sub>4</sub>C<sub>2</sub> AMORPHOUS ALLOY**  
A. Maričić<sup>1</sup>, O. Aleksić<sup>2</sup>, N. Mitrović<sup>1</sup>, D.M. Minić<sup>3</sup>  
<sup>1</sup>*Technical Faculty Čačak, University of Kragujevac, Čačak, Serbia*  
<sup>2</sup>*Center for multidisciplinary studies of the University of Belgrade, Belgrade, Serbia*  
<sup>3</sup>*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia*

## SYMPOSIUM D: COMPOSITES

**P.S.D.1. SYNTHESIS AND MECHANICAL PROPERTIES OF BIOMORPHIC C/SiC COMPOSITES**

I. Djordjević, B. Babić, D. Sekulić, B. Matović  
*Institute of Nuclear Sciences Vinca, Belgrade*

**P.S.D.2. DETERMINATIONS OF MECHANICAL PROPERTIES OF PARTIALLY CARBONIZED CARBON FIBRES AND THEIR CARBON-CARBON COMPOSITES**

Lj. Milovanović, D. Sekulić, B. Kaludjerović  
*Institute of Nuclear Science «Vinča», Belgrade, Serbia*

**P.S.D.3. THE INFLUENCE OF CARBON BLACK AND SILICA FILLER ON THE PROPERTIES OF ACRYLONITRILE-BUTADIENE/ETHYLENE-PROPYLENE-ETHYLIDENENORBORNENE RUBBER BLENDS**

V. Jovanović<sup>1</sup>, J. Budinski-Simendić<sup>2</sup>, S. Samardžija-Jovanović<sup>1</sup>, G. Marković<sup>3</sup>, S. Konstantinović<sup>4</sup>

<sup>1</sup>Faculty of Science, University of Pristina, Kosovska Mitrovica, Serbia, <sup>2</sup>University of Novi Sad, Faculty of Technology, Serbia, <sup>3</sup>Tigar, Pirot, Serbia, <sup>4</sup>Faculty of Technology, Leskovac, Serbia

**P.S.D.4. THE INFLUENCE OF CARBON BLACK AND WOOD FLOUR ON HIGH ENERGY RADIATION RESISTANCE OF COMPOSITES BASED ON NR/CSM RUBBER BLEND**

G. Marković<sup>1</sup>, B. Radovanović<sup>2</sup>, M. Marinović-Cincović<sup>3</sup>, J. Budinski-Simendić<sup>4</sup>

<sup>1</sup>Tigar, Pirot, <sup>2</sup>Faculty of Science, Niš, <sup>3</sup>Institute of Nuclear Science Vinča, Belgrade, <sup>4</sup>Faculty of Technology, Novi Sad, Serbia

**P.S.D.5. POSSIBILITIES OF APPLICATION OF CARBON STEEL-SiC CAST IN CARBIDE COMPOSITES AS WEAR RESISTANCE MATERIAL**

D. Čikara<sup>1</sup>, D. Kalaba<sup>1</sup>, Z. Vasić<sup>1</sup>, D. Čikara<sup>2</sup>

<sup>1</sup>Faculty of Technical Sciences, University of Pristina, Serbia

<sup>2</sup>Faculty of Technology and Metallurgy, University of Belgrade, Serbia

**P.S.D.6. COMPUTER MODEL OF HEAT AND MASS TRANSFER DURING HEAT TREATMENT OF WOOD**

L. Pezo<sup>1</sup>, S. Stanojlović<sup>1</sup>, D. Majstorović<sup>1</sup>, B. Tomić-Tucaković<sup>1</sup>, D. Debeljković<sup>2</sup>

<sup>1</sup>Eng. Dept. Holding Institute of General and Physical Chemistry, Belgrade, Serbia

<sup>2</sup>Faculty of Mechanical Engineering, Belgrade, Serbia

- P.S.D.7. MODELLING OF AIRFLOW THROUGH A WOOD-DRYING KILN**  
L. Pezo<sup>1</sup>, S. Stanojlović<sup>1</sup>, D. Majstorović<sup>1</sup>, B. Tomić-Tucaković<sup>1</sup>, D. Debeljković<sup>2</sup>  
<sup>1</sup>Eng. Dept. Holding Institute of General and Physical Chemistry, Belgrade, Serbia  
<sup>2</sup>Faculty of Mechanical Engineering, Belgrade, Serbia
- P.S.D.8. EXPERIMENTAL INVESTIGATION OF A SOLAR DRYER WITH NATURAL CONVECTIVE HEAT FLOW**  
L. Pezo<sup>1</sup>, S. Stanojlović<sup>1</sup>, D. Majstorović<sup>1</sup>, B. Tomić-Tucaković<sup>1</sup>, D. Debeljković<sup>2</sup>  
<sup>1</sup>Eng. Dept. Holding Institute of General and Physical Chemistry, Belgrade, Serbia  
<sup>2</sup>Faculty of Mechanical Engineering, Belgrade, Serbia
- P.S.D.9. MODELLING OF FRICTION PAIR CONTACT CHARACTERISTICS BY MEANS OF ARTIFICIAL NEURAL NETWORKS**  
D. Aleksendrić, I. Balać, Č. Duboka  
Faculty of Mechanical Engineering, University of Belgrade, Serbia
- P.S.D.10. NONWOVEN GEOTEXTILE COMPOSITES WITH BENTONITE**  
J. Dostanić<sup>1</sup>, A. Milutinović-Nikolić<sup>1</sup>, V. Rizmanoski<sup>1</sup>, S. Lukić<sup>2</sup>, D. Jovanović<sup>1</sup>  
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Lj. Gajić-Krstajić<sup>1</sup>, N.V. Krstajić<sup>2</sup>, V.D. Jović<sup>3</sup>, B.M. Jović<sup>3</sup>,  
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<sup>3</sup>Center for Multidisciplinary Studies University of Belgrade, Belgrade, Serbia
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O. Erić<sup>1</sup>, D. Rajnović<sup>2</sup>, L. Sidjanin<sup>2</sup>  
<sup>1</sup>Institute "Kirilo Savic", Beograd, Serbia  
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L. Gusha  
Technological University "Ismail Qemali", Marine Faculty, Naval Engineering Department, Vlora, Albania
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V. Kasemi

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Department, Vlora, Albania*

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V. Stanić<sup>1</sup>, M. Mitrić<sup>1</sup>, Č. Jovalekić<sup>2</sup>, S. Raičević<sup>1</sup>

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M. Jevtić<sup>1</sup>, M. Mitrić<sup>2</sup>, N. Ignjatović<sup>1</sup>, D. Uskoković<sup>1</sup>

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**P.S.E.3. pH SENSITIVE HYDROGELS BASED ON METHACRYLATES**

M. Mičić<sup>1</sup>, S. Tomić<sup>2</sup>, J. Filipović<sup>2</sup>, D. Djokić<sup>1</sup>, E. Suljovrujić<sup>1</sup>

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K. Andjelković<sup>1</sup>, N. Filipović<sup>2</sup>, T. Todorović<sup>1</sup>, D. Jovanović<sup>3</sup>, S. Tufegdžić<sup>4</sup>, D.

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S. Šolajić<sup>1</sup>, V. Bogdanović<sup>1</sup>, I. Ičević<sup>2</sup>, G. Bogdanović<sup>1</sup>, A. Djordjević<sup>2</sup>

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L. Matija<sup>1</sup>, Dj. Koruga<sup>1</sup>, J. Bandić<sup>3</sup>, Ž. Ratkaj<sup>1</sup>, D. Dobrasavljević<sup>2</sup>

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- P.S.E.7. MEDICINE APPLICATION OF LIQUID CRYSTAL AND FULLERENE-DOPED MATERIALS**  
A.A. Kamanin<sup>1</sup>, N.V. Kamanina<sup>2</sup>  
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<sup>2</sup>*Vavilov State Optical Institute, St. Petersburg, Russia*
- P.S.E.8. FLUORIDE CONTENT, RECHARGE ABILITY AND REMINERALISATION POTENTIAL OF GLASS-IONOMER CEMENT**  
B.B. Petrović<sup>1</sup>, D.Lj. Marković<sup>2</sup>  
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- P.S.E.10. NEURAL MODELLING OF PLLA POLYMER IN HA<sub>p</sub>/PLLA BIOCOSMETIC MATERIAL BEHAVIOUR DURING NANOINDENTATION**  
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- P.S.E.11. IMMOBILIZATION OF SACCHAROMYCES ELLIPSOIDEUS CELLS FOR BIOETHANOL PRODUCTION**  
Lj. Mojović<sup>1</sup>, M. Rakin<sup>1</sup>, S. Nikolić<sup>1</sup>, M. Vukašinović<sup>1</sup>, V. Nedović<sup>2</sup>  
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- P.S.E.12. INVESTIGATION OF ANTIMICROBIAL ACTIVITY OF ESSENTIAL OILS AND MICROBIAL METABOLITS FROM LACTIC ACID BACTERIA FOR IMPREGNATION IN MEDICAL TEXTILE**  
K. Mihajlovski Popović<sup>1</sup>, S. Dimitrijević<sup>1</sup>, Lj. Simović<sup>2</sup>, S. Siler Marinković<sup>1</sup>, P. Škundrić<sup>1</sup>  
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- P.S.E.13. SURFACE MODIFICATION AND CHARACTERIZATION OF METHACRYLATE POLYMER NETWORKS FOR TISSUE ENGINEERING**

R. Hobzova, N. Zhunusbekova, J. Sirc, J. Michalek  
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**P.S.E.14. CHROMATOGRAPHIC STATIONARY PHASES FOR SEPARATION OF BIOACTIVE COMPOUNDS - CORRELATION OF MORPHOLOGY AND SEPARATION PROPERTIES**

J. Sirc<sup>1,2</sup>, Z. Bosakova<sup>1</sup>, J. Michalek<sup>2</sup>, R. Hobzova<sup>2</sup>

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**P.S.E.15. THE INFLUENCE OF THE STERILIZATION PROCESS BY GAMMA RAYS IRRADIATION ON THE ACTIVATED CARBON CLOTH PROPERTIES AS A DRESSING MATERIAL**

D. Sekulić<sup>1</sup>, B.V. Kaludjerović<sup>1</sup>, B.M. Babić<sup>1</sup>, Lj.M. Milovanović<sup>1</sup>, J.M. Stašić<sup>1</sup>, B. Prokić<sup>2</sup>

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**P.S.E.16. HEPATOPROTECTIVE ROLE OF TUNGSTATES**

S. Uskoković-Marković<sup>1</sup>, M. Milenković<sup>1</sup>, A. Topić<sup>1</sup>, I. Holclajtner-Antunović<sup>2</sup>, M.R. Todorović<sup>3</sup>, U.B. Mioč<sup>2</sup>

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**P.S.E.17. ADDITIONAL ENZYME CATALYTIC EFFECTS TO DEGRADATION OF SMART POLYMER BIOMATERIALS**

M.B. Plavšić<sup>1</sup>, M.M. Plavšić<sup>1</sup>, P. Putanov<sup>2</sup>

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**P.S.E.18. RHEOLOGICAL ASPECTS OF STRUCTURED-GEL IMPLANT APPLICATIONS**

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**P.S.E.19. STUDY OF THE RELEASE OF THE HEAVY METALS FROM VARIOUS FIXED DENTURES (APPLIANCES) INTO SYNTHETIC SALIVA, USING ELECTROCHEMICAL STRIPPING ANALYSIS**

B. Kaličanin<sup>1</sup>, Z. Ajduković<sup>2</sup>, S. Najman<sup>3</sup>, R. Nikolić<sup>4</sup>, M. Kostić<sup>5</sup>, M. Andjelković<sup>5</sup>  
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**P.S.E.20. APPLICATION ANALYSIS OF MICRO AND NANO COMPOSITES IN RESTORING OF BONE TISSUE OF THE JAW**

Z. Ajduković<sup>1</sup>, N. Ignjatović<sup>2</sup>, D. Petrović<sup>3</sup>, V. Savić<sup>4</sup>, B. Kaličanin<sup>5</sup>, M. Kostić<sup>6</sup>, M. Andjelković<sup>6</sup>, S. Nikolov<sup>4</sup>

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**P.S.E.21. EVALUATION OF GLASSIONOMER CEMENT APPLICATION FOR PERMANENT BINDING OF PROSTHETIC DENTURES**

M. Andjelković<sup>1</sup>, Z. Ajduković<sup>2</sup>, M. Kostić<sup>1</sup>, N. Krunic<sup>2</sup>, B. Kaličanin<sup>3</sup>, N. Ignjatović<sup>4</sup>

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**P.S.E.22. BOVINE SERUM ALBUMIN (BSA) ION INTERACTION FOLLOWED BY ITC**

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**P.S.E.23. THIN FILMS AND IMPLANT MATERIALS**

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**P.S.E.24. EFFECT OF HYDROGELS BASED ON 2-HYDROXYETHYL METHACRYLATES TO ERYTHROCYTE RESISTANCE TO HEMOLYSIS**

M. Milojević<sup>1</sup>, S. Najman<sup>2</sup>, S. Tomić<sup>3</sup>, Lj. Djordjević<sup>1</sup>

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- P.S.E.25. **EFFECT OF HYDROGELS BASED ON 2-HYDROXYETHYL METHACRYLATES TO VIABILITY AND OXIDATIVE ABILITY OF RAT PERITONEAL MACROPHAGES**  
S. Najman<sup>1</sup>, M. Milojević<sup>2</sup>, S. Tomić<sup>3</sup>, P. Vasiljević<sup>2</sup>  
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- P.S.E.26. **OSTEOGENIC ACTIVITY IN A MICE SUBCUTANEOUS IMPLANT OF POROUS HYDROXYAPATITE/POLY-L-LACTIDE LOADED WITH BONE MARROW CELLS**  
J. Jančićević<sup>1</sup>, S. Najman<sup>2</sup>, N. Beljić<sup>2</sup>, M. Vukelić<sup>2</sup>, N. Ignjatović<sup>3</sup>, D. Uskoković<sup>3</sup>, L.J. Djordjević<sup>1</sup>, P. Vasiljević<sup>1</sup>  
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<sup>3</sup>Institute of Technical Sciences of Serbian Academy of Sciences and Arts, Belgrade, Serbia
- P.S.E.27. **DESIGNING OF THE ALGINATE HYDRO GEL BEADS MORPHOLOGY USING ULTRASONIC SPRAY GELLING METHOD**  
B. Colović<sup>1</sup>, V. Jokanović<sup>1</sup>, B. Bugarski<sup>2</sup>  
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# Abstracts

# Oral Presentation

*PL.S.I.1*

**CHARACTERIZATION AND MANIPULATION OF FUNCTIONAL  
NANOSTRUCTURES USING HIGH RESOLUTION ANALYTICAL TEM AND  
COMBINED SPM-TEM**

E. Olsson

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It is crucial to be able to measure the dynamic properties of nanomaterials on a nanoscale and directly correlate them to the corresponding local microstructure. Both surface and sub-surface structure is important. The scanning tunneling microscope (STM) allows us to image surfaces and measure properties on the nanoscale and also subnanoscale. However, it is not possible to image and measure simultaneously. In addition, the images contain information about the surface while processes below the surface are not directly accessible. The combination of STM and transmission electron microscopy (TEM) enables us to simultaneously image and measure as well as to obtain direct information about both the surface and processes and structures below the surface. This talk will address experiments on carbon nanotubes including electromigration and a nanopipette function using a TEM-STM [1].

Another example concerns gold nanoparticles and the effect of laser irradiation on individual particles as well as ensembles of particles. An intense nanosecond laser pulse can give rise to changes in particle size distribution, morphology, structural and properties. Melting, evaporation and diffusion determine the microstructural modifications [2].

Nanostructures are inherently small and often electron transparent without specimen preparation. However, it may be necessary to develop methods to extract the individual nanostructures or to manipulate and follow the change of individual nanoparticles during dynamical processes. A combined focused ion beam workstation and scanning electron microscope with an in-situ manipulator provides the ability to reach into nanostructures and enables reproducible techniques of local extraction and identification [2, 3].

1. K. Svensson, H. Olin and E. Olsson, “Nanopipettes for Metal Transport”, *Phys. Rev. Lett.* 93, 145901 (2004).
2. L. Eurenus, K. Wettergren, Y. Alaverdyan, M. Käll, B. Kasemo, D. Chakarov and E. Olsson, “Microstructural changes in supported gold particle ensembles and individual particles upon pulsed laser irradiation”, in manuscript.
3. L. de Knoop, K. Svensson, H. Pettersson and E. Olsson, “Extraction of Individual Carbon Nanotubes for Local Probing of Transport Properties”, *AIP*, 786, 118 (2005).

*PL.S.I.2*

**CONTROLLED ASSEMBLY OF EPITAXIAL NANOSTRUCTURES FOR  
NANOELECTRONIC APPLICATIONS**

R. Hull<sup>1</sup>, J. Gray<sup>1,2</sup>, J. Graham<sup>1</sup>, M. Kammler<sup>1,3</sup>, A. Portavoce<sup>1,4</sup>,  
M. Gherasimova<sup>1</sup>, S. Wolf<sup>1</sup>, J. Floro<sup>1</sup>, F.M. Ross<sup>5</sup>

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We are developing new methods for the guided assembly of epitaxial semiconductor systems using low dose focused ion beam pulses to template Si(100) surfaces for subsequent nucleation of Ge(Si)/Si clusters. These methods enable controlled nucleation of either single quantum dots (QDs) or more complex QD "molecules" (that comprise four quantum dots elastically bound to a central shallow pit) to each template site. These methods enable assembly of quantum dot patterns of arbitrary complexity with precision at the 10 nm level. We will review our understanding of the limits of size, spatial control, and uniformity using these approaches, and the ability for simultaneous control of length scales ranging from tens of nm to the macroscopic level. We will also describe the routes we are exploring for nanoscale electronic and magnetic doping of these structures with beams of electrically and magnetically species (e.g. B, As and Mn for Si and Ge nanostructures) using mass-selected filtering from alloy liquid metal ion sources. Our goal is to apply these structures to novel nanoelectronic architectures such as quantum cellular automata and spin exchange switches.

*PL.S.I.3*

**SEMICONDUCTOR NANOWIRE NUCLEATION AND GROWTH KINETICS**

F.M. Ross

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By carrying out chemical vapour deposition of semiconductors in the presence of small particles of a catalytic material, it is possible to grow wirelike structures microns long and below 100nm in diameter. Such nanowires have interesting electronic properties and have already been incorporated into functional devices. Even more applications can be envisaged for branched nanowires or nanowires grown epitaxially at precise locations over an entire wafer. In this presentation we will discuss the growth of epitaxial nanowires in Si and Ge using Au as the catalyst, focusing on the kinetic processes that influence nucleation and final shape. We grow the wires in an environmental TEM, which has capabilities both for evaporating Au onto a clean Si substrate, and for introducing the precursor gases while the sample remains under observation. In situ video rate observations allow us to measure nucleation events and nanowire growth rates, examine the catalyst structure directly, and determine the effects of changes in growth environment on wire shapes. We will focus in particular on the factors that affect shape and the reliability of nucleation, and consider how the in situ results may help in tailoring wire structures for particular applications.

*PL.S.I.4*

**SOME RECENT DEVELOPMENTS IN NANO-MATERIALS**

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Following the discovery of the carbon nano-tube by Iijima in 1991, there have been numerous activities in developing new materials at the nano-scale for scientific and technological purposes. This paper will illustrate some recent advances which both highlight the breadth of applications which can be impacted and the underlying theme of nano-technology whereby new properties can emerge as the dimensions of the material approach that of a few atoms. Firstly we will discuss the synthesis of novel nano-wires from such diverse materials as electrodes for solid-state batteries, optical phase change materials, multi-exciton photovoltaic materials and copper-indium-gallium-selenide (CIGS), the highly efficient solar cell product. We will look at the possible use of ultra-thin silicon nano-wires for light-emitting properties, even though the band gap of bulk silicon is smaller than the energy of visible light, and we will see how the introduction of surface plasmonic effects can be used to probe the functional behavior of monolayer biological molecules. Magnetic nano-particles are being investigated for possible medical application in cancer detection as magnetism is a highly sensitive physical property, and the use of nano-wires and nano-tubes for minute transistor applications will be described. Clearly this represents a whole new area in which materials science plays a critical role.

*PL.S.I.5*

**FINITE SIZE EFFECTS ON DISTRIBUTION AND SHAPE OF SMALL PARTICLES**

D. Chatain

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How do several finite size, small phases like pores or particles distribute in a matrix or at grain boundaries once they have achieved their equilibrium shape? A wealth of configurations can be generated because interfaces with solids are anisotropic and can have facets. These configurations depend on the relative sizes of the phases in contact and on the wetting anisotropy associated with the interface anisotropy. Impact for applications such as self-organization of small particles at interfaces is presented.

*PL.S.I.6*

## **NOVEL METALLIC THIN FILMS FOR NEMS APPLICATION**

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Metal-based NEMS (Nano-Electro-Mechanical-System) components with nm-scale dimensions are traditionally difficult to achieve due to their high intrinsic stress, large surface roughness and grain size, inherent porosity, and low strength. The aim of this report is to describe how to overcome these limitations by using room temperature co-sputtering to synthesize nanocomposite Al-Mo and Ni-Mo alloy thin films. These films were found to exhibit unusually high nanoindentation hardness, nearly zero stress, a sub-nm surface roughness, and large compressive ductility, while maintaining resistivity in the metallic range. A systematic investigation of microstructure and properties as a function of Mo content resulted in optimum film compositions of Al-32at%Mo and Ni-40at%Mo, with a unique microstructure comprised of a dense distribution of nm-scale Mo rich crystallites densely dispersed in an amorphous matrix. We report successfully fabricated and resonance tested fully released NEMS cantilevers of various geometries, using both metallic materials. At a device thickness as low as 4 nm, made of Al-Mo alloy, these are the thinnest released metal cantilevers reported in the literature to date. The interferometer measurements of NEMS devices indicate that the Ni-based cantilevers have excellent resonant properties (frequencies and quality factors) making them competitive to that of single crystal silicon.

O.S.A.1

## PREPARATION AND STUDY OF ZINC – DOPED MAGHEMITE NANOPARTICLES

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Nanoparticles of zinc-doped maghemite were prepared using the ultrasonic radiation. During the experiment the concentration of Zn(OH)<sub>2</sub> in the suspension during sonication was gradually increased. This has a consequence that more zinc was incorporated in the maghemite particles and that the lattice constant gradually increases. The nanoparticles were almost spherical in shape with a diameter of about 20 nm. The HREM imaging showed that the nanoparticles are fully crystalline and confirmed that all analyzed nanoparticles contained both cations, iron and zinc.

At high (Zn(OH)<sub>2</sub> /  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>) ratios during sonication chemical composition of the zinc doped maghemite attains the composition close to zinc ferrite, ZnFe<sub>2</sub>O<sub>4</sub> however, with a lattice constant consistent with the maghemite structure. The magnetic moment per formula unit of zinc doped maghemite is even higher as that of pure maghemite. On heating at 900 °C the magnetization of zinc doped maghemite drastically decreases.

The majority of spinel ferrites exhibit an inverse spinel structure. In this case the resultant magnetic moment of ZnFe<sub>2</sub>O<sub>4</sub> can not show any magnetization. If the zinc ferrite exhibits some magnetization the distribution of the transition cations in the zinc ferrite spinel lattice must be, to a great extent, random.

A completely normal or inverse spinel represents an extreme case. The general cation distribution can be described as: Me<sup>II</sup> <sub>$\delta$</sub> Fe<sup>III</sup><sub>1- $\delta$</sub> [Me<sup>II</sup><sub>1- $\delta$</sub> Fe<sup>III</sup><sub>1+ $\delta$</sub> ]O<sub>4</sub>.

For a completely random distribution the inversion parameter is  $\delta = 1/3$ . Thus, the parameter  $\delta$  is a measure of the inversion. Sample with composition close to ZnFe<sub>2</sub>O<sub>4</sub> exhibits a low-temperature saturation magnetization of 73.5 emu/g and a corresponding magnetic moment per formula unit of 3.21  $\mu_B$  with the formula Zn<sub>0,321</sub>Fe<sub>0,679</sub>[Zn<sub>0,679</sub>Fe<sub>1,321</sub>]O<sub>4</sub>. Thus, in our example the  $\delta$  is 0.321, which is relatively close to the  $\delta$  value expected when the sample is quenched from high temperatures and the cations are completely random distributed.



*O.S.A.2*

**PREPARATION AND MULTILAYERED AGGREGATION OF UNIFORM COLLOIDAL CHOLESTEROL PARTICLES**

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A method for the preparation of stable dispersions of uniformly shaped platelet-type cholesterol crystals of narrow size distribution is described. Such dispersions can serve as model systems to study the effects of versatile physical and chemical environments on the formation, stability and interactions of cholesterol crystals with different solutes and substrates. Various effects on the reported procedure of preparation, based on modifying aging treatments, concentrations of the reactants, ionic strength, temperature and surface charge of the particles, were studied in addition to the standard characterization that involved X-ray diffraction, scanning electron microscopy, zeta potential measurements, infrared spectroscopy and thermal analyses.

O.S.A.3

### DESIGN OF 3D FUNCTIONAL ARTICLES BY USING COMBINED SHS-SLS

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Three dimensional shapes with a wide range of electro-physical characteristics were synthesized via a Selective Laser Sintering process from different oxide powder mixtures: ceramic-plastics (PZT+ PVDF or SiO<sub>2</sub> additives); magnetic systems Ba+M and Li+M (M ~ Fe, Cr) for Li<sub>0.5</sub>Fe<sub>2.52x</sub>Cr<sub>x</sub>O<sub>4</sub> and BaFe<sub>12-2x</sub>Cr<sub>x</sub>O<sub>19</sub> ferrites and high temperature superconductive ceramics YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>, SrFe<sub>12</sub>O<sub>19</sub>. Such materials have promising applications in smart micro devices (Micro Electro Mechanical Systems, or MEMS devices): sensors; filters; piezoelectric detectors and pumps. The concept of connectivity can be used to describe the arrangement of the component phases within a composite. The physical properties of 3D parts can be tailored by changing the phase-structure connectivity, volume fraction, phases distribution and pores within the composite. The optimum regime for laser synthesis of 3D parts and some of their associated electro-physical properties were determined by changing the laser parameters and by conducting the SHS-SLS reactions in applied electric and magnetic fields. An external field applied during SHS alters the interaction mechanism and the product structure by influencing the generation and motion of electrons and chemically ionized particles formed in the reaction front in the transient liquid phase. The mechanical properties and the ability to influence the Shape Memory Effect (SME) in porous nitinol synthesized by means of laser-controlled combination of SLS and SHS was also studied. The strain-stress curves, X-ray, SEM and temperature dependency of electrical resistivity on laser influence parameters are presented. The optimum laser energy input range 100-300 J/cm<sup>2</sup>, the limit of elasticity (0.04 - 0.06 MPa) and bending tensile strength (0.06-0.12 MPa) of 3D NiTi porous products were determined. Measurements of the temperature dependence of specific electrical resistivity on surface laser energy indicate, that in some regimes of synthesis (in the range of ~ 180-240 J/cm<sup>2</sup>) such temperature regions can be found where it is possible to observe a shape memory effect. A comparative study of bone-integration of porous-surfaced NiTi implants with control samples (porous SL-Sintered and commercial used casting Ti) was conducted. There was no significant difference between porous NiTi and Ti implants prepared via SLS in comparison with a cast Ti implant. It was concluded that porous nitinol appears to be suitable for craniofacial applications.

O.S.A.4

### SYNTHESIS AND CHARACTERIZATION OF POLYANILINE-ZEOLITE NANOCOMPOSITE

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Polyaniline-zeolite nanocomposites have been synthesized by the oxidative polymerization of aniline with ammonium peroxydisulfate in aqueous medium in the presence of zeolite HZSM-5. The influence of initial aniline/zeolite weight ratio on the conductivity, molecular and supramolecular structure of prepared composite materials was investigated. The conductivities of polyaniline-zeolite composites for monomer/zeolite weight ratio 1/1 and 1/5 were  $3 \times 10^{-2} \text{ S cm}^{-1}$  and  $3 \times 10^{-5} \text{ S cm}^{-1}$ , respectively. Molecular structure of polyaniline-zeolite was studied by FTIR spectroscopy. Scanning electron microscopy revealed the existence of nanorods with an average diameter of 55–150 nm. Specific surface area of synthesized samples was measured and catalytic activity was tested.

O.S.A.5

### HARD MAGNETIC Co-Pt FILMS PREPARED BY ELECTRODEPOSITION

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Co-Pt thin films of thicknesses up to 500 nm were prepared using the electro-deposition method from a single electrolyte on different substrates. The deposition process was analyzed using current-potential and electrochemical quartz microbalance measurements. As deposited films were annealed up to 700°C and up to 5 h. Phase formation, microstructure and magnetic properties were analyzed and optimum conditions necessary to obtain good magnetic properties were chosen. The maximum coercivity of 1.18 T and the maximum remanence of 0.7 T are achieved. The switching mechanism in the sample with the best magnetic properties was investigated by applying the  $\delta M$  method. The analysis of the hysteresis loop reveals exchange coupling in the annealed film.

O.S.A.6

**SYNTHESIS OF  $\text{Bi}_3\text{Nb}_{1-x}\text{Ta}_x\text{O}_7$  FLURITE - TYPE DIELECTRICS BY POLYMERIC PRECURSOR METHOD**

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The sintering behavior, the thermo-mechanical properties and chemical compatibility with silver has recently significantly increased the interest for  $\text{Bi}_2\text{O}_3$  based fluorite ceramics as potential candidates for use in LTCC (Low Temperature Co-fired Ceramic) technology. Our previous investigations showed that ceramics based on  $\text{Bi}_3\text{Nb}_{1-x}\text{Ta}_x\text{O}_7$  undergoes a phase transformation of cubic-incommensurate to tetragonal-commensurate type that affects profoundly the dielectric properties. By this phase transition tetragonal phase gains dielectric characteristics, which are in accordance for such application in industry. However, the formation of tetragonal-commensurate phase is kinetic dependend and the synthesis of  $\text{Bi}_3\text{Nb}_{1-x}\text{Ta}_x\text{O}_7$  tetragonal-commensurate phase using conventional solid state sintering is relatively slow. The present study aims at investigating a new way of preparing tetragonal analogues of  $\text{Bi}_3\text{Nb}_{1-x}\text{Ta}_x\text{O}_7$  through a polymeric precursor synthesis route. Using a novel synthesis method already allowed us to get nano-sized precursor particles and to influence on kinetics of the phase transition. With this study we compare different synthesis routes and consequently we determine, on the basis of kinetic studies, the conditions of heat treatment that enables optimised synthesis of tetragonal dielectrics.

O.S.A.7

**RHOMBOHEDRAL CALCITE PRECIPITATION FROM CO<sub>2</sub>-H<sub>2</sub>O-Ca(OH)<sub>2</sub> SLURRY  
AT 90 °C AND 90 BAR**

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The formation of solid calcium carbonate (CaCO<sub>3</sub>) from aqueous solutions or slurries containing calcium and carbon dioxide (CO<sub>2</sub>) is a complex process of considerable importance in the ecological, geochemical and biological areas. Moreover, the demand for powdered CaCO<sub>3</sub> is recently very important in various fields of industry: paper, paint, magnetic recording, textile, detergent, adhesive, plastic, cosmetic, food, etc. The aim of this study was then to synthesize fine particles of calcite with controlled morphology.

The morphology of precipitated particles was identified by transmission electron microscopy (TEM/EDS). The Infrared Spectrometry and x-ray diffraction were performed to investigate on the carbonation efficiency and purity of solid product.

The carbonation of dispersed calcium hydroxide ( $Ca(OH)_2 + CO_2 \rightarrow CaCO_3 + H_2O$ ) at 90 °C and 90 bar allowed the precipitation of sub-micrometric isolated particles (<1µm) and micrometric agglomerates (<5µm) of calcite rhombohedral-crystals. The use of high pressure of CO<sub>2</sub> could be desirable for increasing the production rate of CaCO<sub>3</sub> and carbonation efficiency, approximately 92 kg/m<sup>3</sup>h and 98 %, respectively for this study. The dissipated heat for this exothermic reaction was estimated by calorimetry concept ( $\Delta H = -46.1$  kJ/mol).

O.S.A.8

**HYDROTHERMAL PROCESSING OF  
1D –NANOMATERIALS FROM MINERAL SANDS**

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Since the discovery of carbon nanotubes by Iijima in 1991, the synthesis and characterization of inorganic 1D nanostructure materials became an important research subject in scientific community. Among many materials synthesized in this form, titania-based structures have attracted special attention due to their potential applications to semiconductor devices, photovoltaic cells, photocatalysts and carrier of catalysts. Several template-based and electrochemical methods have been employed to synthesize titania-based nanotubes, but generally they involve expensive and complex procedures in which the minimum size of the nanotubes is commonly limited by the template mold dimension. Because of that, the innovative work of producing one titanate-based 1D nanomaterials in the forms of nanotubes, nanorods and nanobelts by hydrothermal process using the low cost precursors like natural rutile and ilmenite sands is developed. Since the synthesis process is a function of the dissolution/precipitation processes, understanding of the exact roles of the temperature, time, pH and precursor physico-chemical characteristics represent the key factor in obtaining of the new materials with tailored morphology and structure.

O.S.A.9

## **FRACTAL ASPECTS OF DISCRETE FRACTURE MECHANICS**

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The basis for the new model of fracture proposed here, the so-called Discrete Fractal Fracture Model (DFFM) is provided by the outcome of the earlier research by Wnuk and Yavari (2003, 2005). The inspiration for the theory developed here stems from the careful analysis of the scatter that occurs in the experimental data of Ippolito et al. (2006). Their theoretical curve, which shows the dependence of the specific energy of fracture  $\gamma$  on the crack length,  $\gamma = \gamma(a)$ , has been derived from the QFM model. Here, we propose a generalized model of fracture that encompasses all the QFM results, but it adds one important characteristic of geometrical nature: fractality of the fracture surface. The latter is usually described either by the fractal dimension  $D$ , or the fractal exponent  $\alpha$ , or the roughness exponent  $H$ . Overall, three essential parameters enter the theory: two are used to describe the micro structure when the discrete fracture is considered (like in the QFM model of fracture), while one of them is suggested by the fractal nature of fracture.

In this way a new mathematical model is constructed, which in addition to the micro structural parameters,  $a_0$  and  $\rho$ , incorporates a geometrical variable, namely the fractal exponent  $\alpha$  or the fractal dimension  $D$ . Therefore, by varying the fractal dimension of the fracture surface one is able to account for all experimental points concerning the  $\gamma$  vs. crack length data as measured in the nano-range of the crack sizes. This matching procedure is fairly simple and it can be accomplished with a high precision.

The new theory not only provides an additional degree of freedom useful in seeking the optimal match between the experimental and theoretical data and in better understanding of the Physics of fracture process, but it also encompasses and generalizes all the previous approaches to the problem of brittle fracture. Some of the unique features of the Discrete Fractal Fracture Mechanics (DFFM) can be outlined as follows: (a) a finite root radius of the blunt crack enters all the pertinent equations, (b) propagation of the crack is viewed not as a continuous process, but rather as sequence of minute jumps, each of which is identified with the finite growth step, the quantum  $a_0$ . Finally, (c), the crack is modeled by a fractal, whose dimension may vary continuously between 1 and 2.

O.S.A.10

**SOLVENT-FREE MECHANOCHEMICAL SYNTHESIS OF SOME  
PHYSIOLOGICALLY ACTIVE SUBSTANCES**

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Solid-state chemistry is a fast-developing science, enhanced by its numerous applications in high-technology industries. The solid-state solvent-free reactions have many advantages: reduced pollution, usability, high conversions and yields, and often short reaction times. The aim of our research was to develop a synthesis of pharmaceutically perspective derivatives of natural and synthetic substances basing on mechanochemical approach. The objects of our study were natural alkaloid lappaconitine and non-steroidal anti-inflammatory drug piroxicam. Lappaconitine possesses high antiarrhythmic activity, drug "Allapinine" was made on its base. We realized mechanochemical oxidation as well as N-deethylation of lappaconitine. Mechanochemical solvent-free reactions were performed in the ball mill SPEX-8000 (USA) and in the planetary centrifugal ball mill AGO-2 (Russia) with water-cooled vials. The reaction course was monitored by HPLC. The interaction of solid lappaconitine and solid 3-chloroperbenzoic acid resulted in lappaconitine N-oxide in good yield. The mechanochemical reaction between solid lappaconitine and solid N-bromosuccinimide led to the target product N-deethylappaconitine in acceptable yield. The best results were achieved when aluminium oxide was added to the mixture of solid reactants. Aluminium oxide prevents conglutination of the reaction mass and absorbs traces of water. In continuation of our searching for anti-inflammatory agents with improved therapeutical properties, we applied the mechanochemical approach in acylation of piroxicam. It was shown that piroxicam transformed into the zwitterion under mechanical activation [1]. We expected piroxicam in the zwitterionic form would be more active in chemical reactions. For acylation solid 4-nitrobenzoyl chloride was used and potassium carbonate or triethylamine adsorbed on aluminium oxide was used as a base. At the first step solid piroxicam was mechanically activated in a ball mill to transform into the zwitterionic form. Then the acylation agent and the basic agent were added and mechanochemical reaction was performed. After a workup procedure the target acylated derivative of piroxicam was obtained in moderate yield. Structures of all the new products were established using spectral data (<sup>1</sup>H and <sup>13</sup>C NMR, IR, MS, UV).

The investigation was supported by the grant of CRDF (No. NO-008-X1) and by the RAS program "Fundamental Research for Medicine".

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*O.S.A.11*

### **MECHANICAL MILLING: EVOLUTION OF CRYSTAL PARAMETER OF IRON POWDER**

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The purpose of the present research was to analyze the evolution of crystal parameter of iron powder exposed to the mechanical milling.

The experiments of iron powder milling were done in a planetary mill with balls of high energy on different time interval. The iron powder with 99.9 % purity was introduced in four vials, having every one an average mass of 1.750 kg, varying the number and the diameter of balls. It was noticed from the experiment that there is a tendency to increase accentuated the crystallographic parameter in the interval of 7.5 – 9 mm ball radius. It also was admitted from the experimental data that the same interval to be more efficiently on milling from point of view of evolution of crystal parameter.

*O.S.A.12*

### **SUPERFICIAL DISTORTION INFLUENCE ON CHARACTERISTICS OF THE IRON-BASED MATERIALS**

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The surfaces superficial distortion process is applied on materials in order to improve the quality, and especially, some mechanical properties. The material surface is in a situation of intense metalworking accompanied by the presence of specific remnant tensions after the process is applied. In addition, the application of the process to the synthesized materials leads to pores closing and by dismissing their negative effect on some properties. Metalworking through rolling or gritting of synthesized materials leads to an important increasing of tiredness resistance.

The effect of rolling on materials properties depends, in an important measure, by the parameters of the process (contact pressure and process length) and by the material structure. Until now, based on technical considerations, the rolling process was applied just on cylindrical samples.

The aim of the paper is to present some experimental results of plane surfaces metalworking influences on synthesized steel properties obtained from different powders blend. There has been observed that some properties (e.g. toughness, traction and flexion resistance) were improved with increasing of the length of rolling, but the relationship was not linear. The materials with a higher plasticity suffer a more intense metalworking process with positive consequences on mechanical properties of interest.

O.S.A.13

**PLASMA POST-PROCESSING IN OXYGEN AND CARBON CONTAINING  
ATMOSPHERES FOR WIND TURBINE COMPONENTS TREATMENT**

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Wind energy conversion to electricity is the most growing renewable energy source industry in the world. Different types of wind generators are in operation but the 'conventional' multi-stage gear-driven wind turbines dominate the market over direct-drive systems without the gearbox. The gearbox fault is a very serious source of today's wind turbines failure. We propose a new pulse plasma surface treatment consisting of plasma nitriding and subsequent plasma post nitrocarburizing, or plasma nitrocarburizing with post-oxidation which improves the fatigue resistance, wear resistance and corrosion resistance and contributes to the lowering of weighted acoustic level. This process is a candidate for surface treatment of wind turbine gears which are exposed to severe working conditions including high mechanical stresses, alternative load, surface wear and corrosion and during the operation they can be source of high sound level which influences the environment. The samples made of steel grades AISI C 1045, 4140 and H 11 were pulse plasma nitrided and plasma post-nitrocarburized. The Vickers's method was used for surface microhardness and depth profiling measurements, while the surface zone morphology was examined by SEM. The surface zone phase analysis was performed by XRD method while the ball-grinding technique was used to measure the compound zone thickness. A low friction, chemically stable single-phase magnetite superficial layer can be formed by plasma post-oxidation. The post treatment in carbon containing atmosphere resulted in formation of a surface layer with gradually increased carbon content and the cementite phase formation, as was found by XRD analyses. Two steps plasma processing in one batch which provides the treatment of complex shape workpieces to obtain nitrided layer with cementite rich zone at the surface was found suitable as a candidate technique for wind turbine gears processing.

*O.S.A.14*

**SYNTHESIS OF OLIVINE-TYPE  $\text{LiFePO}_4$  BY SONOCHEMICAL METHOD**

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Lithium iron phosphate has become of great interest as storage cathode for rechargeable lithium batteries because of its high energy density, low raw materials cost, environmental friendliness and safety. Olivine-type lithium iron phosphate ( $\text{LiFePO}_4$ ) powders were synthesized for the first time by sonochemical reaction. The as-prepared powders were shortly heat-treated at various temperatures under slightly reductive atmosphere. Syntheses were followed by X-ray powder diffraction measurements. X-ray powder diffraction data were used for the crystal structure refinements, based on Rietveld full profile method. All relevant structural and microstructural crystal parameters that could be significant for electrochemical intercalation/deintercalation processes were determined. Electrochemical characteristics were evaluated by using cyclic voltammetry. Particle morphologies of the obtained powders were determined by scanning electron microscopy.

*O.S.A.15*

**SYNTHESIS AND CHARACTERIZATION OF IRON CONTAINING MCM-41  
POROUS SILICA – APPLICATION TO ADSORPTION OF ARSENATES**

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The new family of silica-based mesoporous materials (designated as M41S) that scientists at Mobil Oil Research successfully synthesized in 1992, have very high surface area, ordered pore structure and extremely narrow pore size distribution. Since then, research has focused on the utilization of the M41S or other similar mesoporous materials in various environmental and industrial processes. However, a main drawback of these materials is the relatively low surface chemical reactivity. Partial substitution of silicon by active metal ions (such as aluminum, titanium, etc.) in the silicon oxide network of the parent material can induce acid-base and redox catalytic properties, whereas functionalization of the external surface by grafting of organosilicon groups can provide active sorbents for biological, environmental, sensing and other related processes. In the last years iron-modified mesoporous MCM-41 silica materials have gained large interest as nanostructured materials with interesting catalytic, sorptive, optical and magnetic properties. This work deals with the synthesis, characterization and application of iron containing MCM-41 and iron containing amino-functionalized MCM-41 porous silica materials. The preparation of amino-functionalized MCM-41 was realized using silanes containing mono-, di- and triamino groups via post-synthesis grafting methods. The incorporation of iron to MCM-41 was achieved either by the direct hydrothermal synthesis of Fe-substituted MCM-41 or by impregnation of the calcined material with aqueous solution of iron salts. In the case of the amino-functionalized materials iron cations were anchored on the amino groups. The last step in the current research was the application of the above mentioned (iron containing MCM-41 and iron containing amino-functionalized MCM-41 porous silica) materials for the removal of arsenates from aqueous solutions. Sorption capacity was related to the state (oxide or cationic)/distribution of iron species as well as to the porous characteristics of the iron-MCM-41 materials.

*PL.S.II.1*

**NEW DEVELOPMENTS IN QUANTITATIVE 3D STRUCTURE ANALYSIS OF THIN  
SOLID FILMS BY TRANSMISSION ELECTRON MICROSCOPY**

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Thin solid films play a crucial role in many modern technologies, like microelectronics, solar cells, sensors, and coatings. A key to understanding and controlling thin film growth processes and properties is the knowledge of the variation in structure with distance from the substrate or, in other words, the knowledge of the film's three-dimensional (3D) structure. Transmission electron microscopy (TEM) is known as a powerful tool for characterization of thin films. By combining plan-view and cross-section analysis a qualitative view of the 3D film structure can be obtained. However, neither of the two geometries is compatible with the need for quantitative characterization of the film's 3D structure. Here we present a new sample preparation technique that overcomes these limitations by a double-wedge sample geometry that probes different depths in the thin film and separates depth information in a continuous sequence of thin slices that are spread over a lateral distance in the TEM sample. By large-area characterization of 2D film sections at different film depths a statistical description of the 3D film structure can be obtained. The wide applicability of the technique will be demonstrated by showing examples of quantitative characterization of the 3D grain structure of polycrystalline MEMS films and of 3D dislocation networks in buffer layers of high-efficiency solar cells.

PL.S.II.2

**USING REAL TIME MICROSCOPY TO QUANTITATIVELY DETERMINE  
NUCLEATION MECHANISMS AND KINETICS DURING THE GROWTH OF Si  
NANOWIRES AND CARBON NANOTUBES**

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A comprehensive understanding of growth mechanisms and kinetics is of considerable importance for structural optimization of nanostructured materials with desired properties. Here, we report real time transmission electron microscopy (TEM) measurements of the nucleation kinetics of Au-catalyzed Si nanowires and Fe-catalyzed carbon nanotubes.

Our direct observations of Au mediated Si nanowire nucleation span from initial observations of the pure solid Au catalyst to final nanowire nucleation. Our measurements show that the nucleation time is linearly proportional to the diameter of the AuSi alloy drop – contrary to behavior expected from the Gibbs-Thomson effect – and that the nucleation rate linearly increases with disilane pressure. These two observations indicate that the rate limiting step throughout the process is the thermally activated dissociative adsorption of disilane on the catalyst surface. Furthermore, we classify the subsequent nucleus growth process of Si nanowires into three regimes: an initial rapid growth of the nucleus, a subsequent slow growth of the nucleus, followed by axial growth of the nanowires away from the AuSi drop. We show that for the initial growth, the growth rate ( $dr/dt$ ) is simply proportional to the critical supersaturation required to nucleate the nanowire. Additionally, during the slow growth regime and final nanowire growth, the growth rate is proportional to the ratio between the surface area of the AuSi alloy and the Si nucleus. These observations are in an excellent agreement with a theoretical model we have proposed for nanowire nucleation kinetics.

In the case of Fe catalyzed nanotube growth we have used the alcohol catalyzed chemical vapor deposition process developed by Maruyama to grow carbon nanotubes in-situ to the electron microscope. We will report measurements of Ostwald Ripening of the Fe catalysts during the onset of nanotube growth and the role of this ripening in terminating growth processes. Additionally, or initial measurements regarding the feasibility of determine the interrelationship between catalyst structure and nanotube chirality will be discussed.

These quantitative measurements yield critical data needed for controlling nanowire and nanotube nucleation during the fabrication of high performance nano-electronic devices based on these structures.

PL.S.II.3

## BULK NANOCRYSTALLINE ALLOYS STUDIED BY TEM

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Bulk nanocrystalline metals and alloys attract considerable interest in materials science since their structural changes lead to exciting new features. Transmission electron microscopy (TEM) methods are therefore most appropriate to analyse the structures of these materials. When bulk nanostructured alloys are studied by TEM special care is needed to interpret the images. In alloys processed by severe plastic deformation like high pressure torsion (HPT) the achieved grain size is less than the foil thickness of the TEM sample. Therefore, overlapping grains frequently lead to moiré patterns. This can cause images of bend and interrupted lattice fringes that should not be misinterpreted as arrays of dense dislocations [1].

The evolution of the nanocrystalline structure resulting from HPT deformation was studied in ordered Ni<sub>3</sub>Al. As a precursor blocks and bands are formed containing misoriented fragments in the 100 nm range separated by a three-dimensional array of low angle boundaries. The inhomogeneous deformation leads to localized disorder and a high density of dislocations. Dynamic recovery causes a heterogeneous formation of the nanocrystalline structure. At strains of about 1000% a duplex structure is formed consisting of veins of disordered nanograins that are embedded in the ordered coarse-grained structure; at strains above 50,000% the whole volume transforms to the nanocrystalline structure [2].

In NiTi, a shape memory alloy, the martensitic phase transformations of nanocrystals were investigated. After a HPT deformation of about 1000%, shear bands of an amorphous phase were observed filling the whole volume at larger strains. Since the amorphous phase formed by HPT contains several nanocrystalline debris that can act as nucleation sites, it was used successfully to make a bulk nanocrystalline structure by devitrification. Upon cooling the martensitic transformation of the nanostructures is not complete since the grain boundaries hinder the autocatalytic formation of martensite [3]. In addition, the size effect on the transformation of nanocrystals embedded in an amorphous matrix was studied [4]. In both cases the large transformation strains of the martensite are reduced by very fine compound twins. The observed twin boundaries of very low energy facilitate arrays of compound twins on an atomic scale to overcome the strain energy barrier of the nanograins thus violating the hitherto well established theory of martensite formation [5].

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*PL.S.II.4*

**APPLICATION OF HIGH SPATIAL AND HIGH ENERGY RESOLUTION  
ANALYTICAL TOOLS FOR THE CHARACTERIZATION OF ADVANCED  
MATERIALS**

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Over the last two years, the EAG has rapidly built on the foundation of Charles Evans & Associates to form a network of over 18 laboratories and representatives in nine countries (Europe, Unites States, Japan, Korea, Taiwan, The Peoples Republic of China and Singapore). These laboratories have over 150 major instruments and 300 experienced employees to provide

- Surface and Microanalysis (all three modes of SIMS, XPS, AES/SAM, RBS, etc);
- Advanced Electron Microscopy (SEM, SEM/EDS, TEM, STEM/EDS, SPM, etc.);
- Chemical Analysis (GDMS, ICP-MS, FTIR, Raman, GCMS, etc), and
- Failure Analysis.

This lecture will describe several of these techniques and illustrate their utility with interesting and advanced applications. The applications will cover the areas of microelectronics, biotechnology, and other materials systems that benefit from these advanced analytical techniques.

*PL.S.II.5*

**BIOLOGICALLY ENABLED ASSEMBLY OF NANOSTRUCTURED MATERIALS  
WITH COMPLEX THREE-DIMENSIONAL MORPHOLOGIES AND CHEMISTRIES**

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Ph. Graham, M.B. Dickerson, G. Ahmad

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Nature provides spectacular examples of micro-organisms that self-assemble intricate 3-D structures that, through biological reproduction, are replicated with genetic precision in a massively-parallel fashion. A stunning range of silica structures can be found among the microshells of diatoms (unicellular algae). Each of the thousands of diatom species assembles a silica-based microshell (frustule) with a particular shape and pattern of fine (nanoscale) features. In this presentation, several shape-preserving approaches for converting diatom silica frustules into other functional chemistries will be described: i) fluid/solid reactions, ii) conformational coating methods, and iii) combined reaction and coating approaches. By merging shape-preserving chemical conversion with biological self-assembly, a wide range of nanostructured functional microcomponents of controlled 3-D shape may be mass-produced.



PL.S.II.6

## CHARACTERIZATION OF SOLID/LIQUID INTERFACES BY SURFACE POTENTIAL MEASUREMENTS

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Recently, the method for measurement of the surface potential  $\Psi_0$  was introduced<sup>1</sup>. For that purpose the single crystal electrodes (SCrE) were developed<sup>2</sup>. The problem of evaluation of surface potentials from measured electrode potentials of SCrE was solved<sup>3</sup>. Surface potential, *i.e.* the electrostatic potential at the solid surface (inner Helmholtz plane), affects directly activity coefficients of charged surface species<sup>4</sup> and thus the entire equilibrium within the electrical interfacial layer (EIL). Several metal oxide aqueous interfaces were examined. It was shown that the magnitude of the slope of the  $\Psi_0(\text{pH})$  function is lower than the Nernstian, depending on the type of oxide and the composition of the electrolyte solution. The simultaneous interpretation of electrokinetic potential, surface potential and surface charge data will be presented. Such an approach enables more reliable characterization of interfaces. The application of results to the problem of stability of nano-dispersions will be discussed.

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3. Kallay, T. Preočanin and T. Ivšić, *Determination of Surface Potential from the Electrode Potentials of a Single Crystal Electrode*, J. Colloid Interface Sci., in press.
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PL.S.II.7

## BI-BASED MATERIALS FOR GLASS-FREE LTCC MODULES

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In the last decade a wide variety of wireless applications were found for broadband and high-frequency devices operating from 800 MHz to 2 GHz. New functional properties such as Bluetooth or LAN demand even higher frequencies, up to 5.3 GHz, and WLL (Wireless Local Loop) 20 to 30 GHz. Therefore, advanced materials and process technologies have to be extensively investigated to meet the demands of the communication and sensor modules of the future. These materials and processes must increase the performance and functionality of modules, improve their reliability, and they must have the potential to reduce costs. Multilayer components like those produced by LTCC (Low Temperature Co-fired Ceramics) technology are considered to fulfill these demands. The highlights of LTCC for microwave applications include: *i.*) the integration of antenna-, R-, L- and C-elements; *ii.*) a high density of connections; *iii.*) cost-effective manufacturing using parallel process steps and a reduction of SMD components; *iv.*) a robustness against mechanical stresses and high temperatures. New ceramic materials with improved (di)electric properties and/or a better combination of properties will strongly accelerate the development of new components and devices operating at MW frequencies.

Today performance and size standards are set by other technologies like SAW filters. In order to meet these challenges the application of new design concepts along with new technologies are required. The design concepts range from folded quarter wave length resonators to lumped element designs and are based on a multi-layer, via forming kind of technology. To reach the full potential of this technology it is necessary to develop new materials which have good microwave properties and allow an all-silver co-fire process.

The research in our laboratory has been focused on Bi-containing compounds such as  $\text{Bi}_2\text{O}_3\text{-Nb}_2\text{O}_5$  fluorite-type solid solutions and  $\text{Bi}_2\text{M}_{1/3}\text{M}''_{2/3}\text{O}_7$  ( $\text{M}=\text{Zn, Ni, M}''=\text{Nb, Ta}$ ) pyrochlores, which can be sintered below 900°C. We found that by varying the composition and additives, the permittivity of such ceramics can be tuned from 20 to 90, while keeping the temperature coefficient of resonant frequency in the range  $-20 < \tau_f < +20$  ppm/K, and the Qxf values in the vicinity of 3000 GHz. This has led to a new concept of the glass-free LTCC module.

In the lecture, chemical as well as sintering compatibility issues will be addressed. It will focus on the development of glass-free low sintering materials with dielectric constants between 20 and 90, low losses and low temperature coefficients. The co-fire ability with silver electrodes will be discussed. Applications for these materials will be presented.

*O.S.B.1*

## LITHIUM CONDUCTING PEROVSKITES

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Li-ion conducting materials of the system La-Li-M-O, where M –Ti, Nb, Ta with the perovskite structure have been studied, and will be discussed. Various structural prerequisites responsible for the cation conductivity in the perovskite La-Li-M-O which include structural channels as well as the cation vacancies were considered. The crucial role of structural channels, formed by oxygen octahedral, in the charge transport processes in Li-conducting perovskites has been shown. The increase in the size of the conducting channels was found to not directly result in the increase in lithium-ion conductivity. It has been concluded that the alkali ions are not rigidly connected with the perovskite lattice framework La-M-O and may contribute to the conductivity. The size effect of the structural environment of Li ions on the type of lithium ion motion will be also discussed.

*O.S.B.2*

## LOW-LOSS MICROWAVE DIELECTRICS BASED ON THE COLUMBITES $A^{2+}Nb_2O_6$ AND PEROVSKITES $Ba(A_{1/3}^{2+}Nb_{2/3})O_3$ : THE EFFECT OF COMPOSITIONAL VARIATION

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Due to their high quality factor in the microwave (MW) range the columbites  $A^{2+}Nb_2O_6$  and perovskites  $Ba(A_{1/3}^{2+}Nb_{2/3})O_3$  can found a variety of applications in the MW engineering. However, the attainment of low-microwave-loss structure of the above compounds is rather complicated task, and their MW properties may vary significantly due to the structural inhomogeneity. In this work the effect of slight compositional non-stoichiometry on the microstructure and MW dielectric properties of the columbites  $A^{2+}Nb_2O_6$  and perovskites  $Ba(A_{1/3}^{2+}Nb_{2/3})O_3$  has been studied and will be discussed. The effects of the quality of starting reagents as well as the synthesis conditions were also considered. The non-linear dependence of the  $Q$ -factor magnitude on the chemical composition has been found and associated with the evolution of the microstructure.

O.S.B.3

### MOLDING FLUORESCENCE EMISSION BY PHOTONIC BAND GAP ENGINEERING

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The fluorescence of dye molecules embedded in a photonic crystal is known to be inhibited by the presence of a pseudo-gap acting in their emission range. Here we present the influence of the pseudo-gap on the fluorescence of simple dye as fluorescein and up to our knowledge the first account of the influence that a photonic pseudo-gap has on the fluorescence resonant energy transfer. The FRET investigations were possible due to a combination of photonic band gap engineering based on the self assembly process with oligonucleotide technology. Oligonucleotide double strands were infiltrated in a photonic crystal as a tool to investigate the influence of a pseudo-gap on FRET between two dyes covalently attached to the oligonucleotides. By inserting synthetic, donor (D)- acceptor (A)-labeled oligonucleotide structures in self-organized colloidal photonic crystals, we were able to measure simultaneously the emission spectra and lifetimes of both donor and acceptor by confocal microscopy. Our results clearly show an inhibition of the donor emission together with an enhancement of the acceptor emission spectra. These results are mainly attributed to a decrease of the number of available photonic modes for radiative decay of the donor in a photonic crystal in comparison to the effective homogeneous medium. The fluorescence decay parameters are also dominated by the pseudo-gap acting on the energy transfer efficiency.

O.S.B.4

### PROPERTIES OF $\text{NdCr}_3(\text{BO}_3)_4$ BORATE: SPECTROSCOPIC STUDY

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We present the first high-resolution spectroscopic investigation of the  $\text{NdCr}_3(\text{BO}_3)_4$  single crystal. The members of the family  $\text{RM}_3(\text{BO}_3)_4$  with  $M = \text{Al}$  and  $\text{Fe}$  have earlier been shown to possess a device potential. Up to now, only little was known about the properties of the rare-earth chromium borates  $\text{RCr}_3(\text{BO}_3)_4$ . We have found that the structure of  $\text{NdCr}_3(\text{BO}_3)_4$  is described by the R32 space group in the whole range of temperature 1.8 – 300 K. At  $T_N=8\text{K}$ , the optical spectroscopy data imply long-range spin order of the  $\text{Cr}^{3+}$  subsystem in  $\text{NdCr}_3(\text{BO}_3)_4$ , since in the ordered state the  $\text{Nd}^{3+}$  Kramers doublets are split by the internal staggered magnetic field. In the spin-ordered phase, we estimate the value of this field as 3 Tesla at 1.8 K.

*O.S.B.5*

**EXITON-IMPURITY ENERGY TRANSFER DYNAMICS IN NEW LOW PHONON ENERGY LASER MATERIALS**

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The RE-doped low phonon energy alkali-lead halide crystals are promising new material emitting in a wide spectral region from UV up to mid IR [1]. We report on the results of the study of energy transfer dynamics in RE<sup>3+</sup>:KPb<sub>2</sub>Cl<sub>5</sub> crystals under UV excitation at low and room temperature. UV excitonic or host excitation at 12 K leads both to excitonic and RE ions emission. Recombination of self-trapped exciton is followed by broad-band emission in visible spectral range with nanosecond decay time and a series of narrow lines corresponding to RE ion emission. In spite of the strong quenching of exciton emission at room temperature, RE ions emission was observed in wide spectral ranges. It was shown that exciton recombination is followed by fast energy transfer to RE centers independently on temperature. Possible ways of exciton → impurity energy transfer are discussed.

*O.S.B.6*

**NEW RE DOPED FLUORIDE AND CHLORIDE CRYSTALS FOR EFFICIENT OPTICAL CONVERTERS**

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The rare earth doped low phonon crystals, such as fluorides and chlorides, demonstrate efficient conversion of IR light into the visible region and are promising for use in optical converters designed for enhancement of solar cells efficiency or IR light visualization, as well as for use in the laser diode pumped solid state lasers, emitting in the visible spectral range. In this work we report on the comparative study of upconversion processes in RE-doped double fluoride crystals and new low phonon chloride crystals KPb<sub>2</sub>Cl<sub>5</sub>:RE (RE=Er<sup>3+</sup>, Yb<sup>3+</sup>). The mechanisms of upconversion population of Er excited levels upon LD pumping are investigated both experimentally and theoretically. Estimations of IR to VIS up-conversion efficiency are presented.

O.S.B.7

## MAGNETIC PHENOMENA IN THE 4f-ELECTRON INTERMETALLIC COMPOUNDS

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The work focuses on the magnetic properties of the ternary intermetallic compounds containing 4f electron elements (rare earth elements, denoted here as R), transition d-electron elements (denoted as T) and the elements of the fourth or fifth group (denoted as X). The intermetallic  $R_mT_nX_p$  phases crystallize in a wide range of composition (m:n:p) and show a large variety of crystal structure types and magnetic properties [1]. The influence of the crystal structure on the magnetic properties is discussed.

In the work the magnetic properties of new  $R_mCu_nSn_p$  systems with the stoichiometry 1:1:1, 1:1:2, 1:2:2 and 3:4:4 are discussed. The 1:1:1, 1:1:2 and 3:4:4 compounds crystallize in different orthorhombic structures while the 1:2:2 compounds have tetragonal crystal structures. In the case of the 3:4:4 compounds the rare earth atoms occupy two nonequivalent crystallographic sites. In all these structures the atomic framework can be described as a sequence of monoatomic planes perpendicular to a crystallographic axis. This suggests strongly anisotropic properties.

The magnetic and neutron diffraction data suggest that the majority of the studied compounds order antiferromagnetically with different magnetic structures (collinear or modulated). In these compounds the magnetic moment are localized on the rare earth atoms. The values of the magnetic moment are close to the free  $R^{3+}$  ion values in the paramagnetic state and are smaller in the ordered state. The latter suggests strong influence of the crystal electric field. Thermal dependence of resistivity indicates metallic character of these compounds. For all discussed systems stability of the magnetic ordering is due to interactions via conduction electrons (the RKKY model). However, the de Gennes scaling ( $T_N$  vs  $(g-1)^2J(J+1)$ ) is not fulfilled, which suggests the influence of the crystal electric field [2]. In the case of the 3:4:4 compounds the magnetic moments in the two rare earth sublattices appear to order entirely independently with different critical temperatures of the magnetic ordering and different magnetic structures. In some compounds the magnetic neutron diffraction and specific heat measurements indicate an additional phase transition in the ordered state.

The influence of external magnetic field on changes in the magnetic structure is reported and the magnetocaloric effect is also investigated. Finally the electronic structure and its influence on the magnetic properties of these compounds is discussed. Larger values of the hybridization energy between localized 4f states and the conduction electrons are observed for compounds with the light rare earths (Ce, Pr, Nd).

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*O.S.B.8*

**THE DISPROPORTIONATION PROCESS IN RARE-EARTH-TRANSITION-METAL-BASED MATERIALS: AN EXPERIMENTAL AND MODELING APPROACH**

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Rare-earth permanent magnets have taken a large share of the market because of their outstanding magnetic properties and their versatility when it comes to processing. Sintered Nd-Fe-B-based magnets dominate the market, but there are considerable niches held by melt-spun materials, hot-pressed materials, and magnets produced by the hydrogen-disproportionation-desorption-recombination (HDDR) process. As with all forms of processing, the more we understand about what is happening during the various stages of producing the material the better the position we are in to improve the properties. In this investigation the HDDR process for the production of permanent magnets was evaluated from the kinetic point of view. Phase transformations can be investigated by isothermal and isochronal (non-isothermal) experiments and the experimentally obtained data are usually described by the Johnson-Mehl-Avrami model, or models similar to it. The best fit is chosen to be the appropriate model for the reaction investigated. The disproportionation reaction was monitored using a modified VSM that enabled us to follow the progress of the reaction in a hydrogen atmosphere under isothermal conditions and with gravimetric measurements. The behavior in hydrogen was evaluated for two different Sm-Fe-based alloys –  $\text{Sm}_{13.7}\text{Fe}_{86.3}$  and  $\text{Sm}_{13.8}\text{Fe}_{82.2}\text{Ta}_{4.0}$ . The purpose of this kinetic study was to obtain information about the reaction mechanism through comparisons of measured values – transformation and time – and theoretical functions, which have been derived from models based on the geometry of the interface's initiation and advance and/or diffusion process occurring in the solid. The disproportionation behavior differs depending on the alloy composition. With the addition of Ta the reaction kinetics is changed. Whereas in the binary alloy the behavior can be described with the sigmoid rate equation, the disproportionation of the ternary alloy suggests that the process is decelerator in its nature.

O.S.B.9

### MESOPOROUS TITANIUM DIOXIDE: SYNTHESIS AND PHOTOCATALYTIC ACTIVITY

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Porous titania with high surface area have received a great deal of attention as a perspective photocatalytic material and catalyst support. Here we suggest non-hydrothermal approach which allows to obtain titania with high surface area and narrow pore size distribution via hydrolysis of  $\text{Ti}(\text{O}^i\text{Pr})_4$ ,  $\text{Ti}(\text{O}^n\text{Bu})_4$ ,  $\text{TiCl}_4$  and  $\text{TiO}(\text{NO}_3)_2$  in presence of cetyltrimethylammonium bromide and P123 triblock copolymer. It was found out that ultrasonic treatment promotes polycondensation and allows getting mesoporous structures with better thermal stability due to thicker pore walls. After optimization of synthesis conditions we have obtained mesoporous titanium dioxide with high surface area up to  $580 \text{ m}^2/\text{g}$ , nanocrystalline pore walls and significant photocatalytic activity. This work was supported by RFBR (grants 06-08-01443-a and 06-03-89507-HHC\_a).

O.S.B.10

### INCOMMENSURATE-COMMENSURATE PHASE TRANSFORMATION IN THE $\text{Bi}_2\text{O}_3\text{-Nb}_2\text{O}_5$ SOLID SOLUTION

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The partial substitution of Bi with Nb in  $\text{Bi}_2\text{O}_3$  stabilizes the fluorite-type  $\delta\text{-Bi}_2\text{O}_3$  crystal structure down to room temperature. The resulting solid solutions exhibit high oxygen mobility, which makes them promising materials for applications in solid-oxide fuel cells (SOFCs), electrochemical sensors, dual-phase membranes and catalysts. Furthermore, we have shown that these materials can be successfully applied as high-permittivity layers in LTCC-based LC filters. There are two crystal-structure modifications, differing in terms of their structural modulation, which we found interesting for tuning the dielectric properties. The incommensurately modulated structure forms during the solid-state synthesis at temperatures above  $700^\circ\text{C}$ . We established that this modification is in fact stable only above a certain temperature, which depends on the composition of the solid solution. Upon annealing at lower temperatures it transforms to a commensurately modulated modification exhibiting a  $3 \times 3 \times 7$  superstructure with respect to the incommensurate one. The kinetics of the transformation is unusually slow since it appears to require a certain induction time before its commencement. The results of the XRD and TEM analyses of the transformation will be presented.



*O.S.B.11*

**SOL-GEL SYNTHESIS AND CHARACTERIZATION OF A NEW BISMUTH  
TITANATE PYROCHLORE CERAMIC**

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The dielectric properties of bismuth-based pyrochlores have demonstrated that they are promising materials for LTCC applications. In our study, various powder compositions of bismuth titanate pyrochlore (BT-pyrochlore) were synthesized using the sol-gel method and fired under different sintering conditions. The fired samples were characterized using X-ray powder diffractometry (XRD), scanning electron microscopy (SEM) with energy-dispersive spectroscopy (EDS) and wavelength-dispersive spectroscopy (WDS). At low temperatures we confirmed the existence of the BT-pyrochlore solid solution and above 1150°C we observed the formation of a new BT-pyrochlore,  $\text{Bi}_{1.65}\text{Ti}_2\text{O}_{6.5}$ . In the report we will discuss the thermal stability of the BT-pyrochlore solid solution and the dielectric properties of the new BT-pyrochlore ceramic.

O.S.B.12

**INFLUENCE OF CRYSTAL SYMMETRY ON THE VOLTAGE-TUNABILITY OF  
Na<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub>-BASED SYSTEMS**

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The voltage-tunability of materials critically depends on their behavior in static and dynamic electric fields and is determined by the susceptibility of the dielectric constant to the DC-bias field ( $n_r = (\epsilon(0) - \epsilon(E)) / \epsilon(0)$ ). The behavior relates to the material's polar order, while most of the commercially available tunable materials are in a paraelectric phase, since in general they exhibit lower dielectric losses with respect to materials in the ferroelectric phase. However, promising tunable properties of ferroelectrics have been shown recently, especially above the relaxation frequency of the domain-wall motions. In contrast to paraelectric materials the tunability of polar phases has not yet been extensively studied. Therefore, we focused our study on the Na<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub> relaxor ferroelectric, which is a polar compound and exhibits a broad dielectric maximum at 320°C, related to dielectric relaxation at the microwave frequencies. In addition, relaxor ferroelectrics are described by their polarization rotation, which is remarkably susceptible to the DC-bias field, and thus considerable tunability of the Na<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub> is expected. The temperatures of the Na<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub> phase transitions were optimized by Li<sub>3x</sub>La<sub>(2/3-x)</sub>TiO<sub>3</sub> ( $0.03 \leq x \leq 0.167$ ) and NaTaO<sub>5</sub>, which have characteristics similar to incipient antiferroelectrics and ferroelectrics, respectively. Prior to an electrical characterization the mechanisms of solid-state synthesis and sub-solidus phase relations in the selected systems were determined. The dielectric, ferroelectric and tunable properties of the compounds from the homogeneity regions were measured at different temperatures, frequencies and electric fields. The differences in the tunable properties were related to the variation in the remanent and saturated polarizations, which further depend on the crystal chemistry and the stoichiometric properties across the homogeneity regions, which will be the main focus of our contribution.

O.S.B.13

**PHYSICO-CHEMICAL CHARACTERISTICS OF Rb<sup>+</sup> AND Cs<sup>+</sup> SALTS OF 12-TUNGSTOPHOSPHORIC ACID**

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As good candidates for design at the atomic and molecular level, heteropoly catalysts have been proven as valuable in both fundamental and practical applications. Counteranions have great influence on the secondary and tertiary structure and thus on physicochemical properties of heteropoly compounds (HPCs). Salts of large cations such as K<sup>+</sup>, Cs<sup>+</sup> and Rb<sup>+</sup> are insoluble in water, have high surface area and thermal stability which is of importance for heterogeneous catalysis.

As the results for potassium salts of 12-tungstophosphoric acid are published yet [1], in these study physicochemical characteristics of Rb<sup>+</sup> and Cs<sup>+</sup> salts of 12-tungstophosphoric acid, neutral and acid ones were investigated. The salts were prepared by conventional techniques of ion exchange. In order to improve catalytic properties of HPCs, Al-pillared interlayer clays were doped with these salts and their characteristics were studied by FTIR, XRPD, thermal and microscopic techniques. Textural properties of obtained products were studied by N<sub>2</sub> adsorption-desorption isotherms.

The obtained solids were tested as catalysts in wet oxidation of toluene by hydrogenperoxide. Removal of toluene from water by catalytic wet oxidation with hydrogen peroxide is environmentally important process.

[1] M. Todorović, I. Holclajtner-Antunović, U. Mioč and D. Bajuk-Bogdanović, Mat. Sci. Forum 555 (2007)

*O.S.B.14*

**CARBON/CARBON-SILICON-CARBIDE DUAL-MATRIX COMPOSITES FOR  
BRAKE DISCS**

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Composite ceramic materials reinforced with carbon fibers are interesting materials because of their excellent mechanical and thermo-physical properties, which make them appropriate for many applications, including re-entry shields, rocket nozzles, disc brakes and prosthetic devices. For all these purposes many different types of such materials have been developed, for example, carbon/silicon-carbide or carbon/carbon-silicon-carbide composites that are commonly produced from carbon/carbon composites impregnated with liquid silicon by the liquid-silicon infiltration (LSI) process. The aim of our work was to develop a friction material for brake discs that will combine a high fracture toughness with good oxidation and abrasion resistance, good thermal conductivity and the appropriate friction characteristics, without the use of the expensive and time-consuming LSI process. For the production of such materials the "dual-matrix" approach was used. The discs were first prepared using phenolic resin with active and passive fillers to prepare the C/C-SiC composite by pyrolysis. These discs were finally impregnated with ceramic-forming polymers to obtain superior mechanical and tribological properties.

O.S.B.15

## DETECTION OF THE DEGREE OF BRANCHING IN HYPERBRANCHED POLYMERS

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Hyperbranched polyesters based on 4,4-bis(4-hydroxyphenyl)pentanoic acid were synthesized for the application as a potential additive in processing of linear polymers. The investigation of the polymers was carried out by using size exclusion chromatography (SEC) with triple, light-scattering, viscosity and concentration, detection. Using the Flory-Fox method the radii of gyration of the dendritic and linear polymers were determined. By comparing the radii of gyration of the hyperbranched polyesters with those of the linear-chain copolyesters based on bisphenol-A and 3-phenylglutaric acid [1] the degrees of branching (DB) were calculated applying the Zimm-Stockmayer theory of branching. In comparison to the maximum value of DB of 0.368, found by (the equation of) Hölder et al. [2], our values of DB are somewhat below. Furthermore with increasing molecular weight a decrease of DB was observed (0.33-0.25). This result suggests the presence of some structure irregularities, although the linear Mark-Houwink plot with a slope of  $a = 0.34$  confirms a hyperbranched structure of the polymer.

### Reference

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2. D. Hölder, A. Burgath, H. Frey, Acta Polym., 48 (1997) 30-35.

W.S-S.BC.1

### PHONONS IN MoS<sub>2</sub> AND WS<sub>2</sub> NANOTUBES

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Phonon dispersions of all the single-wall MS<sub>2</sub> nanotubes with diameter range 1-20 nm, are calculated using full symmetry implemented valence-force-field model. Using simple coupled-spring like model, for the same symmetry modes of walls, the frequency shifts for double-wall tubes are estimated. Infrared and Raman active modes are singled out, in order to clarify possible application of these methods in the experimental sample characterization. A prescription for experimental distinction of zig-zag, armchair and chiral tubes, based on their different symmetry and resulting selection rules, is proposed. Furthermore, it is shown that the displacements significantly depend on the chiral angle only for two modes in Mo S<sub>2</sub> nanotubes, namely twisting in-phase (rigid layer) and breathing out-of-phase, and none of W S<sub>2</sub> modes. Heat capacities of the nanotubes and layer are similar.

References:

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W.S-S.BC.2

### STUDIES OF APPLICATION AND CHARACTERIZATION OF PLASMAS USED IN TREATMENT OF POLYMERS AND ORGANIC MATERIALS

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Studies of treatment and deposition of polymers have been carried out in Laboratories in Ljubljana and Belgrade as a part of bilateral collaborative project. At Institute Jožef Štefan inductively coupled plasma source was used for deposition of a wide range of polymers on surfaces. At the Institute of physics in Belgrade large size capacitively coupled reactors have been employed in treatment of surfaces of polymers, treatment of textiles and living tissues. In addition a plasma needle has been developed operating at atmospheric pressure which allows superficial treatment of different organic materials without using the low pressures. Diagnostic techniques have been developed and implemented including derivative probes for voltage and current measurements and ICCD detection of emission, that allow non-intrusive control and diagnostics of plasmas. At the same time applicability of such sources in treatment of surfaces has been tested and optimized.

W.S.-S.BC.3

**PULSED LASER ABLATION OF PVD MULTI-LAYERED COATINGS:  
PROFILOMETRIC ANALYSIS**

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Multilayered physical (PVD) vapor deposited coatings have some advantages over single layers as they combine the properties of several materials and show some new properties. Multilayered (TiN/TiAlN) possesses better physico-chemical properties than single layered TiN or TiAlN hard coatings (HC). Due to its high hardness and brittleness, mechanical micro structuring is difficult, thus the laser beam processing is one of possible solutions. Pulsed laser beams are suitable for local ablation of coatings layer from substrate material. Roughness and thickness of HC are commonly measured by a profilometer. Data obtained with diamond tip give real 2D surface profile. A 3D topography of the surface can be obtained with this procedure, too. In this work we compared effects of focused TEA CO<sub>2</sub> (ns regime) and Nd: YAG (ps regime) lasers ablation of TiN/TiAlN coatings. The TiN/TiAlN (2.7 microns thick; consisted of 45 layers) was deposited on the hot work tool steel. The results of profilometer analysis using Taylor\_Hobson Talysurf 2 profilometer, of laser-ablated area are presented. Profilometer analysis describes effects of laser ablation well and it would be supplement to the results obtained by microscopy analysis

W.S.-S.BC.4

**TEM STUDY OF TiAlN/CrN NANOLAYER COATINGS**

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TiAlN/CrN nanolayer coatings with ~25 nm thick layers were prepared by unbalanced magnetron sputtering. Transmission electron microscope (TEM) was used to study microstructure, crystal structure, interfaces and chemical composition of the coating. Conventional TEM studies revealed columnar microstructure. X-ray diffraction and selected area electron diffraction showed NaCl-type crystal structure of TiAlN and CrN layers. Epitaxial growth inside columnar grains was observed with high resolution TEM. Boundaries between the grains were low-angle and high-angle. Between certain grains voids were also present. Chemical composition of layers performed by energy-dispersive X-ray spectroscopy showed well separated layers with no substantial intermixing.

W.S.-S.BC.5

### SYNTHESIS AND MAGNETIC PROPERTIES OF Fe<sub>2</sub>O<sub>3</sub> NANOPARTICLES IN A SILICA MATRIX

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Fe<sub>2</sub>O<sub>3</sub> nanoparticles in a silica matrix with different concentrations of iron-oxide in the 10-45 wt.% range were synthesized by the sol-gel method. Transmission electron microscopy studies showed that the average particle sizes were about 4-20 nm with a narrow size distributions. Depending on the Fe<sub>2</sub>O<sub>3</sub> concentration and temperature treatments different iron oxide polymorphs were obtained showing a variety of magnetic characteristics. Investigation of the magnetic properties by DC magnetization and AC susceptibility measurements indicated behavior typical of a superparamagnetic system, such as the existence and frequency dependence of a blocking temperature, irreversibility of the zero-field-cooled (ZFC) and field-cooled (FC) curves, and emergence of magnetic hysteresis below the blocking temperature. Quantitative analysis of the DC magnetic data indicated that the system consisted of an assembly of superparamagnetic nanoparticles with a narrow size distribution, while the AC data, depending on iron oxide concentrations, implied the existence or absence of inter-particle interactions.

W.S.-S.BC.6

### SOL-GEL PRODUCED THIN FILMS FOR PHOTOCATALYSIS

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Titanium dioxide has become the material of choice for photocatalytic and hydrophilic self-cleaning surfaces. Transparent TiO<sub>2</sub>-anatase films, pure or containing low concentrations of other elements (Si, Zr, Ag, Fe), were produced by two different sol-gel processing routes on soda-lime glass supports: (i) dip coating from alcoholic sols containing surfactants and followed by heat treatment at 500°C; (ii) dip coating from aqueous sols after extended refluxing treatment and followed by heating at considerably lower temperatures, which brings certain advantages from the application point of view. In both cases the starting precursor was titanium isopropoxide and the final coatings consisted of a dominant anatase crystalline phase. The as-prepared films were characterized by standard microscopic and spectroscopic characterization techniques, showing their nanostructural features. They are correlated with their self-cleaning performance and photocatalytic activity in various tailor-made systems and photoreactors.



W.S-S.BC.7

**ON THE PREPARATION OF METAL-ORGANIC FRAMEWORKS (MOF) AS  
POTENTIAL MATERIALS FOR HYDROGEN STORAGE**

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Hydrogen adsorption on porous materials is a method of hydrogen storage. Materials based on metal-organic frameworks (MOF) are now considered as suitable materials for the storage. MOF are crystalline solids having cavities of uniform size and large internal surface. They are built by connection of rigid rod-like organic moieties with inorganic clusters that act as joints. The resulting void spaces are defined by the length and functionalities of the organic units. Tailoring of the MOF's properties depends on the appropriate choice of starting materials. This presentation expounds the use of oxalate, malonate and benzene-1,4-dicarboxylate ions for bridging and/or chelation of metal cations to produce rigid, geometrically defined clusters.

*PL.S.III.1*

**NANOSTRUCTURED MATERIALS FOR INTERMEDIATE TEMPERATURE SOLID OXIDE FUEL CELLS (IT-SOFCs)**

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Environmental problems lead to the need for new technologies for sustainable energy production and storage, to reduce pollutant emissions from fossil fuel combustion and to increase energy safety. Solid oxide fuel cells (SOFCs) are promising as electrochemical power sources: the technology is proven, but costs are too high for general use. The major trend in the present research activities on SOFCs is the reduction of operation temperature to reduce costs and improve lifetime. This can be achieved either by reducing the thickness of the YSZ electrolyte to reduce ohmic drop, or by using alternative electrolytes such as ceria, lanthanum gallate, or bismuth oxide. The main drawback of reducing operation temperature is the increase in polarization drops at the electrode/electrolyte interfaces. An increase in the triple phase boundary (TPB) at these interfaces can improve the electrode performance. Operating SOFCs at temperatures below 700°C allows the use of stable nanocrystalline oxides as electrode (both anode and cathode) materials to extend the TPB length. This talk will summarize examples of recent works on the study of electrolyte (ceria), cathode (pyrochlore and perovskite oxides), and anode materials (Ni-YSZ cermets), performed in the lab of the author, in which the electrochemical properties are affected by the reduction of grain size at the nanometer level.

*PL.S.III.2*

**TRANSPORT PROPERTIES OF NANOSTRUCTURED ANTIMONY-DOPED TIN OXIDE FILMS**

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Transparent conductive oxides (TCOs) have been extensively studied due to their important technological applications, such as electrochromatic displays, solar cells, and other optoelectronic devices. In this work it is described the preparation of antimony doped tin oxide thin films with thickness of 40 to 988 nm by using chemical solutions. Two main routes were used to prepare these films, one based on aqueous colloidal suspensions of 3-5 nm crystalline oxides and other based on polymeric precursor solutions both deposited on amorphous silica substrates by spin coating. Concentrations of antimony ranging from 0 to 18mol% were used in this study. Morphological characterization revealed films with round-shaped grains, nanometric size and low roughness. These films display high transmittance (~ 80%) in the visible range of transmittance spectra, which is desirable for transparent conductive oxide films. Semiconductor behavior was observed in all studied films, but the transport mechanism showed to be strongly thickness dependent making difficult to a proper adjust to well-known models. In thicker films the mechanism was revealed as an intermediary system, with thermal activated and hopping contributions, depending on the measuring temperature.

PL.S.III.3

**NO<sub>x</sub> ABATEMENT OVER SUPPORTED BINARY OXIDE CATALYSTS CONTAINING  
CuO COUPLED WITH Ga<sub>2</sub>O<sub>3</sub> AND SnO<sub>2</sub>**

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Emissions of nitrogen oxides (NO<sub>x</sub>) discharged into the atmosphere from the burning of fossil fuels have significant adverse effects on human health and the environment, contributing substantially to the formation of acid rain, and ground level ozone. Substantial NO<sub>x</sub> reductions from current levels are necessary to address these problems.

Encouraged from the promising results obtained using highly dispersed CuO phases over modified silica supports as catalysts in different reaction paths for the NO<sub>x</sub> abatement, in this work we report on the preparation, characterization and catalytic activity of Cu/Ga and Cu/Sn binary oxides deposited over a silica-alumina support with high surface area and acidity. In particular, different reaction paths for the NO<sub>x</sub> abatement are reported, as the direct decomposition of N<sub>2</sub>O, and the SCR of NO, and N<sub>2</sub>O by C<sub>2</sub>H<sub>4</sub>, and CH<sub>4</sub>. Emphasis will be put on the original mode of preparation by sol-gel for the supports and adsorption for the simple and binary supported oxide catalysts.

Catalytic systems containing the same number of total metal atoms ( $6 \cdot 10^{20}$  atom $\cdot$ g<sup>-1</sup>) distributed in different proportions on a silica-alumina support (Cu:Me=1:0.25, 1:0.50, 1:0.75 with Me = Sn or Ga) were prepared by a successive adsorption method starting from molecular precursors.

The catalytic tests were performed in a laboratory continuous reaction line equipped with a quartz tubular microreactor working at variable contact time ( $\tau = 0.2 - 0.5$  s) and temperatures ( $T = 250 - 650^\circ\text{C}$ ).

Amorphous high surface area materials ( $350 - 500$  m<sup>2</sup> $\cdot$ g<sup>-1</sup>) with well-dispersed oxide phase (around 5 nm) were obtained, as shown by the XRD, N<sub>2</sub>-BET, TEM and SEM analyses. The addition of the second metal oxide phase of gallium or tin to that of copper gave rise to remarkable differences in the catalytic activity. Both the binary oxide catalysts showed higher activity in the C<sub>2</sub>H<sub>4</sub>-SCR of NO than the CuO containing catalyst, with 10 % higher NO conversions. The CuO phase was the most active when N<sub>2</sub>O reactivity was concerned, while the presence of Ga<sub>2</sub>O<sub>3</sub> enhanced the reducing properties of the copper oxide phase.

The resistance towards water was enhanced in the catalyst associating CuO with SnO<sub>2</sub>: once restored the dry feed after exposure to humid reactants the Cu/Sn binary catalysts rapidly recovered their activity, while the catalysts of the Cu/Ga series showed a decreased conversion of more than 10 %.

The surface and catalytic properties of dispersed copper oxide were influenced by addition of a second metal oxide. It is possible to tune the spectrum of activity of copper oxide centers by addition of a second component that can impart specific catalytic behaviors.

PL.S.III.4

## ELECTRICAL RELAXATIONS DUE TO ELECTRONS IN OXIDES

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The electrical response of a material is due to charge density fluctuations, when it is submitted to a time-dependent electric field. These fluctuations are either expressed by the frequency-dependent complex permittivity  $\epsilon$ , conductivity  $\sigma$  or resistivity  $\rho$ . They are generally described by relaxations up to millimeter waves. The time scale (or relaxation time) of the fluctuations depends on the scale at which they occur. In electronic conductors, the electrical relaxations are generally depending on their crystal structure, microstructure and nanostructure.

At the interatomic scale, the dielectric relaxations are due to small-polaron hopping in transition-metal oxides ( $V_2O_5$ ,  $LiNiO_2$ ,  $Li_xV_2O_5$ , etc.). In this case, the dielectric relaxation time corresponds to the hopping time of the charge and is thermally activated.

However, the study of electrical transport properties becomes more difficult when the materials are under form of powders or thin films. The conductivity measurements by usual dc or low frequency techniques cannot give any information on their transport properties owing to the existence of nano- and microstructures inside the materials. In this way, the presence of grain aggregates and grain boundaries can influe on the electronic mobility. Particle size effect has been evidenced, giving rise to stronger electron localisation on the nanometric particles (for exemple  $WO_3 \cdot H_2O$  powder). Moreover, during the insertion of lithium ions in oxide nanoparticles, a lithium segregation occurs on their surface giving rise to surface conductivity.

We showed that the electrical (resistivity, conductivity and permittivity) spectra are only interpreted providing that the electronic properties, the nano- and microstructures are first known.

PL.S.III.5

**SURFACE REACTIVITY OF METAL OXIDES: SORPTION AND ADHESION  
PROCESSES**

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The surface reactivity of metal oxides particles plays a role in several processes, as the sol-gel synthesis of materials for example, since it controls the stability and the coagulation of suspensions and the growth of particles. The surface reactivity of particles or oxide layer is also a major concern in problems of fouling of industrial plants. In this talk, we will report on our recent results about reactivity of the metallic oxides particles: the sorption of inorganic ions, as sulfate or nitrate, on iron, aluminum and titanium oxide, and the adhesion on massive metal substrates. To understand and quantify the common theoretical basis of these processes, as surface charge, acido-basicity, or electrostatic double-layer structure, we have developed several experimental setups. To record *in situ* spectra of species at the solid/solution interface, attenuated total reflectance – IR spectroscopy is used with a home-made circulation cell. The adhesion properties of metallic substrates towards particles have been determined with a method based on the turbidimetric measurement of the adhesion rate. Thus, we have studied the surface charge of several metals (stainless steel, aluminum,...) and the effect of the surface treatment on their adhesion properties. Finally, the fouling phenomenon in industrial plants is also controlled by hydrodynamics, so we have built a circulation setup to study the deposition of particles in a turbulent flow. The experimental results have been compared with predictions from a computer code taking into account both hydrodynamical and chemical phenomena.

*PL.S.IV.1*

**THE FIRST INORGANIC NAOBUDS AND PEA-PODS: WS<sub>2</sub> AND MoS<sub>2</sub>  
FULLERENES GROWN BY DIFFUSION PROCESS**

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The W<sub>5</sub>O<sub>14</sub> nanowires, which were reported as homogeneous phase only in 1978 by McColm et al., and in meantime declared as the compound, which may hardly exist, have been synthesized by chemical transport reaction and used as precursors for synthesis the WS<sub>2</sub> nanotubes by sulphurization in the mixture of 1% H<sub>2</sub>, 1% H<sub>2</sub>S in argon. The produced nanotubes are mainly closed and of very regular structure. Their diameter is much smaller than the wideness of precursor nanowires revealing a splitting of the precursors, while the length up to several hundreds microns frequently matches the length of the W<sub>5</sub>O<sub>14</sub> nanowires. Beside nanotubes, the WS<sub>2</sub> fullerenes grow simultaneously. This is the first evidence that the WS<sub>2</sub> fullerenes can grow by diffusion process without spherical precursors. The details of the transformation process will be presented revealing the importance of hexagonal 2Hb stacking. The fullerenes grown on the surface of the nanotubes represent the first case of WS<sub>2</sub> nanobuds, while in the isomorphous MoS<sub>2</sub> system we found the first quasi pea-pods. Results of transmission electron microscopy and diffraction will be combined with ultra high vacuum atomic force microscopy and scanning tunnelling microscopy observations.

*PL.S.IV.2*

**PROCESSING AND CHARACTERIZATION OF MAGNETIC NANOSTRUCTURED  
MATERIALS**

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The microstructure of magnetron sputtered magnetic thin films used for data storage is sensitive to processing conditions such as substrate temperature and sputter bias. Grain size distribution, crystallographic texture, defect density, and composition inhomogeneities all strongly influence the magnetic properties and resulting areal data density. Typical CoPtCr magnetic recording alloys utilize a non-magnetic grain boundary layer in order to break the magnetic exchange between grains. Traditional longitudinal magnetic recording media employ a Cr seedlayer to produce an in-plane easy-axis of magnetization [0001] of the hexagonal Co grains and rely on Cr grain boundary segregation for magnetic isolation between grains. Recent perpendicular magnetic recording media are processed using reactive sputtering to form intergranular oxide layers between the granular CoCrPt grains grown with their c-axis normal to the thin film plane. Understanding the relationship between the microstructure and magnetic recording properties requires characterization with nanoscale resolution. High resolution imaging in the transmission electron microscope (TEM) is combined with analytical methods, such as energy-filtered transmission electron microscopy (EFTEM) and energy dispersive x-ray + electron energy loss spectrum imaging using a field-emission gun scanning TEM, to develop these structure-property relationships.

PL.S.IV.3

**SYNTHESIS AND PROPERTIES OF METAL-CARBON NANOCOMPOSITES.  
SOME PERSPECTIVE APPLICATIONS IN CATALYSTS CHEMISTRY AND  
MEDICINE (PHOTO-THERMAL THERAPY OF TUMORS)**

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The investigation of metal carbon-encapsulated nanoparticles has attracted attention due to technological potential applications in medicine and as catalyst materials for protection of environment. The very important factor of such nanocomposites is that the carbon-coated nanoparticles could be protected from the environmental degradation.

However, up to now the investigations of carbon-encapsulated metal nanoparticles have mainly devoted to the preparation method and characterization of nanocomposites. Practically we have very little known about their real applications.

In the talk the novel preparation method and several perspective encouraging results concerning the selective catalytic activity in hydrogenation and hydrodechlorination have been presented. Besides, the phototherapeutic application (hyperthermia) of the light activated nanoparticles on the base of the relatively stable carbon-encapsulated metal nanoparticles (Ni@C) for treating tumors, have been demonstrated.

1. The nanocomposites (Me@C) on the base of different metals ((Me-Ni, Fe, Co, Al, Bi, Ag, Mg, Pd, Cu and others) which are encapsulated (@) in carbon matrix C were synthesized by novel method. It was shown that in dependence from the synthesis regimes and type of metal the structural state of carbon and quality of coating is varied. The thickness of carbon coating is equal about few nanometers depending on type of metal while the carbon structure is an amorphous ("glassy") carbon (C<sub>m</sub>) for all metals. The average particle size of metals encapsulated in carbon matrix is changing in the range of few nanometers up to tens nanometers with narrow size distribution.

2. Investigation of catalytic activity of the nickel-carbon nanocomposites Ni@C<sub>am</sub> was performed as a hydrogenation and hydrodechlorination catalyst. The abnormal highest catalytic activity of carbon-encapsulated nickel catalyst in hydrogenation reaction at ball-milling of Mg in hydrogen atmosphere was revealed. The rate of hydrogenation reaction using Ni@C<sub>am</sub> catalyst was much more faster in comparison with the best well-known catalyst on the base of V<sub>2</sub>O<sub>5</sub>. In the gas reductive transformations (at 50 - 300°C) of chlorobenzene to benzene or cyclohexane in H<sub>2</sub> using nanosized Ni and Pd particles encapsulated in carbon matrix was shown that these catalysts were very selective in benzene or cyclohexane formation respectively.

3. Laser photothermolysis is a new promising therapeutic method of tumors treatment. In that case the light absorbing nanoparticles on the base of Ni@C nanoparticles are used instead of photosensitizers (molecular dyes). During the time when sufficient nanoparticles accumulation in tumor is attained the tumor spot is activated by pulsed laser. In the result of the addressed laser beam interaction with nanoparticle the high temperature in nanoparticle goes up to several hundreds Celsius degree. In the nearest vicinity of nanoparticle the tumor is destroyed due to overheating.

PL.S.IV.4

**Fe<sub>3</sub>O<sub>4</sub> NANOPARTICLES FOR BIOMEDICAL APPLICATIONS:  
THE ROLE OF THE SURFACTANT**

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Magnetic nanoparticles [1] have attracted much research over the recent years due to their potential interest in a variety of biomedical applications [2]. Uniform magnetite Fe<sub>3</sub>O<sub>4</sub> nanoparticles of 6, 10 and 17 nm in diameter were synthesised by thermal decomposition at high temperature of an iron organic precursor in an organic medium [3]. Oleic acid was used as surfactant in all cases and the organic solvent was chosen in each case so as to maximise size and shape uniformity. The particles, as revealed by transmission electron microscopy, are very uniform in size, with polydispersion below 20%, and x-ray patterns show that they consist of highly crystalline particles with an inverse spinel structure and lattice parameters similar to those of magnetite. Surprisingly enough, for all samples studied, saturation magnetization  $M_s \approx 82$  emu/g almost reaches the expected value for bulk magnetite at low temperature, in contrast to results in small particle systems for which  $M_s$  is usually much smaller due to surface spin disorder (for example,  $M_s \approx 50$  emu/g for 4 nm particles in [4]). The coercive field for the 6 nm particles is also in close agreement with that of bulk magnetite (175-210 Oe). Both results suggest that the oleic acid molecules covalently bonded to the nanoparticle surface yield a strong reduction in the surface spin disorder, such that the new O<sup>2-</sup> surface ligands partially reconstruct the crystal field of the surface Fe cations, as suggested by x-ray photoelectron spectroscopy in the Fe 2p, 3p and 3s, and O 1s core levels. These findings may be of relevance in biomedical applications since they may reduce the strength of the magnetic field required to obtain a high value of the magnetisation and they open the question of whether  $M_s$  above the bulk value may be obtained by taking advantage of the orbital contribution to the magnetic moment, for example, due to the interplay of the surface cations in the particles and the ligands in the surfactant. XMCD, Mossbauer and time-dependent thermo-remanent experiments are currently in progress in order to ascertain the nature of the magnetic moments in the particles.

The funding from the Spanish MEC through the projects NAN2004-08805-CO4-02, NAN2004-08805-CO4-01, CONSOLIDER CSD2006-12 and MAT2006-03999, and from the Catalan DURSI (2005SGR00969) is acknowledged.

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*PL.S.IV.5*

### **3-D SCAFFOLDS FOR 3-D TISSUE ENGINEERING**

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Tissue engineering and tissue regeneration are both exciting and rapidly expanding fields that are making an impact on the healthcare sector. In general, the tissue engineering approach is to seed a patient's cells on to a sector, apply appropriate signals and stimuli via a bioreactor and then implant the generated tissue. Clearly, the scaffold is key to the whole process.

The scaffolds that are created at Oxford are based on the natural tissues themselves. The aim is now to mimic not only the biofunctionality of the original tissue but also to mimic the structure and biology. We achieve this aim through control of the scaffolds' architecture and biochemical functionality over several length scales.

For example, for the work on bone analogues, we use type 1 collagen and hydroxyapatite – the two major components of bone, organised to mimic natural bone, as our scaffolds. At the molecular level we control the stoichiometry and substitution levels of the hydroxyapatite. At the nanoscale we control the mineral size, shape and crystallographic orientation. At the microstructural level we control the volume fraction and distribution of the hydroxyapatite within the collagen scaffold. At the mesoscale we control the porosity of the collagen and the extent and dimensions of microchannels to aid vascularisation. At the macroscopic level we control the external shape to fit the proposed defect site.

This, in effect, is a platform technology.

Further examples, include work on other aspects of the musculoskeletal system: cartilage (both meniscal and articular) and osteochondral devices. We have further initiated research on applications related to the cardiovascular system (e.g., heart muscle, aortic heart valves, capillary formation)

These studies highlight the importance of fundamental science by materials scientists, working in close collaboration with surgeons, in helping the health care sector and patients.

PL.S.IV.6

## BIOACTIVE PEPTIDE DESIGN USING THE RESONANT RECOGNITION MODEL

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Biological processes in any living organism are based on selective interactions between particular biomolecules, mostly proteins. The rules governing the coding of the protein's biological function, i.e. its ability to selectively interact with other molecules, are still not elucidated. The Resonant Recognition Model (RRM) is one attempt to identify the selectivity of protein interactions within the amino acid sequence. The RRM model interprets protein's linear information using signal analysis methods including spectral and space-frequency analysis. It has been found that the spectrum of the distribution of the energies of free electrons along the proteins is critical for protein's function (interaction). As there is evidence that charge can travel along the protein, then this charge moving through the protein backbone and passing different energy stages caused by different amino acid side groups can produce sufficient conditions for the specific electromagnetic radiation or absorption. These results lead to the conclusion that specificity of protein interactions are based on the resonant electromagnetic energy transfer between interacting molecules with a specific frequency for each observed function/interaction. The estimated range of these processes includes IR, visible and UV light. These computational predictions were confirmed by comparison of: a) Absorption characteristics of light absorbing proteins and their characteristic frequencies, b) Frequency selective light effects on cell growth and characteristic frequencies of growth factors and c) light effects on kinetics of LDH enzymes. All these results lead to the conclusion that the specificity of protein interactions is based on the resonant electromagnetic energy transfer at the frequency specific for each interaction observed. Given the existence of these resonant effects, we consider here the possible interactions of the weak electromagnetic radiation (EMR) in the frequency range of IR, visible and UV with biomolecules particularly proteins. Once the characteristic frequency for a particular protein function/interaction is identified, it is possible then to utilize the RRM approach to predict the amino acids in the sequence, which predominantly contribute to this frequency and thus, to the observed function as well as to design *de novo* peptides having the desired periodicities. As was shown in our previous studies of FGF peptidic antagonists and HIV envelope agonists, such *de novo* designed peptides express the desired biological function. The RRM is based on the finding that proteins with the same biological function or interactive activity do have the same periodic components in the distribution of delocalised electron energies along the protein molecule. Mathematical and physical background of the RRM model will be discussed. A number of examples of bioactive peptide design and active site predictions will be presented as well.

*O.S.C.1*

**ATOMIC RESOLUTION HAADF-STEM: APPLICATIONS IN MATERIALS SCIENCE**

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Atomic resolution high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM), known also as Z-contrast imaging, has become a promising technique to assess chemical information on the atomic scale. The HAADF-STEM images are recorded in a FEG (S)TEM with an annular detector at large inner angles. In this way the contribution of Bragg reflections is minimized and incoherent thermal diffuse scattering (TDS) becomes the prevailing contribution to the image intensity. Such incoherent STEM images are almost insensitive to defocus and/or thickness change, contrary to the HRTEM images, and the atom columns always appear as white dots. Since intensity of TDS is related to the average atomic number  $Z$  of the atomic columns, qualitative interpretation of HAADF-STEM images is relatively straightforward. Namely, the atom columns with higher average atomic number exhibit higher intensity. On the other hand, quantitative interpretation of the observed atom columns intensities, i.e. determination of chemical composition of individual atom columns based on their intensity, is much more complicated and requires image simulations and image matching. Recently it was shown that quantitative interpretation is additionally complicated due to changes in atom columns intensities arising from local distortions of crystal lattice in case of solid solution and/or interfaces. In order to perform correct quantitative interpretation of HAADF-STEM images, the exact structure (atom positions) of investigated structural phenomena should be known. In our presentation an overview on qualitative and quantitative HAADF-STEM technique will be given and illustrated by examples of characterization of various inorganic materials.

O.S.C.2

## NANOCATALYST ENGINEERING ON EXTENDED AND NANOSCALE SURFACES

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In this report we investigate extended polycrystalline PtM alloys ( $M=Ni, Co, Fe, V, Ti, Re$ ) as well as  $Pt_3Ni(hkl)$  and  $Pt(hkl)$  single crystalline surfaces for various catalytic reaction. All surfaces were prepared in ultra-high vacuum by sputtering/ annealing cycles, and well characterized before transfer into liquid environment. PtM alloy surfaces were characterized in UHV: by AES, LEIS and UPS. We observed enhanced catalytic properties induced by the second metal, which may occur through several effects: (1) *Electronic effect*, due to changes in the metallic d-band center position vs. Fermi level; and (2) *Structural effect*, which refers correlation between surface atom arrangements, and/or corrosion-induced dissolution – surface roughening.

We have found that for each alloy it was possible to form surfaces with two different compositions. Due to surface segregation, annealed alloy surfaces form the outermost *Pt-skin* surface layer, which consists only platinum atoms, while the sputtered surfaces have the bulk ratio of alloying components. Post-electrochemical UHV surface characterizations revealed that Pt-skin surfaces are stable after immersion to an electrolyte, while sputtered surfaces formed Pt-skeleton outermost layers due to dissolution of transition metal atoms. Therefore, three different near-surface compositions (Pt-skin, Pt-skeleton and polycrystalline Pt) all having pure-Pt outermost layers are found to have different electronic structures, which originates from different arrangement of subsurface atoms of the alloying component. Modification in Pt electronic properties alters adsorption/catalytic properties of corresponding bimetallic alloy. -For instance, the most active systems for the electrochemical oxygen reduction reaction (ORR) are established to be the Pt-skin near-surface formation. The very same levels of catalytic enhancement have been established between extended surfaces and corresponding cubooctahedron nanoparticles. In addition to the d-band center position, we have found how catalytic activity is affected by the arrangement of surface atoms. Results for  $Pt_3Ni(hkl)$  single crystal alloys showed that the  $Pt_3Ni(111)$ -skin surface has a superior catalytic activity for the ORR. In particular *the rate of the ORR on the Pt-skin-Ni(111) electrode is increased 15 times (!!!) relative to a polycrystalline Pt surface (the highest that has ever been observed for the ORR)*. In order to engineer catalysts with the physicochemical properties that are similar with the  $Pt_3Ni(111)$ -skin surface we have found from Monte-Carlo simulation that nanoparticle with *octahedral* shape, which consists 8 (111) facets, 12(111)-(111) step-edges and 6 vertices, was predicted to be thermodynamically stable.

Therefore, the ultimate goal in the catalysts engineering would be to *tune the electronic and structural properties of nanoparticles* in order to achieve superior catalytic enhancement of the  $Pt_3Ni(111)$ -skin surface.

O.S.C.3

**PREPARATION OF AMINE-FREE SILICA-COATED AgI NANOPARTICLES  
WITH A MODIFIED STÖBER METHOD**

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In recent years, we studied on fabrication of silica-coated AgI nanoparticles with a Stöber method toward new X-ray contrast agents. In the Stöber method, amines are often used as catalysts for silica-formation, so that it is probable that amine is left in the silica-coated particles. Since amines are harmful to the human body, amine-free particles are desired for medical use. From this viewpoint, amine-free silica-coated AgI nanoparticles were prepared with a modified Stöber method using NaOH as catalyst instead of amine in a present work. The AgI nanoparticles were prepared from AgClO<sub>4</sub> and KI with the use of 3-mercaptopropyltrimethoxysilane as a silane coupling agent and NaOH catalyst for alkoxide hydrolysis. The silica-coating was performed at  $4.5 \times 10^{-6}$ - $4.5 \times 10^{-5}$  M MPS, 11-20 M water, 0.002-0.1 M NaOH and 0.005-0.04 M tetraethylorthosilicate at AgI concentrations of 0.1-1 mM. Consequently, AgI-silica core-shell particles as small as ca. 30 nm could be prepared with the use of  $4.5 \times 10^{-5}$  M MPS, 20 M water, 0.0011 M NaOH, 0.001 M AgI and 0.04 M TEOS. This successful fabrication of particles is expected to open an opportunity for a further study on their properties of X-ray contrasting.

O.S.C.4

### CHARACTERIZATION OF NANOPARTICLES BY FLUORESCENCE CORRELATION SPECTROSCOPY

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Fluorescence correlation spectroscopy (FCS) is an experimental technique based on the monitoring of time fluctuations of fluorescence intensity originating from random, diffusive motions of fluorescent particles both in solutions or on surfaces. Unlike a similar and more widely used photon correlation spectroscopy method, dynamic light scattering, FCS is selective because it is sensitive only to particles bearing a fluorescent label which is excitable with the used light. This feature makes FCS a promising tool for studies of diffusive motions in turbid environments, e.g., biological systems including living cells. In this presentation, we demonstrate how FCS can be used for basic characterization of various nanoparticles such as block copolymer micelles or phospholipid vesicles in solutions.

O.S.C.5

### MULTILAYER POLYMERIC NANOPARTICLES BASED ON SPECIFIC INTERACTIONS IN SOLUTION: LIGHT SCATTERING AND ATOMIC FORCE MICROSCOPY STUDY

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The nanoparticles formed after the addition of poly(2-vinylpyridine), PVP, to block copolymer micelles of polystyrene-*block*-poly(methacrylic acid), PS-PMA, were studied by light scattering, LS, and atomic force microscopy, AFM. Due to the strong hydrogen bonding between PVP and PMA segments, complex structures form in organic media. However, the aggregated structures dissolve in basic buffers and stable soluble nanoparticles reform in aqueous media. The behavior of their solutions was studied in a broad pH range by LS, AFM and capillary zone electrophoresis, CZE. Further, advantages and disadvantages of LS and AFM measurements of kinetically frozen nanoparticles will be discussed in this communication.

O.S.C.6

### POLYURETHANE NETWORKS WITH INORGANIC NANO-BUILDING BLOCKS

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Polyurethane networks containing as additive the stannoxane cluster dication  $[(n\text{BuSn})_{12}\text{O}_{14}(\text{OH})_6]^{2+}$  with two functional groups attached as anions were prepared. The stannoxane building blocks are of interest for several reasons: they can act as mechanical reinforcement via cluster-cluster interaction, they can stabilize chemically the modified polyurethane, and they could influence the catalytic mechanism of the polyurethane reaction. In this contribution, results concerning the mechanical (DMTA) characterization of the stannoxane-modified polyurethanes, their thermal stability (TGA), and the influence of the stannoxane on the polyurethane formation are presented.

Acknowledgement: The authors thank the Ministry of Industry and Trade of the Czech Republic, grant FT-TA3/034 for the financial support of this work.

O.S.C.7

### EPITAXIAL GROWTH BY MONOLAYER RESTRICTED GALVANIC DISPLACEMENT

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In this work we present a "proof-of-concept" study realizing a monolayer-restricted galvanic displacement as a "building block" in the growth of smooth, epitaxial, thin metal films. Electrochemical methods and ex-situ surface characterization techniques (scanning tunneling microscopy, x-ray photoelectron spectroscopy and x-ray diffraction) are employed for studying the growth kinetics of layers. Replacement schedules are optimized with respect to sacrificial layer identity (Tl, Pb or Bi), specific polarization regimes and rate of deposition in order to yield a working protocol for growth of crystallographically well-defined, morphologically flat and inclusion-free silver thin films on gold single crystal substrates.

O.S.C.8

### THIN SEMI-CONDUCTOR FILMS FORMED BY PULSED ION DEPOSITION

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The research results of semi-conductor films of complicated composition of InP and GaAs are presented in the report. The films were applied out of the ablation plasma generated from massive targets of InP and GaAs under the action of series of high-power pulses of nanosecond duration. The number of pulses in the series varied from 20 to 200. The beam parameters at the film deposition were the following: accelerating voltage was 250 kV, current density at the target was 250 A/cm<sup>2</sup>, and pulse duration of the accelerating voltage at the half-height was 80 ns. The films were applied to the substrates made of Silicon (Si <100>), Mylar and Cu at the room temperature. The preservation of stoichiometric composition of deposited films relatively to the initial target was checked by the methods of Rutherford back-scattering and Auger-spectroscopy. The morphology of film surface was determined by the methods of optical and atomic force microscopy. The phase composition of films was investigated by the X-ray phase analysis, low-angled X-ray scattering and transmission electron microscopy. The thickness of film deposited for a pulse was from 2 to 10 nm depending on the target material, target-substrate and target anode distance at the constant ion current density. It was shown that the deposited films have the composition close to the stoichiometric composition of the targets. The InP films are polycrystalline with an average grain size of about 8-10 nm. The GaAs films have as polycrystalline phase with an average grain size of 20 nm so amorphous one.

O.S.C.9

### LASER-INDUCED CHANGE IN THE REFRACTIVE INDEX IN THE ORGANIC SYSTEMS DOPED WITH NANOOBJECTS

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The drastic laser-induced change in the refractive index in the nanoobjects-doped organic  $\pi$ -conjugated electrooptical structures, including liquid crystal ones, has been studied. The increase in the local and total polarizability has been found. The promising way to improve the dynamic properties of the nanostructural materials has been discussed. It has been established that the systems doped with nanoobjects can be considered as a good candidate to apply them in laser and display techniques as well as in the information processing.

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O.S.C.10

**RAMAN SPECTROSCOPY METHOD FOR DETERMINATION OF PARTICLE SIZE DISTRIBUTION IN ANATASE TiO<sub>2</sub> NANOPOWDERS**

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Raman study was performed on titania (TiO<sub>2</sub>) nanopowders in anatase phase synthesized by a laser-induced pyrolysis as well as on commercial nanosized TiO<sub>2</sub> powder with a particle size less than 10 nm. The mean particle sizes (14.4-20.6 nm) estimated from specific surface area of the synthesized powders coincide well with the crystallite sizes (12.3-17.4 nm) determined by XRD measurements. The particle size distribution in TiO<sub>2</sub> nanopowders was estimated from the low frequency Raman spectra, using the fact that the phonon modes in nanosized TiO<sub>2</sub> observed in the low frequency region ( $\omega < 40 \text{ cm}^{-1}$ ) can be well described by the elastic continuum model, assuming that nanoparticles are of perfect spherical shape and isotropic. The nanosized particle distribution obtained by this methodology is used for the calculation of the frequency and shape of the most intensive  $E_g$  Raman mode in anatase TiO<sub>2</sub> by the phonon confinement model. The calculated broadening of this mode, associated with the particle size distribution, coincides well with the characteristics of  $E_g$  mode observed in measured Raman spectra of TiO<sub>2</sub> nanopowders. This confirms the Raman spectroscopy method as a powerful tool for determination of particle size distribution in nanosized materials.

O.S.C.11

**LUMINESCENT PROPERTIES OF EUROPIUM DOPED YTTRIUM AND GADOLINIUM SESQUIOXIDE PREPARED USING POLYETHYLENE GLYCOL ASSISTED COMBUSTION METHOD**

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Phosphors based on Eu<sup>3+</sup> doped rare-earth (RE) sesquioxides such as yttrium and gadolinium are important materials with many applications in different fields. In particular, Eu<sup>3+</sup> doped Y<sub>2</sub>O<sub>3</sub> and Gd<sub>2</sub>O<sub>3</sub> are well-known luminescent material widely used to provide red light emission for modern optoelectronic devices. In present work we prepared these materials in nanocrystalline form using polyethylene glycol (PEG) assisted combustion method. We investigated influence of different particles morphology and size, achieved by variation of PEG molecular weight and concentration, on luminescence emission of Eu<sup>3+</sup> ions embedded in nanoparticles. In particular, we analyzed  $^5D_0 \rightarrow ^7F_1$  spin forbidden f-f transitions and emission kinetics. Also, we analyzed the asymmetry ratio of the integrated intensity of the  $^5D_0 \rightarrow ^7F_2$  and  $^5D_0 \rightarrow ^7F_1$  transitions to find asymmetry of the coordination environment around the Eu<sup>3+</sup> ion. For the same purpose we measured the splitting of Stark components of the  $^7F_1$  manifold induced by crystal field.

O.S.C.12

**SYNTHESIS AND CHARACTERIZATION OF HIGH-QUALITY ORGANIC BASED  
MAGNETIC FLUIDS**

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Magnetic fluids or ferrofluids represent colloidal suspensions of monodispersed superparamagnetic nanoparticles with a mean particle size of around 10 nm, coated with a thin layer of dispersive agent (carboxylic acids, silica, etc.) and dispersed in a variety of carrier liquids, water or organics. Ferrofluids have become a subject of a great interest of recent years due to their high specific magnetization and long-term stability, which make them useful in a wide range of technological and biomedical applications. The objective of the present work was the preparation and characterization of ferrofluids based on ferrite nanoparticles that were prepared in a two step procedure. In the first step, the particles were coprecipitated by alkalinizing mixtures of Fe(II) and Fe(III) at elevated temperature. In order to prevent the aggregation of the synthesized material in the next step, the particle surface was covered with a thin layer of carboxylic acid as a dispersive agent and finally dispersed in an organic medium to obtain high-quality organic based ferrofluid of a long-term stability.

O.S.C.13

## HIGH PRESSURE SINTERING OF NANOCRYSTALLINE TITANIUM CARBONITRIDE

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Recently the interest in nanocrystalline materials based on high-melting point compounds has increased. It is hope that new materials with higher physical and mechanical properties in comparison with the microcrystalline ones can be obtained. Conventional regimes in sintering and hot pressing are not suitable for their production due to intense recrystallization. Nowadays high-energy methods of consolidation of nano-particulate materials are the most promising ones. High pressure sintering is one of such methods. It allows to keep the nanostructure of initial powder and to obtain sintered highly dense material with small grain size.

Titanium carbonitride Ti(CN) constitutes high interest as component of hard alloys. Carbon and nitrogen atoms can replace each other in its crystalline lattice, forming unlimited TiC-TiN solid solutions. At that its physical and mechanical properties depend on nitrogen and carbon ratio. It has higher hardness in the field of TiC rich compositions on the Ti-C-N diagram in comparison with pure TiC and TiN. Previously the possibility to increase physical and mechanical properties of titanium nitride at the expense of its nanocrystalline structure created at high pressure sintering has been demonstrated. The properties of nanocrystalline titanium carbonitride did not studied yet. The goal of present work is obtaining of compact samples by high pressure sintering Ti(CN) nanopowder and investigation of its physical and mechanical properties.

Ti(CN) nanopowder with surface area of 24.7 m<sup>2</sup>/g prepared by method of plasmochemical synthesis in Joint-stock Neomat Co (Latvia) was used as initial. The compaction of TiCN nanopowder at pressures from 0.5 to 4 GPa at room temperature is investigated. The evolution of structure, phase composition, density, hardness and fracture toughness of Ti(CN) depending on sintering temperature up to 1800 °C and pressure up to 4 GPa is studied. The dense material based on titanium carbonitride with hardness of 23 GPa and fracture toughness of 4.1 MPa·m<sup>1/2</sup> is obtained. The peculiarities of the consolidation and physical and mechanical properties of nanocrystalline titanium carbonitride in comparison with ones of materials fabricated by other methods of sintering are discussed.

O.S.C.14

**Fe-C BULK NANOCOMPOSITES PREPARED BY MECHANICAL ALLOYING AND  
MAGNETIC PULSE COMPACTION**

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X-ray diffraction, atomic force microscopy (AFM), density, microhardness and coercivity measurements have been used to study iron-cementite bulk nanocomposites prepared by magnetic-pulse compaction (MPC) of the mechanically alloyed (MA) powders with total carbon content from 5 to 25 at.%. MA was performed by milling elementary Fe and C mixtures (Fe+C) and Fe powder in the heptane plus vinyltriethoxysilane solution (H+VTES). The resulting samples were discs of 15 mm in diameter and 1-2 mm of thickness, with the best results obtained at compression temperature 500°C and pressure in pulse 3 GPa. The ratio of  $\alpha$ -Fe and Fe<sub>3</sub>C phases in (Fe+C) samples was in fair correspondence with the total C content at MA. The grain size in all phases was 40-50 nm. The sample density ( $\rho$ ) decreased monotonously from 7.4 g/cm<sup>3</sup> (95% of X-ray density) for the sample with 5 at.% C to 6.3 g/cm<sup>3</sup> (82% of X-ray density) for the sample with 25 at.% C. The dependence of microhardness H versus C concentration is a curve with the maximum H~9 GPa at 15 at.% ( $\rho = 6.8$  g/cm<sup>3</sup>). The amount of cementite in (H+VTES) samples was ~ 40 wt.%, i.e. corresponded to the total C content in 10-15 at.%. Along with  $\alpha$ -Fe and Fe<sub>3</sub>C a small amount (~ 1 weight %) of Fe<sub>2</sub>SiO<sub>4</sub> phase was detected. It is possible that its presence resulted in the reinforced internal morphology of the cementite and, respectively, unexpectedly high characteristics of the MPC sample:  $\rho = 7.3$  g/cm<sup>3</sup>, H = 13–14 GPa. The work has been done under financial support of the project of the RAS Presidium based on the section "Fundamental problems of physics and chemistry of nanosized systems and nanomaterials", and a joint project of UrB RAS – SO RAS "Mechanocomposites-precursors for the creation of materials with new characteristics".

O.S.E.1

**POTENTIALITIES OF MAGNETOLIPOSOMES AS INTRACELLULAR  
THERANOSTICS**

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Magnetoliposomes (MLs) consist of nanometre-sized magnetite cores, wrapped by a bilayer of phospholipid molecules. In the past we showed that these nanocolloids can be exploited as powerful biocompatible T<sub>2</sub>\* MRI contrast agents. In the present work we report on the partitioning of the amphiphilic drug, (*R/S*)- propranolol, within the lipidic envelope of MLs. It is found that the amount of sorbed molecules can be fine-tuned by changing the phospholipid composition of the ML coat. Furthermore, it is also shown that MLs are easily internalised by 3T3 fibroblasts, used as a representative cell model. Overall, the results prove that drug-loaded MLs have great potential as unique intracellular *theranostics*, i.e. as a nanoscale delivery systems with combinatory *therapeutic-diagnostic* imaging modalities.

O.S.E.2

**CHEMICAL AND PHYSICAL CHARACTERIZATION OF REGULAR AND ULTRA THIN CHITOSAN FILMS STORED AT VARIOUS TEMPERATURES**

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The second most abundant polysaccharide on earth - chitin is similar to cellulose with the only difference on C2 having acetylated amino group instead of hydroxyl group. Like cellulose, which is the structural polysaccharide in plants, chitin is the structural polymer in arthropod exoskeleton and fungal cell walls. Although chitin is insoluble in common solvents and, thus, has no practical applications, its simple deacetylation yields chitosan, a polycationic polysaccharide with many functional properties. Due to its antimicrobial, protein-, lipid- and metal binding properties, and the fact that it is biodegradable and easily hydrolyzed by lysozyme, chitosan finds many applications in medicine - in bandages and wounds coverings, in pharmacy - as a dietary supplement for weight reduction, in food industry - as an edible packaging material, and thickening and/or antimicrobial agent, etc. The overall goal of our research was to develop and fully characterize chitosan films that can be used as wound covers and/or packaging material in pharmaceutical and food industry. The films were produced from pure chitosan or from a mixture of various ratios of chitosan and polyethylene oxide (PEO) by solution casting or by spin coating. The thickness of the cast films were 0,03 to 0,15 mm, while spun films were 50 to 300 nm thick. Ultra-thin films were prepared using spin-casting method. Surface composition and morphology of films were characterized by XPS, SEM, AFM, and XRD. The physical and mechanical properties of the films were evaluated by measuring water solubility, water vapor permeability, puncture strength, tensile strength and elasticity. Potential development of films crystallization was monitored by polarized microscope, and film uniformity was assessed by ATR-FTIR. Antibacterial properties were tested against *Escherichia coli*, and metal binding capacity with Cr(VI). Furthermore, the effects of acid used for film preparation and the storage conditions and age of films on the crystallinity development and chemical stability of the films were evaluated. Our results showed development of crystallinity in the films kept at higher humidity for long duration as opposed to fresh films where the crystallinity was absent. Glass-rubber transition of fresh acetic-acid-films occurred at 165°C and decreased to 65°C after 1 year storage at 50% RH while T<sub>g</sub> of fresh chitosan-lactic-acid-films was at 155°C and decreases to 120°C after aging. Generally, storage modulus of the films slightly increased with aging, but the values for acetic-acid-films were about 10 folds higher than values for lactic-acid-films. Interestingly, acetic-acid-films shrunk for about 1% after being heated at ≥100°C regardless on the age of the films, while lactic-acid-films shrunk for 12% when tested fresh, and stretched for 20% when tested after being stored for 1 year. The detail overview of the results will be given in the presentation.

O.S.E.3

**NANOBIOLOGICAL ATOMIC FORCE MICROSCOPY STUDY OF THE  
SPORULATION OF *BACILLUS SUBTILIS***

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Atomic force microscopy can yield valuable information concerning changes in material properties of living organisms. *Bacillus subtilis* is a single celled bacterium commonly found in soil. It can sporulate, i.e. reversibly form a tough and protective endospore that allows the organism to tolerate extreme environmental conditions. *B. subtilis* is not harmful to human health and its robust spores may therefore serve as safe model organisms for pathogenic microorganisms in drinking water. Thus, this organism is used to evaluate water disinfection devices that utilize UV radiation.

By inducing adverse environmental conditions to living *B. subtilis* cells while imaging them with the atomic force microscope, the sporulation procedure was successfully recorded over a time span of about 50 hours. Given this promising result, the recording time of material properties shall be extended to a week, thereby covering the entire sporulation procedure from the vegetative cell to the spore. Two methods of spores production resulting in different types of spores were included in the investigation. One type of *B. subtilis* spores is highly resistant to UV irradiation, whereas the other type shows a low UV resistance. By means of the atomic force microscopy technique differences in the characteristics of the different spores may be elucidated. Detailed scientific understanding of the sporulation of this organism shall provide information regarding the development of novel biomimetic UV resistant materials.

O.S.E.4

**NANOMEDICINE PERFORMED WITH THE  
ATOMIC FORCE MICROSCOPE ON HUMAN RED BLOOD CELLS**

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Atomic force microscopy can yield valuable information concerning basic physical properties as well as alterations of human red blood cells due to environmental factors. Erythropoietin is a hormone that is naturally produced in the kidney to stimulate the growth of red blood cells. Administration of genetically engineered synthetic erythropoietin stimulates the production of even more red blood cells. Therefore erythropoietin is used in doping in serious sports. In this study, differences in the structure and stiffness of red blood cells which are produced body own or with synthetic erythropoietin were investigated for several nanomechanical properties. The samples were prepared via standard methods, and atomic force spectroscopy with trigger forces of three micronewtons was performed in ambient air. The penetration depth does not reveal statistically relevant differences in the two types of red blood cells. Furthermore, cells with a penetration depth four times as large as healthy ones were encountered. In this case, the atomic force microscope served as a nanomedical tool and revealed a rare type of diabetes in the donor of that sample.

O.S.E.5

### SYNTHESIS AND CHARACTERIZATION OF DLPLG NANOPARTICLES FOR CONTROLLED DELIVERY OF WATER-SOLUBLE VITAMINS

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Biodegradable polymers have become the materials of choice for a variety of biomaterials applications. In particular poly (DL-lactide-co-glycolide) (DLPLG) nanoparticles have been studied for controlled released drug delivery. In this paper we are describing new method of obtaining the system for targeted and controlled delivery of the folic acid in the body. Folic acid (pteroyl-L-glutamic acid, vitamin B<sub>9</sub>) is a water-soluble vitamin essential in the human diet. It is an important cofactor in the synthesis of DNA and RNA, of dividing cells, particularly during pregnancy and infancy when there is an increase in cell division and growth. The DLPLG particles were obtained by chemical solvent/non-solvent method with PVP as a surfactant. The obtained DLPLG particles are non-agglomerated, uniform and with particles size in the submicron scale. The folic acid has been encapsulated into the polymer matrix by means of homogenization of the water and organic phases. The concentration of the folic acid in the water has been varied in order to obtain nanoparticles with different ratio of DLPLG and folic acid. The samples were characterized by Infrared Spectroscopy (IR) and Scanning Electron Microscopy (SEM).

O.S.E.6

### GENOTOXICITY OF THE POLY-D,L-LACTIDE MICROPARTICLES ON THE HUMAN LYMPHOCYTES

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Particles generated of biodegradable material are extensively investigated as carriers for sustained drug delivery. Studies have been mainly focused on the monitoring of the drug release and of the rate of the particle degradation. However, the influence of the carrier particles on the human immune cells was only rarely addressed. In this work, the influence of the microparticles made of poly-D,L-lactide (PDLLA) on the function of human lymphocytes in a three-day culture was investigated. PDLLA microparticles have been prepared by a modified precipitation method and human lymphocytes were isolated from the blood of healthy volunteers by a Ficoll – density gradient centrifugation. Lymphocyte proliferation test and the cytochalasin B micronucleus test were used to assess the PDLLA particle effect on the lymphocytes. Results showed that PDLLA particles did not influence on the proliferation of the human lymphocytes. On the other hand, changes in the nuclei form, as well as nucleus buddings were observed. Moreover, the appearance of micronuclei could be detected. All together, these results might imply genotoxicity of the PDLLA particles, or some of the chemicals used for the particle preparation/stabilization on the human lymphocytes.



O.S.E.7

**NONLINEAR EXCITATIONS IN Q1D STRUCTURAL POLYMER TRANSITIONS**

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The experimentally and theoretically established phenomenon of quantum-mechanical resonance in structural polymer transitions, points out the significant role of quantum-mechanical properties of the electronic and nuclear subsystems. The exact quantum-mechanical solutions for polyatomic systems do not exist, but in adiabatic approximation when nuclear and electronic movements are separable, the Schrödinger equation of this complex system can be splitted into successively solved Schrödinger equations for the electrons and nuclei, the later being coupled with the former via parametrically obtained electronic energy vs. chemical coordinates hypersurface. On this quantum-chemical line the problem can be treated even in the non-adiabatic region, when electronic and nuclear movements are entangled. In our paper a possibility of appearance of the soliton-like nonlinear excitations will be examined in Q1D structural transitions of non-saturated hydrocarbon polymers.

O.S.E.8

**PARAMAGNETIC/DIAMAGNETIC DYNAMICS OF BIOMOLECULES-WATER  
COMPLEXES ON NANOTESLA SCALE**

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Water molecule itself is matter with diamagnetic properties. Also, deionized water in bulk fluid state and in solid state (ice) are diamagnetic. However, when water contains ions than under certain conditions dynamics of ions-water clusters formation and disappearing may generate magnetic field fluctuation from weak diamagnetic to weak paramagnetic states. Phenomenon of paramagnetic/diamagnetic dynamics on pico and –nanotesla level occurs during biomolecules (which surfaces are rich with polar amino acids) - water interaction. Experimental results strongly indicate that clusterized water may generate paramagnetic/diamagnetic dynamics on pico and –nanotesla scale. This property of water opens a new possibility for consideration water role in biomolecular conformation change and molecular recognition.

O.S.E.9

**OBTAINING NANO CALCIUM PHOSPHATE/POLY(DL-LACTIDE-CO-GLYCOLIDE) COMPOSITE BIOMATERIAL BY SONOCHEMICAL DEAGGLOMERATION**

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Nanoparticles have several advantages over the microparticles in interactions of the biomaterial with the organism. The response of the organism depends on the interaction of the biomaterial with the surrounding tissue and its adhesion to cells. Besides composition and morphology, the size and size distribution of the composite particles plays a key role in these phenomena.

This paper shows possibilities of synthesizing composite biomaterials calcium phosphate/poly-(dl-lactide-co-glycolide) (CP/DLPLG) formed as nanoparticles (NPs) powders. Each CP nanoparticle was coated with amorphous DLPLG polymer. In dispersion, particles can be deagglomerated by ultrasound treatment.

The size distribution of calcium phosphate coated with poly-(dl-lactide-co-glycolide) (CP/DLPLG) was obtained by dynamic light scattering (DLS). Agglomerate of CP/DLPLG was investigated by atomic force microscopy (AFM) before and after ultrasound treatment.

Results obtained at different time of ultrasound treatment showed a significant influence of ultrasound treatment on deagglomeration of powder CP/DLPLG. Fine particle fractions were found to increase time of ultrasound treatment from 30 to 120 minutes.

O.S.E.10

## SIMILARITIES ANALYSIS ON HYDROXYAPATITE-ZIRCONIA COMPOSITES

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Hydroxyapatite ( $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ ) is one of the implants materials with medical applications due to its higher biocompatibility. The hydroxyapatite found complete utilization after proper preparation of composite. The influence of zirconia ( $\text{ZrO}_2$ ) on the phase composition and on mechanical properties of hydroxyapatite-zirconia composites has been investigated and reported by Rapacz-Kmita et al [1]. Starting with the experimental data reported in [1], hierarchical cluster analysis methods were applied in order to assess the similarities of four different types of composites. Four classes of composites: HAp (hydroxyapatite), HAp-CGz (CGz = Coarse-Grained Zirconia), HAp-FGZ (FGZ = Fine-Grained Zirconia), and HAp-NGZ (NGZ = Needle-Grained Zirconia) cumulating a total number of sixteen experiments were analyzed. A number of nine quantitative variables were included into analysis: sintering temperature ( $^{\circ}\text{C}$ ), Vickers hardness (GPa), bending strength (MPa), characteristic strength (MPa), Weibull modulus, anisotropy (%), Young's modulus (GPa), rigidity modulus (GPa), and Poisson ratio. Data were analyzed with SPSS software (average linkage between groups as cluster method and squared Euclidean distance as measure of analyzed variables). The analysis revealed interesting information regarding similarities between studied hydroxyapatite-zirconia composites.

### References

[1] Rapacz-Kmita, A.; Ślósarczyk, A.; Paszkiewicz, Z. Mechanical properties of HAp- $\text{ZrO}_2$  composites. *Journal of the European Ceramic Society* 2006, 26(8), 1481-1488.

# Poster Presentation

*P.S.A.1*

**THE SYNTHESIS IN COMBUSTION MODE OF COMPLEX OXIDE FOR GAS SENSING MATERIALS**

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The combination of high sensitivity, selectivity and performance causes the wide application of semiconductor gas sensors. Searching of ways of creation new gas sensing materials and already modification available for today is one of actual problems of modern materials science. In the presented work experimental results on synthesis by method SHS (self-propagating high-temperature synthesis) stannate transitive metals of general formula  $M_2SnO_4$  ( $M = Cr, Fe, Co, Ni, Cu, Zn, Cd$ ) and connections  $Sn_{1-x}Ti_xO_2$  ( $x = 0.3, 0.5, 0.7$ ) are resulted. Synthesis of stannates was carried out according to two reactionary schemes: as fuel the powders of corresponding transitive metals were used; as fuel the powder of tin was used. Properties of the synthesized products have been investigated by means of X-ray analysis, electronic microscopy and other physical and chemical methods. Testing of gas sensitivity was spent with the use of microfilm technology. For the testing some gases were used: hydrogen, monoxide carbon, propane.

*P.S.A.2*

**THE EFFECT OF AN APPLIED ELECTRIC FIELD ON SELF-PROPAGATING HIGH-TEMPERATURE SYNTHESIS OF FERRITES**

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One of the perspective ways to government of Self-propagating High-temperature Synthesis (SHS) is an application of external physical fields of electromagnetic nature. Studying the influence of these fields not only on process course parameters, but also on physico-chemical properties and crystal structure of the products is an actual problem for creation of new functional materials. Ferrimagnetic materials based on manganese ferrites  $BaFe_{12}O_{19}$  and  $MnFe_2O_4$  have the unique combination of interesting magnetic properties. They are used for recording head fabrication, core of transformers, elements of computer memory. Besides that manganese ferrite has an effect of giant magneto resistance (GMR), i.e. the considerable change of resistance of a conductor by application of magnetic fields. Ferrite  $BaFe_{12}O_{19}$  belongs to the group of hard ferrites that are used for permanent magnets production. These ferrites have extremely high coercive force, rather high magnitude of residual and saturation magnetization that is the major requirement for the properties of permanent magnets. Influence of dc electrical field applied without contact to a sample, on SHS process  $MnFe_2O_4$  and  $BaFe_{12}O_{19}$  and properties of the final product has been investigated.

P.S.A.3

### **TiO<sub>2</sub> COATINGS PREPARED BY SOL-GEL METHOD FOR POTENTIAL USE FOR AIR DEODORIZING**

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Sol-gel method was used to synthesize polymer titanic material. Sol-gel processed titanic materials display unique properties i.e. the high refractivity, low density, high permittivity and they are chemically stable, mechanically strength and resistant to environment hazards. Sol-gel processed titanic materials are widely used in optics for processing of antireflection coatings, optical filters and sensors and planar optical wires. Due to relatively simple technique of processing sol-gel synthesized TiO<sub>2</sub> are applied as anticorrosive and abrasion-resisting coatings. In their midst applications in fuel cells, gas sensors ceramic membranes and for photocatalytic purification of water and air stand apart. TiO<sub>2</sub> properties are determined by its crystal phase (anatase, rutile or brookite). Anatase displays the best catalytic properties and potentially is the most suitable for applications for air deodorizing.

In this work, TiO<sub>2</sub> material obtained by hydrolyzing at room temperature alcoholate precursor: n- butoxytitanium (TBT Ti[O(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>]<sub>4</sub>) with the use of sol-gel method. Ethanol and water were used as solvents and acetylacetone was the stabilizer of the titanic precursor. TiO<sub>2</sub> in the form of thin film deposited on ceramic substrate in spintop hydrocyclone at 3000 r.p.m. Thin TiO<sub>2</sub> films were then annealing in air at 500 °C for 1 hour and subjected to the X-ray diffraction examination. In the measuring pattern, besides reflexes coming from the substrate at 29.6 angle, there was the strong peak identified as coming from anatase phase what makes obtained TiO<sub>2</sub> material potentially suitable for applications for deodorizing the air by decomposing odorous organic compounds present in the ambient.

This work was partially supported by Polish State Committee for Scientific Research KBN under grant No PBZ-ME i N-5/2/2006.

P.S.A.4

**BIOMETIC METHOD SUITABILITY FOR PROCESSING OF TiO<sub>2</sub> COATINGS  
APPLICABLE FOR AIR DEODORIZING**

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TiO<sub>2</sub> thin film due to its oxidizing ability could actively decompose organic odorous compounds present in the air. However TiO<sub>2</sub> properties depend strongly on its crystal phase (anatase, rutile or brookite). Rutile is mostly used as pigment. Anatase displays the best catalytic properties and potentially is the most suitable for applications for air deodorizing. Biomimetic method was used to synthesize titanic coating on ceramic substrate. The advantage of biomimetic processing over sol-gel method and other thin-film deposition techniques is that it does not require the post-deposition heat treatments to convert the coatings to structurally stable TiO<sub>2</sub>. The biomimetic deposition technique consists in providing energetically favorable interfaces for heterogeneous nucleation and growth of inorganic films from supersaturated solutions.

TiO<sub>2</sub> thin films were grown on functionalized interfaces (to promote mineralization) from aqueous solution of diammonium salt of dihydroxy titanium lactate (NH<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>Ti(C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>)<sub>2</sub> at strictly controlled solution conditions including ionic concentrations (supersaturation levels), pH and temperature.

The deposited thin TiO<sub>2</sub> films were subjected to the X-ray diffraction examination. In the measuring pattern there were some peaks coming from the ceramic substrate and no peaks characteristic for any crystal phase of TiO<sub>2</sub> and thermographic measurements carried out in the temperature range 23 °C – 1050 °C showed no exothermic peak characteristic to morphic- to crystal phase transition. The thickness of the deposited films was determined by measuring of absorption of radiation and was calculated as 2.7 μm thick. Although the morphic character of TiO<sub>2</sub> coating processed by this method put in doubt its suitability for air deodorizing the biomimetic method of thin film deposition for its indifference on substrate shape is worth considering for other applications.

This work was partially supported by Polish State Committee for Scientific Research KBN under grant No PBZ-ME i N-5/2/2006.

P.S.A.5

**ELECTRICAL PROPERTIES OF TiO<sub>2</sub> THIN FILMS WITH Eu AND Pd DOPANTS  
PREPARED BY MAGNETRON SPUTTERING ON SILICON**

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In this work, investigations of electrical properties of Eu and Pd-doped TiO<sub>2</sub> thin films have been outlined. It has been shown that incorporation of Pd and Eu dopants into TiO<sub>2</sub> matrix could modify its properties to obtain electrically and optically active oxide-semiconductor with specified type of electrical conduction at room temperature. Pd dopant changes the electrical properties of TiO<sub>2</sub> from dielectric oxide to oxide-semiconductor.

Thin films were deposited by low pressure hot target reactive sputtering from metallic Ti-Eu-Pd mosaic target on conventional silicon wafers.

For electrical characterization of TiO<sub>2</sub>(Eu,Pd) thin films four parallel TiSi-Ag electrodes were deposited through the metallic mask into the thin films.

Samples were examined by means of thermoelectrical, current-voltage (I-V) and capacitance-voltage (C-V) measurements.

On the basis of the measurement of d.c. electrical resistivity ( $\rho_{dc}$ ), in a temperature range from 300 K to 800 K, the activation energies were estimated. Negative sign of Seebeck coefficient has been determined, what indicates the electron-type (*n*) conduction.

I-V and C-V measurements indicated formation of electrically active heterojunction at the interface of semiconducting TiO<sub>2</sub>(Eu,Pd) thin film and silicon substrate.

I-V characteristics displayed a strong non-linear (diode-like) behavior of prepared heterojunctions and C-V characteristics exhibit large variation of capacitance with applied voltage.



*P.S.A.6*

**A STUDY OF MICROSTRUCTURAL CHANGES IN TiN THIN FILMS INDUCED BY ION IMPLANTATION**

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Titanium-nitride layers are interesting as hard coatings, wear and corrosion protection materials. In general, their functional properties depend on their microstructure, i. e. the mean grain size, grain boundaries, crystalline defects, preferred orientation, surface and interface morphology, etc. Here we present a study of the micro-structural changes induced in TiN layers by irradiation with argon ions. Titanium nitride thin films were deposited by reactive ion sputtering on (100) Si to a thickness of ~250nm. After deposition the films were implanted with 120keV argon ions to the fluences of  $1 \times 10^{15}$  and  $1 \times 10^{16}$  ions/cm<sup>2</sup>. Structural characterisation of the samples was performed by cross-sectional transmission electron microscopy, x-ray diffraction and Rutherford backscattering spectrometry. It was found that ion irradiation induces local micro-structural changes, formation of nanoparticles and defects. We also measured their electrical resistivity with a four point probe. The induced crystalline defects yield an increase of electrical resistivity after ion irradiation.

*P.S.A.7*

**INFLUENCE OF NITROGEN ION IMPLANTATION ON THE MECHANICAL PROPERTIES OF C1045 STEEL**

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Ion implantation is a very powerful technique for improving tribological properties of different materials. We have studied the effect of the energy of implanted nitrogen ions on the mechanical properties of construction steel C1045. Ion energies were 50 and 100 keV per atom, and ion fluence was  $2 \times 10^{17}$  ions/cm<sup>2</sup>. Structural examinations were performed by grazing incidence X-ray diffraction at different angles of incidence, and microhardness was measured by the Vicker's method. Nitrogen implantations induced the formation of Fe<sub>2</sub>N iron nitride in the near surface region of the samples, accompanied by a significant increase of microhardness. These effects were found to be more pronounced in the case of a combined implantation of nitrogen with both energies, to a total fluence of  $3 \times 10^{17}$  ions/cm<sup>2</sup>.

P.S.A.8

## **SURFACE MODIFICATION WTi SYSTEM INDUCED BY TEA CO<sub>2</sub> LASER BEAM**

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The WTi alloy as a refractory material possesses very good physicochemical characteristics such as thermochemical stability and high melting temperature. Conventional processing of this material is extremely difficult because of its hardness and brittleness, and the use of a laser is a possible solution. In this work interaction of a transversely excited atmospheric carbon dioxide (TEA CO<sub>2</sub>) laser with tungsten-titanium (WTi) alloy deposited on different substrate is considered. During WTi system irradiation with nanosecond laser pulses the main part of the absorbed energy was rapidly transformed into heat thus the intensive modifications on the target surface was occurred. The WTi thin film/coating deposition was done by plasma-beam-sputtering process. Good quality layers on different substares (steel and silicon) was obtained. Various analytical techniques were used for characterization of the samples. The phase composition and crystallite structure of coating and substrate were determined by X-ray diffraction method. Surface morphology was monitored, by optical microscopy (OM), by scanning electron microscopy (SEM). In the experiment typical laser output parameters were: wavelength – 10.6 μm; pulse duration of initial spike (FWHM) – 100 ns; peak power density – 120 MW/cm<sup>2</sup>. Multi-pulse laser irradiation was conducted in air atmosphere. Modification of WTi can be summarized as: (i) thin film/coating, (ii) morphological patterns in form of periodical structures (iii) apperance of resolidified material-droplet in central spot area and on the periphery and (v) plasma creation in front of samples.

P.S.A.9

**STUDY OF SUBSTRATE PRETREATMENT ON TOPOGRAPHY AND DEFECTS IN  
DEFECTS IN PVD-HARD COATINGS**

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It is well known that the adhesion of hard coatings is not only dependent on deposition process parameters (substrate temperature, ion bombardment during growth), but also critically depends on the tool material (composition, structure and morphology) and its pretreatment. It is thus important to choose the substrate material and its pretreatment very carefully. The topography of tool steel substrates (M2, D2 and H11) was analysed after polishing, ion beam etching and after deposition of PVD hard coatings by scanning electron microscope (SEM), atomic force microscope (AFM) and stylus 3d-profilometer. Focused ion beam milling system built in QUANTA 200 3D microscope (FEI) was used to prepare cross-section through the defects, while field emission scanning electron microscope (SIRION 400 NC, FEI) were used for study of the coating microstructure and defect morphology in planar surface view and cross-sectional fracture view. The substrates were ion etched and coated by different hard coatings in the termionic arc ion plating BAI 730 (Balzers) and the CC800 (CemeCon) unbalanced magnetron deposition systems. The roughness of all substrates was compared after polishing, ion etching and deposition, as well as the distribution of pit depths and hillock heights.

P.S.A.10

**THEORETICAL CALCULATION OF PARTITION AND THERMODYNAMIC  
FUNCTIONS OF B<sub>2</sub>C AND BC<sub>2</sub> GAS PHASE MOLECULES**

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One important technique to produce solid boron carbide (and also other solids with similar characteristics) is chemical vapour deposition (CVD) in particular thermal plasma CVD. In the vapour, used in the synthesis, different species (atoms, molecules, ions and electrons) are formed, among of them B<sub>2</sub>C and BC<sub>2</sub> molecules. They appear in the reaction (gas) mixture with considerable concentration in the large temperature zone (1000-4000 K).

In this paper we present the results of the calculation of partition functions, Gibbs energies and enthalpies of B<sub>2</sub>C and BC<sub>2</sub> molecules (these data are not available in the NIST-JANAF tables), for temperature range between 500 and 6000 K. The computation is performed by using the results of theoretical *ab initio* studies of the structure of these molecules (B<sub>2</sub>C and BC<sub>2</sub>) carried out by Martin *et al.*

*P.S.A.11*

### **THE INFLUENCE OF THE GAS DISCHARGE ELECTRICAL PROPERTIES ON UNIPOLAR PULSE PLASMA SYSTEM RESPONSE**

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New film deposition technologies like HIPMS (High Power Impulse Magnetron Sputtering) are based on modern pulse power supply development. The understanding of various discharge characteristics as a load is of crucial importance for further advances in material processing. The measurements of the gas discharge electrical signal waveforms in the case of unipolar pulse plasma have shown that the gas discharge electrical properties are closely related with the operating pressure value, cathode temperature, working gas mixture composition and vacuum chamber properties. Based on measurements, a variable voltage controlled impedance gas discharge electrical model was introduced. The model includes different discharge electrical behavior during the process of the gas discharge spreading over the cathode surface and the process of gas discharge transition to the stationary state. The analysis of the electrical signal waveforms obtained by the simulation of the equivalent circuit response, confirms the waveform details found by measurement, as well as the overall system behavior in case of different system parameters variation. Thus, the simulation results have shown that the dynamic as well as static gas discharge properties influence the shape of the unipolar pulse plasma electrical system response.

*P.S.A.12*

### **SILICON SURFACE PROCESSING BY QUASISTATIONARY PLASMA FLOW**

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In this work, modification of silicon single crystal surface by the action of nitrogen quasi-stationary compression plasma flow (CPF) generated by magneto-plasma compressor is studied. It was found that, as a result of single pulse surface treatment, regular fracture features are obtained on the Si (100) surface, on the central part of target. These regular formations can be related to the cleavage phenomena. Highly-oriented silicon periodic cylindrical shape structures are produced on the periphery part of target. The periodical structures formation can be related to the driven capillary waves, quenched during fast cooling and re-solidification phase of the plasma flow interaction with silicon surface. These surface phenomena are results of specific conditions during CPF interaction with silicon surface: high plasma flow energy density, large dynamic pressure, thermodynamic parameters gradients and quenching effects.

*P.S.A.13*

**INFLUENCE OF THE LASER PROCESSING PARAMETERS ON STRUCTURAL CHANGES OF SUPER ALLOY HASTELLOY**

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The state of the material after long exploitation in hard working conditions is considered. The Hastelloy X alloy is used for jet plane's combustion chamber construction. Even Hastelloy alloy has a great resistance to high temperatures and pressures, after long time use, the material will obtain damages of corrosive and macrospore types. In order to obtain more precise detailed analysis of material's degradation, laser techniques with various parameters: energy, wavelength and repetition rate will be applied.

*P.S.A.14*

**THE INFLUENCE OF LASER BORONIZING ON THE SURFACE LAYERS STRUCTURE OF 500-7 NODULAR IRON**

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In this paper the effect of the laser boronizing on surface layer structure of the nodular iron was studied. Laser treatment was performed with molecular CO<sub>2</sub> continuous Triumph laser TLF 2600t. Different laser beam power density was used. Three zones: melted, transition and hardened from solid state were found after laser boronizing in all cases. It was showed that microhardness of melted zone is about 5 times higher than the core microhardness. Boron existence in melted zone was confirmed by Auger Electron Spectroscopy (AES). Moreover, microstructure photographs (optical microscope), microhardness distribution (Vickers tester), boron, carbon and iron distribution (AES) in melted zone on the section from the surface certify that melted zone is almost utterly homogenous, whereas two other zones below: transition and hardened are totally heterogeneous. Martensite, ferrite, graphite and ledeburite were found in those zones, at least.

*P.S.A.15*

**THE EFFECT OF TEMPERATURE AND ZINC CONCENTRATION ON ZINC COATINGS DEPOSITED WITH PACK CEMENTATION**

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Zinc coatings are proved to be corrosion resistant as they react with several atmospheric compounds and form bulk adherent. They maintain their protection to steel even in cases when are mechanically locally damaged as they offer cathodic protection. This work aims to investigate the feasibility of zinc deposition on low alloy steels at temperatures from 380 up to 450°C by pack cementation process aiming to increase their corrosion resistance without affecting their mechanical properties. A series of experiments were undertaken to investigate the effects of pack composition and the deposition temperature of the process. The pack zinc content varied from 10 to 50 wt.%. The duration of the process was 2h. It was observed that the parameter of the zinc content only affected the coating thickness, but not the phase composition of the as produced coating referring to  $\Gamma$ -Fe<sub>11</sub>Zn<sub>40</sub> and  $\delta$ -FeZn<sub>10</sub> phases of the Fe-Zn phase diagram. It was also deduced that there is an exponential correlation between the coating thickness and the zinc concentration.

*P.S.A.16*

**STUDY OF THE GROWTH MECHANISM OF ZINC HOT-DIP GALVANIZING COATINGS**

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Zinc hot dip galvanizing is one of the most effective methods for the corrosion protection of ferrous materials. However, although its efficiency is undisputable, the exact growth mechanism of these coatings is still under question. In the present work, the diffusivity of liquid zinc in carbon steel was measured with electron microscopy. Furthermore, the change of the free Gibbs energy was calculated for each phase of the coating. Nevertheless, the coating structure was microscopically studied for extremely short immersion time (about 1 sec). This way, it was deduced that the coating growth begins with the nucleation of the zeta phase of the Fe-Zn system. Gamma and delta grow with zinc diffusion through this phase. Eta phase is mechanically drifted due to surface tension of the liquid metal.

*P.S.A.17*

**EXAMINATION OF THE MICROSTRUCTURAL FEATURES OF ZINC PROTECTIVE COATINGS ON LOW CARBON STEEL FORMED IN A FLUIDIZED BED REACTOR**

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Corrosion protection of several metal substrates is very often achieved by the formation of zinc layers on its surface. For this reason zinc coatings are widely applied especially in metal fabrication industry and in the construction field. Galvanizing is the most industrially used process for this purpose but there are alternative methods with less environmental impact such as CVD fluidized bed process (FBR). In this work the structure of Zn coatings formed with FBR technique, at 400°C for 30min/1h/1h30min/2h holding time, has been studied. Several experiments were carried out using a convenient halide activator in form of powder or pill. The coated samples were observed with SEM microscopy and they were characterized with EDS and XRD analysis which showed that a two-layered coatings were formed corresponding to gamma and delta phase of the Fe-Zn phase diagram. Also some of the as-received coatings are likely to provide sufficient anticorrosive protection while others are of low quality, as many porous areas are present in their mass depending on the state of the activator.

*P.S.A.18*

**FORMATION AND GROWTH OF COPPER DEPOSITS UNDER HYDROGEN CODEPOSITION**

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Electrodeposition of copper under conditions of hydrogen codeposition has a large technological significance. The formation of powder particles and disperse but adherent deposits with the extremely high surface area suitable for electrodes in electrochemical devices takes place in the range of overpotentials and current densities where there is a parallelism between copper electrodeposition and hydrogen evolution. Except overpotentials and current densities, parameters of electrolysis of the significance for the formation of these deposits types are primarily concentration of copper (II) ions, concentration of supporting electrolyte (H<sub>2</sub>SO<sub>4</sub>) and temperature. Having to view the high technological significance of these copper deposits, the optimization of these parameters of electrolysis is necessary. The aim of this work will be to do it.

*P.S.A.19*

### **CHARACTERIZATION OF CARBON FIBROUS MATERIALS MODIFIED BY RUBY LASER RADIATION**

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The interaction of ruby laser ( $\lambda=694.3$  nm), working in the Q-switched regime, with carbon fibrous materials was investigated. Materials were of different textile shapes and in various process stages, therefore having different mechanical and optical properties. Structural and morphological changes, caused by high temperatures arising in the material during short laser pulses, were examined using scanning electron microscopy and X-ray diffraction. The experiments show that changes strongly depend on the material, and also on the laser working regime (energy and power density of the laser beam etc.). This type of laser radiation influences mostly on turbostratic carbon fiber structure, leading to its better arrangement. Destructive and nondestructive changes, as well as approximate laser radiation thresholds for destructive changes were assessed. Numerical modelling of the temperature changes in the material was also conducted. It has been established that the porous nature has a strong impact on the heat conduction when the material is subjected to laser beams.

*P.S.A.20*

### **RAPID QUENCHED METAL FIBRES AND POROUS FIBROUS MATERIALS**

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Application of rapid quenching provides reception of some new metastable phases and micro-, nanostructures. In the Centre of Powder Materials Science the way of extraction of a melt from the hanged drop with electron beam heating is realized. As a result of extraction RQ-product is received as continuous and discrete fibres. Influence of technological parameters on geometry of a fibre is investigated. The reasons of occurrence of wavy changes of a cross-section of metallic fibers are analyzed at extraction of a melt from the hanged drop. One of examples of application of metallic fibers is creation of permeable non-woven materials (metallic felt). A key feature of materials at use as filters and elements of noise-reduction designs is its high permeability at a wide range of porosity and high specific characteristics.



P.S.A.21

### PREPARATION OF $\text{Al}(\text{OH})_3$ POWDER BY FIB FOR TEM INVESTIGATION

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Crystallization of  $\text{Al}(\text{OH})_3$  from caustic soda solution is the most important part of Bayer process for alumina production because the properties of precipitated  $\text{Al}(\text{OH})_3$  mainly depend on several phenomena which occur during this process: nucleation agglomeration and crystal growth. Investigation of mechanism of  $\text{Al}(\text{OH})_3$  crystals growth by Transmission Electron microscopy requires special way of preparation. In this case we prepared powder samples for TEM investigations by FEI Strata Dual Beam FIB.

The dual-beam FIB system combines multiple experimental systems within the same chamber so that combinations of different techniques can be accommodated by unique sample preparation, manipulation and analysis methods. The system contains both a focused Ga<sup>+</sup> ion beam and a field emission scanning electron column. The ion column can be used for selective removal of material by ion beam milling. In addition, the ion beam can be used for ion-enhanced imaging of fine texture analysis in crystalline materials.

P.S.A.22

### MASS-SPECTROMETRIC DIFFERENTIATION OF SULFUR CONTAINING ELECTRON-RICH HETEROCYCLES

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Selected, highly delocalized 2-alkylidene-4-oxothiazolidines, 1,2-trithiazapentalenes and 1,3-thiazines, exemplified by general structures **1**, **2** and **3**, respectively, have received considerable synthetic attention as model compounds for studying electronic materials based on organic matter.

The mass spectrometry behavior of these compounds, which exhibit in most cases a high-intensity molecular ion peak, depends on the nature of the heterocyclic ring, and position of the substituents within specific ring system. In terms of the characterization, a good correlation between the structure and the fragmentation pathways, investigated under EI and CI conditions, was established for all three classes of heterocyclic compounds. The mass spectrometry results will be presented with respect to the spectroscopic and electronic properties of the materials **1-3** which were studied previously via UV-Visible spectroscopy and cyclic voltammetry.

*P.S.A.23*

### **POINT OF ZERO CHARGE AND ISOELECTRIC POINT OF ALUMINA**

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The point of zero charge,  $\text{pH}_{\text{pzc}}$ , and the isoelectric point,  $\text{pH}_{\text{iep}}$ , of a commercial alumina sample ( $\text{Al}_2\text{O}_3$  AKP-30, Sumitomo, Japan) was investigated in  $\text{KNO}_3$  solutions. The point of zero charge was determined by the batch equilibration technique, while the isoelectric point was determined by a potentiometric method using a Zetasizer Nano equipped with a MPT-2 Autotitrator (Malvern, UK). The influence of the electrolyte concentration as well as of the alumina/solution ratio on  $\text{pH}_{\text{pzc}}$  and  $\text{pH}_{\text{iep}}$  was investigated. The obtained results are compared with those published in literature.

*P.S.A.24*

### **STABILITY OF ZIRCONIA SOL IN THE PRESENCE OF VARIOUS INORGANIC ELECTROLYTES**

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The stability of zirconia sol in the presence of various inorganic electrolytes ( $\text{LiCl}$ ,  $\text{NaCl}$ ,  $\text{KCl}$ ,  $\text{CsCl}$ ,  $\text{KBr}$ ,  $\text{KI}$ ,  $\text{KNO}_3$ , and  $\text{K}_2\text{SO}_4$ ) was studied by a potentiometric titration method. Zirconia sol was prepared from zirconyl oxychloride solutions by forced hydrolysis at  $102^{\circ}\text{C}$ . The prepared sol consisted of almost spherical, monoclinic, hydrated zirconia particles 48 nm in diameter. Dependence of the critical concentration of coagulation (CCC) on the dispersion pH was determined for all studied electrolytes. For all investigated electrolytes, the critical coagulation concentration values are lower at higher pH. These values for all 1:1 electrolytes are equal in the range of experimental error. For a given pH value, CCCs of  $\text{Na}_2\text{SO}_4$  are 3-4 orders of magnitude lower than the corresponding values for 1:1 electrolytes

P.S.A.25

**SYNTHESIS OF  $\text{Li}_{1+x}\text{Mn}_{2-x}\text{O}_4$  CATHODE MATERIAL USING GEL-COMBUSTION METHOD**

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$\text{LiMn}_2\text{O}_4$  spinel is widely used cathodic material for lithium-ion batteries, but suffers of rapid capacity fade during electrochemical cycling. Usually, capacity fade was reduced by replacing a part of Mn by other transition metal. In this study, capacity fade was reduced by adjusting initial molar ratio Li/Mn. This adjustment was carried out by adjusting the composition of precursor solution used for material synthesis. The powdery materials  $\text{Li}_{1+x}\text{Mn}_{2-x}\text{O}_4$  was synthesized by glycine-nitrate gel-combustion method. The XRPD analysis evidenced that for all compositions, with  $0 < x < 1$ , pure spinel phase was obtained. The material with  $x=0,05$  used as the cathodic material provided initial discharge capacity of 104 mAh/g and retained 94% of its initial discharging capacity after 50 charging/discharging cycles.

P.S.A.26

**HYDROTHERMAL SYNTHESIS OF CATHODE MATERIALS FOR LITHIUM-ION BATTERIES**

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A series of spinel structured and layered structured materials have been synthesized by the hydrothermal procedure. Hydrothermal treatment was carried out in a Parr floor stand pressure reactor 4530 in aqueous medium, with the reactor vessel volume of 2 liters. By varying synthesis condition, that is working temperature and pressure, as well as starting materials, the optimal parameters for obtaining monophased samples were found. Phase identifications of the as-prepared powders were checked by the use of X-ray diffraction measurements. X-ray diffraction data were also used for the structural refinement. Particle morphology was revealed by scanning electron microscopy.

*P.S.A.27*

**MODELING OF EMULSION PROCESS GENERATION USING REAL TIME MEASUREMENTS**

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There are many developed strategies in emulsion evaluation, in purpose to determine the quality and life circle of emulsions. Most of them are based on the reological properties of emulsions. There are very few which relay on the direct emulsion observations. In this paper we present the developed method for emulsion process generation evaluation by the direct observation of particle size distribution. Method is based on the measure of emulsion transmittance properties, and the partcle projection on the screen which are directly dependent on the emulsionprocess generation. Emulsion properties were measure with the application of system for acquisition of visual information's, which is based on the CCD camera and fast PC configuration equipped with the capturing software. The acquired sets of visual information's were analyzed by the OZARIA software package. As the measure for emulsion properties the mean particle diameter,ferets shape factor, and particle density were used. Two differently formed emulsion were tested, one formed by ultrasound dispersionand the other formed by clasical mixing. The obtained results shows difference in all selected paramaters, which proved the assumption that direct emulsion obseravtions could give data for the modeling of emulsion process formation.

P.S.A.28

## INNOVATIVE MATERIALS FOR H<sub>2</sub> STORAGE

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This paper reports on the study of H<sub>2</sub> generation via catalytic hydrolysis of NaBH<sub>4</sub>, for "start and stop" and on-board applications. Up to now, most studies were performed on systems in which the hydrolysis of a stabilized borohydride solution takes place on a solid catalyst. However, in such systems the excess water and the presence of a stabilizing agent significantly lower the amount of hydrogen that can be produced compared to the theoretical 10.8 wt.%. In order to approach this value, the present work investigates the reaction of solid NaBH<sub>4</sub> with the stoichiometric amount of water in presence of a catalyst either in aqueous solution or mixed with solid NaBH<sub>4</sub>.

In a first stage, less costly catalytic systems were compared with the commonly used noble metal based catalysts such as Ru. The metals or their salts were studied in water solution or deposited on the borohydride surface in the form of well-dispersed metallic nanoparticles. The activities of different acidic and metallic catalysts and the corresponding evolved energies were studied under atmospheric pressure by means of calorimetry coupled with hydrogen quantity measurements.

Information on the reaction mechanism was obtained by analyzing the solid products of the hydrolysis and the used catalyst using different complementary physico-chemical techniques (XRD, TEM, SEM, XPS and TGA).

The main properties and challenges of these systems will be discussed in terms of catalytic active phase, water diffusion, and reaction rate.

P.S.A.29

## THE INFLUENCE OF EXCESS SODIUM CATIONS FROM LTA ZEOLITE ON HIGH TEMPERATURE CRYSTALLIZATION AND STABILITY OF LOW-CARNEGIEITE

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High temperature transformations of sodium LTA zeolites are known methods for nepheline and carnegieite preparation. Sometimes, a new phase, which is not characterized, appears in those systems. In this paper we are studying the influence of sodium excess on the appearance of a new phase in investigated systems. Sodium LTA zeolites were synthesized by gel route in different reaction conditions Na<sub>2</sub>O(2.4-3.9):Al<sub>2</sub>O<sub>3</sub>(1):SiO<sub>2</sub>(1.5-2.0):H<sub>2</sub>O(90-170). The excess of sodium was removed after washing several times with water. Unwashed, partially washed and several times washed samples were thermally treated in temperature range from room up to 950°C. Obtained high temperature phases were investigated by various methods including chemical analysis, XRPD analysis, thermal (DT/TG) analysis, FT-IR spectroscopy and SEM.

*P.S.A.30*

### **PREPARATION AND CHARACTERIZATION OF ZEOLITE ENCAGED ENZYME-MIMETIC COPPER HISTIDINE COMPLEXES**

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Histidine, a naturally occurring amino acid, was incorporated inside the supercages of FAU (NaY or HY) type zeolite in a form of Cu-complex entity. It is already known from the literature that such complexes mimic the active centre of natural enzymatic counterparts, such as galactose oxidase. In the form of complexes incorporated into the inorganic support, such systems have already exhibited promising catalytic activity, for example, in the case of epoxidation of alkenes with peroxides. Possible catalytic activity was the main interest in this work for investigation of this kind of systems. The preparation was done either by ion-exchange procedure, or previously prepared Cu-histidine complex was incorporated into the  $\alpha$  cages of Y zeolite by occlusion; pH was found to be very important factor, as well as the amount of copper complex loaded on the zeolite. The characterisation of obtained samples was performed using Diffuse Reflectance Ultraviolet-Visible Spectroscopy (DRUV-Vis), Electron Paramagnetic Resonance (EPR), Infrared Spectroscopy (IR) and Raman Spectroscopy (RS). The structure of the complexes is found to be highly dependent on the synthesis conditions.

*P.S.A.31*

### **STRUCTURAL DESTABILIZATION IN MAGNESIUM HYDRIDE**

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As hydrogen storage is the main technological problem of a practical hydrogen economy, most research is focused on storing hydrogen in a lightweight, compact manner for mobile applications. Much attention is devoted to hydrogen storage in magnesium hydride and related alloys. The problem of magnesium based alloys is that hydriding/dehydriding reaction takes place at high temperature and the kinetic is relatively slow. One way to improve the kinetics of magnesium based alloys is to modify compositions and/ or their structure. The aim of this study was to investigate the structural modifications in magnesium hydride caused either by mechanical alloying with diatomite or by irradiation with light ions. A systematic study has been conducted on pure MgH<sub>2</sub> irradiated by light ions and MgH<sub>2</sub> doped with different amount of diatomite by SEM, X-ray diffraction and DTA. The result shows significant improvement of reaction kinetics.

P.S.A.32

### EFFECTS OF ORGANIC SURFACTANTS ON MECHANOCHEMICALY SYNTHESIZED ZnO PARTICLES

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Nanocrystalline ZnO powders were prepared by the mechanochemical method followed by a heat-treatment in a planetary ball-mill using a agate jars and alumina balls. The frequency of the rotation of jars around the common axis was 180 revolutions per minute, activation times were from 30 min to 4 h.

Mechanochemical processing involves the mechanical activation of solid-state displacement reaction at low temperatures. In this experiment the starting materials were ZnCl<sub>2</sub> and Ca(OH)<sub>2</sub>. We studied influence of addition of different types of organic surfactants to the reactant mixture on the morphology of the synthesized particles. Selected surfactants used in these experiments were: oxalic acid, SDS (sodium dodecil sulphate) and PEG (polyetilene glycol).

After milling, the powder was calcinated at different temperatures from 1h to 3h and washed with ethanol and deionized water using an ultrasonic bath and a centrifuge to remove all the residual reaction by-products. Powders characterization was preformed using X-ray diffraction method (XRD) and scanning electron microscopy (SEM).

P.S.A.33

### THEORETICAL APPROACH FOR DEVELOPMENT OF ANTIMICROBIAL MATERIALS BASED ON Ag-APATITES

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Antimicrobial materials are becoming increasingly important because of their wide range of applications including biomaterials, fabrics, cosmetics, etc. These materials consist of metal-ions such as silver Ag<sup>+</sup> ions, and substrate, based on calcium phosphate, zeolite or amorphous silica. Stability of antimicrobial materials which prevent the fast dissolution of the substrate and subsequent fast release of Ag<sup>+</sup> ions, represent an essential prerequisite for their practical application. Hydroxyapatite (HAP) is a material which is able to incorporate different metal-ions in its structure. Here we performed the theoretical assessment of HAP/Ag system stability based on calculation of the ion-ion interaction potential. The obtained results indicate that Ag forms a stable solid-solution by substitution of the calcium ions in the HAP lattice. This result points out HAP as a suitable substrate for development of the Ag-based antimicrobial materials.

*P.S.A.34*

### **INFLUENCE OF MgO ADDITION ON THE SYNTHESIS OF ZINC-TITANATE CERAMICS**

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Starting mixtures of ZnO, TiO<sub>2</sub> and MgO (0, 1.25 and 2.5wt.%) powders were mechanically activated for 15 minutes in a planetary ball mill. The powders obtained were sintered non-isothermally to temperatures between 800 and 1100°C and then held at that temperature for 120 minutes. Analysis of the influence of MgO addition on the synthesis of zinc-titanate ceramics showed that its addition increased the temperature at which the reaction process started and also the temperature at which the sintering process started but it resulted in higher sample densities. These results were correlated with the results of structural characterization using XRPD and SEM analysis.

*P.S.A.35*

### **ARSENIC (V) SORPTION BY IRON MODIFIED NATURAL ZEOLITE TUFF**

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Iron modified natural zeolite is a prosperous and relatively inexpensive material for removal of arsenic (V) from drinking water. The composition and thermal stability of natural zeolite were investigated by the X-ray diffraction and the thermal analysis (DTA/TGA). The natural zeolite was treated with iron (III) chloride solution. During this process the zeolite surface has been laden with iron (III) oxo(hydroxides) whose high affinity for the arsenic (V) adsorption is well known. The surface of starting as well as iron modified zeolite was analysed using scanning electron microscopy (SEM). Kinetics of As(V) adsorption on this material showed that up to 96% of As (V) was removed after a contact time of 30 minutes. The As(V) adsorption experimental data were fitted with Freundlich, Langmuir and Langmuir-Freundlich adsorption isotherms.



P.S.A.36

### ORIENTATION-INDUCED CHANGES IN MICROSTRUCTURE AND CRYSTALLINITY OF DIFFERENT PEs

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This paper studies the influence of orientation on polyethylenes (PEs) with different structural peculiarities in accordance with Peterlin's molecular model of drawing. For this reason, low density polyethylene (LDPE), linear low density polyethylene (LLDPE) and high density polyethylene (HDPE) were oriented via solid-state stretching at an elevated temperature. In order to investigate orientation-induced changes in morphology, surface microstructures were analyzed by optical (OM) and scanning electron microscopy (SEM). Differential scanning calorimetry (DSC) and wide-angle X-ray diffraction (WAXD) measurements were used to determine changes in crystallinity. The presented results reveal a two-stage evolution of crystallinity (of pristine PEs) due to orientation; the first stage is characterized by a significant increase in crystallinity, following saturation occurs with a further increase of the draw ratio at the second stage. The critical draw ratio, which separates these two stages and corresponds to the transformation from the initial to the developed fibrillar structure, was influenced by the structural peculiarities of each PE.

P.S.A.37

### THE STUDY OF NUCLEATION OF SECONDARY PHASE IN GLASS WITH PRIMARY CRYSTALLIZATION

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In this paper the results of investigation of aluminosilicate glass which crystallize by primary crystallization. In the case of primary crystallization, the composition of the crystal phases is different than that of parent glass. The results of investigation shown, that leucite as primary phase, and diopside as secondary one were nucleated heterogeneously. The secondary phase phlogopite shown homogenous mechanism of nucleation. By using DTA method for study of such complex nucleation process was shown that crystallisation peak temperature  $T_p$  and crystallisation peak height  $(\delta T)_p$  are time functions of previous heat treatment of the sample. The heat treatment for the time which corresponds to the maximum of DTA parameters enables the complex curve of  $T_p$  i  $(\delta T)_p$  change as the function of nucleation temperature of this glass to be obtained. Also, this enables to study the nucleation of phlogopite as secondary crystalline phase.

*P.S.A.38*

### **CONJUGATED POLYMER CHARACTERISATION USING LASER BEAM SCATTERING TECHNIQUES**

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Theoretical study of laser beam scattering in characterization of MEH-PPV (2-methoxy,5-(2'-ethyl-hexoxy)-1,4-phenylene vinylene) in solution will be presented in this paper. Some equations for static and dynamic light scattering intensities will be obtained in terms of system structure factor. The intermolecular contribution to light scattering by polymer solutions will be considered for spin casting process characteristic concentrations. The degree of polymer molecules aggregation and interchain interactions, related to the solution parameters, will be analysed, too.

*P.S.A.39*

### **COMPARISON OF SELECTIVE CATALYSTS FOR POLYURETHANE FOAMS**

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Polyurethane foams were prepared from polypropylene glycols and toluene diisocyanate (TDI) or diphenylmethane diisocyanate (methylenediphenylisocyanate, MDI). Commercially available amines and substituted morpholine were tested as single catalysts for the foam formation as well as in catalyst mixtures (amine-amine and amine-tin compound mixtures). Some first results with acidic blocked amine catalysts (amine-acid mixtures) also will be presented. The aim was to compare the catalysts and catalyst mixtures in view of economic and environmental (search for a suitable replacement of organo-tin compounds) aspects.

Acknowledgement: The authors thank the Ministry of Industry and Trade of the Czech Republic, grant FT-TA3/034 for the financial support of this work.

*P.S.A.40*

### **CURING REACTIONS OF SEMI-DRYING OILS ALKYDS WITH MELAMINE RESIN**

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Alkyds modified with melamine resins are mainly used in industrial baking enamels. In this paper the kinetics of curing reactions of alkyd resins based on hydrogenated castor oil and soybean oil with melamine resin have been studied by DSC. The kinetic parameters obtained by the transformation of dynamic DSC results into isothermal data through the Ozawa kinetic model are equivalent to those determined by the isothermal DSC method used. The ratio of hydroxyl equivalent to carboxylic equivalent in the alkyd/melamine formulation determines the extent of curing. The combination of semi-drying oil alkyd with used melamine resin gives a cured film of enamel with good flexibility, while at the same time being characterized by the high hardness in dependences on the type of oil in the alkyd resin and the ratio of reaction components.

*P.S.A.41*

### **DEGRADATION OF SOLAR CELLS DUE TO DIFFERENT WORKING ENVIRONMENTS**

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Solar cells, the basis for photovoltaic power conversion are made of various materials and structures with the main goal of improvement of the properties and cost reduction of solar cells and systems. Basically relatively stable (except perhaps amorphous silicon solar cells), solar systems are (like any other electronic devices) susceptible to the effects of aging, which usually means deterioration of their characteristics. Changes of the main characteristics of solar cells such as efficiency, fill factor, short circuit current etc. due to the exposure of solar systems to different (sometimes hostile) working environment are the aim of this paper's investigation. All of these effects ultimately influence the output characteristics of solar cells, and better understanding of these parameters would lead to the improvement of high-efficiency solar systems and also, larger scale application of solar energy in the near future.

P.S.A.42

### INFLUENCE OF COMPOSITION OF BORONISING MIXTURE ON THE DEPTH OF BORIDE LAYERS PRESSED AND BORIDED SAMPLES FROM IRON POWDER

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During sintering and chemical-thermal treatment-boriding of samples from iron powder generates adequate boride layer, way in this paper are presented results of research dependence of depth of boride layer from composition of mixture which are used for boronising process. Basic mixture used for boriding of investigated samples from iron powder is modified by addition of activators different chemical composition and in different percentage rate. The obtained boride layers vary in depth and quality (porosity, the contact with metal). In order to obtain better boride layers and to show certain appearances during boriding, it was necessary to choose mixture for boriding and to determine the most useful activators and their ratio. Processing of experimentally obtained results is carried out by using Simplex method. Results of investigation and mathematical processing allow us to choose composition of mixture for boriding with depth change which is given in advance. It has been observed that simultaneously with boriding also sintering occurred, and this fact offers a wide application possibility in the chemical-thermal treatment for sintered materials. It is possible to completely avoid sintering process of products which are obtained with powder metallurgy.

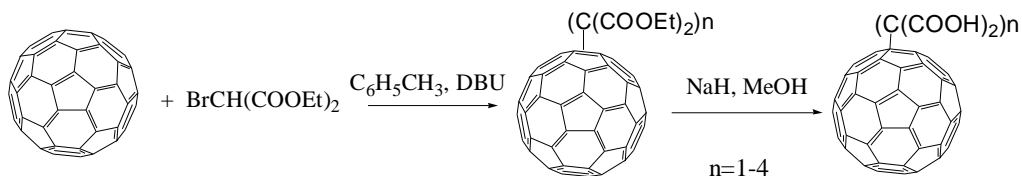
P.S.A.43

### SYNTHESIS OF OLIGOADDUCTS OF MALONIC ACID C<sub>60</sub>

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Water soluble fullerene C<sub>60</sub> derivatives hold promise for medical application. Malonic acid trisadduct C<sub>60</sub>[C(COOH)<sub>2</sub>]<sub>3</sub> of C<sub>3</sub> symmetry which is highly water soluble and prime drug candidate for various neurological diseases. In this paper we presents in two steps, synthesis different regiostructure malonate derivatives of C<sub>60</sub> C<sub>60</sub>[C(COOH)<sub>2</sub>]<sub>n</sub> n=1-4.



*P.S.A.44*

**CHEMICAL SYNTHESIS AND CHARACTERIZATION OF LITHIUM  
ORTHOSILICATE (Li<sub>4</sub>SiO<sub>4</sub>). CO<sub>2</sub> ABSORPTION CAPACITIES.**

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Carbon dioxide is one of the most known atmospheric pollutants, flame combustion of fossil fuels being its common source. The increasing CO<sub>2</sub> emission has been identified as main contributor to global warming. Therefore, removal of carbon dioxide at a variety of different temperatures is imposed as a very serious task to scientific community, all over the world. Recently, Toshiba Company has developed a series of lithium-containing oxides as CO<sub>2</sub> absorbents at high temperatures. These materials have been also probed for the absorptions of CO<sub>2</sub> at near room temperatures. In this work, the synthesis of Li<sub>4</sub>SiO<sub>4</sub> has been performed; the obtained oxide was characterised by means of chemical analysis, the structure was proven by FTIR and XRD. Besides, its absorption capacity towards CO<sub>2</sub> has been probed at different temperatures. The samples were placed in a crucible of thermo balance (TG) and exposed to a flow of CO<sub>2</sub>/He. The absorption capacities were estimated through the obtained mass changes. Absorption capacities have been found as dependent on absorption temperature.

*P.S.A.45*

**SIMILARITY AND DIFFERENCE BETWEEN EXPLOSION WELDING AND LASER  
HYBRID ON STRUCTURAL LEVEL**

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In this paper we investigate the methods of welding metals: explosion welding and laser hybrid, with results of authors' own experimental investigation. In this processes we followed basic structural changes and morphology of welding joints. Structural changes of welding joints have been studied by X-ray diffraction and morphology changes of joints by optical microscopy and EDEX. Attention is particularly on HAZ and microstructural irregularity. The analysis of results gives possibility for improving welding technology.

P.S.A.46

### EXPERIMENTAL RESEARCH OF EFFECTS OF AIR PRESSURE TO THE WALLS OF BYPASSING HIGH SPEED TRAINS

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This paper is review of experimental studies in aerodynamics of high speed trains the passing by each other in opposite direction on open tracks. The paper describes measurement of aerodynamic pressures produced by the trains. The focus of this study is to determine the localized effects such as potential damage to windows. Experimental researches of train models carried out in wind tunnel in our country are presented. Results of the experiment are compared with the pressures predicted by a computational fluid dynamics simulation. Theoretical calculation is based on the FEA (finite element analyses), which is used for flow field prediction of two high speed trains. Speed of each train was 250 km/h.

P.S.A.47

### THERMAL STABILITY AND FRAGILITY PARAMETERS OF Fe-M-Al-Ga-P-C-B (M=Nb) AMORPHOUS ALLOYS

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The thermal stability and crystallization processes of multicomponent metallic glasses with compositions  $\text{Fe}_{72-x}\text{Nb}_x\text{Al}_5\text{Ga}_2\text{P}_{11}\text{C}_6\text{B}_4$  ( $x=0, 2$ ) was investigated by isochronal differential scanning calorimetry (DSC) and X-ray diffraction (XRD). Thermal stability was discussed in terms of the width of supercooled liquid region ( $\Delta T_x = T_x - T_g$ ; where  $T_x$ -crystallization temperature and  $T_g$ -glass transition temperature), as well as reduced glass-transition temperature ( $T_{rg} = T_g/T_1$ ). The replacement of Fe by Nb leading to a slight decrease in  $\Delta T_x$  from 65 K to 63 K. Glass-forming ability (GFA) of studied alloys was estimated with respect to two fragility parameters: ( $D^*$ ) obtained from the dependence of the glass transition on the heating rate described by Vogel-Fulcher-Tamman (VFT) relation as well as ( $m$ ) fragility parameter (at a particular temperature  $T_g$ ) that can be classified under the Angell's concept of glass-formers selection. The fragility parameter of the Nb-free alloy ( $D^*=2.98$ ) is about four times larger than that for the minor Nb-added alloy ( $D^*=0.86$ ). The calculated values of  $m$  at  $T_g$  corresponding to heating rate 20 K/min is around 53 for  $x=0$ , and about 69 for  $x=2$ . Therefore, obtained values for  $m$  indicates that the investigated alloys can be associated into the intermediate category according to the Angell's classification scheme on fragile, intermediate and strong glass-formers. The both values of fragility parameters indicated the better GFA of the Nb-free alloy.

This work was partially financed by Serbian Ministry for Science under the Project No: 142011.

P.S.A.48

## XRD ANALYSIS OF HIGH-COPPER AlCuMg ALLOYS

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In this paper we have examined the as-cast microstructure in the AlCuMg system over a wide range of magnesium and titanium contents in order to determine the effect of the content of both elements on the microstructure and properties of AlCuMg alloys. Depending on the alloy composition (say Cu content and Cu/Mg ratio), different phase distribution and consequently different material characteristics can be obtained. Characterization of six different AlCuMg alloys having a copper content 15 wt.% was performed with X-ray powder diffraction, optical and electron microscopy. Hardness and compression strength were determined, also. Using X-ray diffraction we established that the tetragonal intermetallic compound Al<sub>2</sub>Cu and orthorhombic intermetallic compound Al<sub>2</sub>CuMg are formed across the whole range of magnesium additions. From the X-ray diffractograms the following microstructural parameters have been calculated: the average sub-grain size, the microvoltage and the dislocation density.

P.S.A.49

## TRICALCIUM ALUMINATE HEXAHYDRATE (TCA) FILTER AID IN THE BAYER INDUSTRY

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Tricalcium aluminate hexahydrate (TCA) is used within the Bayer industry as a filter aid during purification of sodium aluminate liquors — a role in which the TCA morphology and particle size are particularly important. In spite of this usefulness, no studies have been reported in the open literature examining the influence of reaction variables on the morphology of TCA prepared at 100°C under conditions of interest to the Bayer industry. In this paper, we examine the influence of sodium hydroxide concentration, gibbsite ( $\text{Al}(\text{OH})_3$ ) charge, CaO charge, reactant addition procedure, added salts ( $\text{Na}_2\text{CO}_3$ , NaCl and  $\text{Na}_2\text{SO}_4$ ) and reaction time on the formation and morphology of TCA at 100°C. Our results indicate the reactant addition procedure significantly influences the TCA purity and particle size. For example, reaction between CaO (15 or 60 g/L) and a sodium aluminate solution yields TCA crystals with a median particle size of  $\approx 6 \mu\text{m}$  but with  $\text{Ca}(\text{OH})_2$  as an impurity, while reaction between CaO and gibbsite in a sodium hydroxide solution can give pure TCA with a median particle size of  $\approx 11 \mu\text{m}$ . The CaO loading or liquor alumina/caustic ratio do not significantly affect the particle size for TCA formed by reaction between CaO and a sodium aluminate solution. The morphology of TCA formed by addition of CaO and gibbsite to a sodium hydroxide solution is significantly affected by the  $\text{CaO}/\text{Al}_2\text{O}_3$  ratio. In particular, a molar  $\text{CaO}/\text{Al}_2\text{O}_3$  ratio between 1.8 and 3 forms TCA with a morphology similar to that of a rhombic dodecahedron, while a molar  $\text{CaO}/\text{Al}_2\text{O}_3$  ratio less than 1.8 forms TCA of a less well defined morphology. Conducting the reaction between CaO and gibbsite in a sodium hydroxide solution containing added  $\text{Na}_2\text{CO}_3$ , NaCl and  $\text{Na}_2\text{SO}_4$  forms hexagonal plates of a calcium aluminate carbonate hydrate with the approximate formula  $4.1 \text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 0.75 \text{CO}_2 \cdot 11 \text{H}_2\text{O}$ . This compound subsequently reacts to well defined TCA crystals with a median particle size of  $\approx 11 \mu\text{m}$ .



*P.S.A.50*

**AN INFLUENCE OF MICROSTRUCTURE OF SCREEN FORMED BY LASER  
EXPOSURE OF LIGHT-SENSITIVE FILM ON TON VALUE INCREASE IN  
PRINTING**

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In this paper an influence of microstructure of screen, formed by laser exposure of light-sensitive film, on ton value increase in printing was investigated. Test forms containing a 50% tints were made by exposing the photosensitive emulsion containing AgX crystals. Photosensitive emulsion was exposed using red laser diode (680 nm), with various diameter of the laser beam (various resolution) with the same screen ruling. In order to produce printing forms and control prints, films were copied to positive printing plates coated by photosensitive cresol-formaldehyde layer. An influence of laser beam diameter, i.e. output resolution on dot sharpness was investigated by analyzing the microscopic pictures of dots formed in thin layer of photo emulsion, photosensitive coating of the printing plate and thin layer of printing ink. The geometric characteristic of screen dots was determined: a dot perimeter / dot surface ratio, dot contour shape and length, screen ruling and ton value, and their influence on the ton value increase in printing.

*P.S.A.51*

**EXPERIMENTAL ANALYSIS OF CRACK INITIATION AND GROWTH IN WELDED  
JOINT OF STEEL FOR OPERATION AT ELEVATED TEMPERATURES**

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Successful application of steel for operation at elevated temperatures, designed for highly loaded welded structures operating under conditions of elevated temperatures and high pressures, depends on the properties of critical regions of a welded joint. Heat affected zone (HAZ) and weld metal (WM) are potential locations of crack initiation, i.e. the locations where local brittle zones may form to whom crack initiation is ascribed.

For better understanding of the cause and mechanism of crack initiation and growth in welded joints of steel designed for operation at elevated temperatures and high pressures, it is necessary to establish how does the heterogeneity of the structure and mechanical properties of a welded joint affect the crack initiation and growth and to express quantitatively the parameters affecting-controlling the local strain behaviour and crack growth. In the analysis, we shall use critical stress intensity factor, i.e. critical J-integral, as the parameters of fracture mechanics, as well as the fatigue-crack parameters. Determination of these parameters in parent metal and identification of the location and structure of critical regions in heat affected zone provide higher degree of structural safety.

*P.S.A.52*

**THE POSSIBILITIES OF USING ELECTRO FILTER ASH OF STEAM POWER PLANT „PLJEVLJA“ AS RAW MATERIALS MIXTURE COMPONENT FOR OBTAINING SINTERED PRODUCT**

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The aim of the investigation was to examine the possibilities of using electrofilter ash of steam power plant „Pljevlja“ as raw materials mixture component for obtaining sintered product. The second component of raw materials mixture was an illite-kaolinite clay type. The raw materials mixture was prepared with different contents of electrofilter ash (10 mass%, 20 mass%, 30 mass%, 40 mass% and 50 mass%). The specimens were formed by plastic shaping in a parallelepiped mould with the dimensions 7.7 cm x 3.9 cm x 1.6 cm. The clay and electrofilter ash characterisation was performed by the determination of mineral content by x-ray analysis, determination of chemical content and granulometric analysis for determination of particle size distribution. The linear and volume shrinkage during drying to the constant mass in air and dryer were determined. The specimens were fired at the temperatures of 800<sup>0</sup>C, 900<sup>0</sup>C, 1000<sup>0</sup>C, 1100<sup>0</sup>C, 1200<sup>0</sup>C.

The investigation results demonstrate that the electrofilter ash of steam power plant „Pljevlja“ can be used as raw materials mixture component for obtaining sintered product with satisfactory characteristics for total porosity, volume shrinkage and compression strength.

P.S.A.53

**INFLUENCE OF BASICITY OF ELECTRODES COVERING AND WIRE  
COMPOSITION OF ELECTRODES KERNEL ON THE STRUCTURE AND  
PROPERTIES OF WELD OF LOW ALLOY STEELS**

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Production of covered arc welding electrode present very complex research work and technological process what means processing of receipt (composition of electrode covering) for metal arc hand welding. Role of electrode covering is complex because it use for stabilization of electric arc, degassing, deoxydation and for additional alloying as well. An electrode covering has refinement effect on weld and micro alloying effect, as well. Primary alloying is realized trough electrode wire. System electrode covering – wire request exactly calculation of oxygen potential of electrode covering, because small diapason of oxygen content is existing in a weld of low alloy steels providing a creating more than 80% of acicular ferrite in the structure.

Electrodes belong to program range of Electrodes Plant "Piva - Pluzine". Changeing of composition of electrode covering ( basicity) and electrode kernel intended for welding of low alloy steels.

Results of investigation are related to qualitative and quantitative analysis of type and content of nonmetallic inclusions and structural components, and their influence on the properties, as well.

Increase of content of acicular ferrite in the structure of weld and decreasing of content of nonmetallic inclusions are realized upon increase of basicity of electrodes covering.

P.S.A.54

## NEW DIRECTION IN SOLID STATE SCIENCE

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It is necessary to attract attention of scientific community to the following facts. In 1969 a hypothesis had been formulated concerning existence of an elementary unit of crystal substance – a "crystal quantum". In 1970 this work has been published. In 1994 on the basis of it a sequential theory of secondary crystal structure (SCS) was built. Since 1994 different applications in chemistry, physics, mechanics of solid have been developed<sup>1-3</sup>. It was shown that the SCS theory reflects real processes in solid quite adequately both qualitatively and quantitatively. For example, it is known that properties of crystal particles with dimensions  $\sim 10^{-6}$  cm and less (nanoparticles) differ considerably from properties of massive crystals. Materials containing sufficient quantity of such particles have unusual properties important for practice. That is why all developed countries have national programs on nanoparticle science and technology. Though unusual situation takes place here. Existing theories of condensed matter can not explain why nanoparticle properties differ from properties of massive substance. All over the world nanoparticles and materials on the basis of them are produced to an increasing extent (thousands of tons per year), but the nanoscience is still guessing about this difference in properties. Therefore, the work on the national programs is carried out on the basis of empirical approach to the problem of nanoparticles. The SCS theory explains nanoparticle properties on the basis of a term "Elementary crystal unit". This unit ("minimal crystal – mic") is an analog of molecule, i.e. giant molecule of solid with the approximate size 300 Å. A particle of smaller size is "subcrystal", an analog of molecule-radical. As any radical, the subcrystal has increased energy content and reactivity. Many properties of nanoparticles become understandable. For example, a discussion takes place about the upper limit of nanoparticle dimensions. The SCS theory gives clear answer:  $300 \pm 100$  Å.

Another example. In mechanics of solid one of the basic concepts is dislocation. The existing theory considers it as defect of crystal atomic structure. The dislocation theory is developing more than 50 years – thousands of papers, tens of teaching courses etc. Now this theory, apparently, isn't capable to explain and predict correctly many facts. The SCS theory considers dislocation as defect of the secondary crystal structure – one of manifestations of boundary gaps between elementary crystal units. To explain plastic deformation, the existing theory introduces artificial concepts: edge dislocation, screw dislocation, Burgers vector etc. According to the SCS theory, plastic deformation is mutual displacement on mic boundaries.

Similar examples exist in other sections – isomorphism, catalysis, electron transport – as well. So, on the basis of the concept "subcrystal" there was proposed a new mechanism of heterogeneous catalysis. There was proposed new mechanism of Gunn effect in semiconductors. Now a new scientific trend is formed: "Secondary crystal structure – theory and its applications in chemistry, physics, mechanics of solid". It is represented by many publications: theses (more than 40 conferences in Europe and Russia), papers, the monograph "Secondary structure and properties of crystals". Further development of the SCS theory as well as creation of valuable apparatus of the theory give us new useful results in different branches of Solid State Science.

*P.S.A.55*

**PREPARATION OF BORON CARBIDE NANOWIRES VIA EPITAXIAL VLS GROWTH**

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At first polydispersed Nickel nanocrystalline islands were electrochemically deposited on a graphite surface. This catalyst deposited surface acts as growth substrate which placed in a crucible that carbothermal reduction of boric oxide occurs. Boron carbide nanowires synthesized via a VLS mechanism. X-Ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared spectrum (FTIR) were employed to study the crystal phase, morphology, stoichiometry and structure of the prepared nanowires.

*P.S.A.56*

**SYNTHESIS OF BORON CARBIDE NANOWIRES AND NANORODS VIA CARBOTHERMAL-VLS ROUTE**

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Boron carbide nanowires have been synthesized through a carbothermal reaction in an induction furnace by using of boric oxide and carbon black as the starting mixture small amounts of Ni nanoparticles added to the mixture which caused the formation of nanowires via VLS mechanism also small amounts of NaCl was added to facilitate the nanowires formation and catalyst transportation in the reaction environment. X-Ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared spectrum (FTIR) were employed to study the crystal phase, morphology, stoichiometry and structure of the prepared nanowires.

*P.S.A.57*

**STRAIGHT BORON CARBIDE NANORODS VIA A CARBOTHERMAL TEMPLATE ASSISTED METHOD**

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Straight Boron carbide ( $B_4C$ ) nanowires have been prepared through a template assisted route via a VLS mechanism. At the first step slight amount of Ni is deposited at the bottom of AAO (Anodic Aluminum Oxide) channels by AC deposition and in the second step nanowires synthesized via a VLS mechanism. The mechanism involves carbothermal reduction of the boric oxide and subsequently transport of boron and carbon via gas-phase species to the melted Nickel which acts as catalyst metal at the bottom of AAO channels. X-Ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared spectrum (FTIR) were employed to study the crystal phase, morphology, stoichiometry and structure of the prepared nanorods.

*P.S.A.58*

**SYNTHESIS OF TITANIUM DIBORIDE NANOWIRES AND NANORODS VIA CARBOTHERMAL-VLS ROUTE**

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Titanium diboride nanowires have been synthesized through a carbothermal reaction in an induction furnace by using of Titanium oxide boric oxide and carbon black as the starting mixture. Small amounts of Ni nanoparticles added to the mixture which caused the formation of nanowires via VLS mechanism also small amounts of NaCl was added to facilitate the nanowires formation and catalyst transportation in the reaction environment. X-Ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared spectrum (FTIR) were employed to study the crystal phase, morphology, stoichiometry and structure of the prepared nanowires.

*P.S.A.59*

**PREPARATION OF BORON CARBIDE NANOWIRES VIA A TEMPLATE ASSISTED POLYMERIC PRECURSOR**

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Straight Boron carbide ( $B_4C$ ) nanowires have been prepared through a template assisted method by a low temperature pyrolysable polymeric precursor of boron carbide in a conventional furnace. The precursor prepared from low cost materials and its ceramic conversion is possible at 400-800°C. An open pore anodic aluminum oxide template was filled by the polymeric precursor subsequently the filled templates heat treated at ceramic conversion temperature of the polymeric precursor which yields a boron carbide filled template then the template removed by immersing in HF acid and yield straight Boron carbide nanowires. X-Ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared spectrum (FTIR) were employed to study the crystal phase, morphology, stoichiometry and structure of the prepared nanowires.

*P.S.A.60*

**PREPARATION OF BORON CARBIDE NANOFIBERS VIA A THREE STEP METHOD FROM PAN NANOFIBERS**

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Boron carbide ( $B_4C$ ) nanofibers have been prepared through a three step method. At first electro-spinning process was used for the fabrication of PAN nanofibers, and in the second step PAN nanofibers carbonized in a conventional furnace and in the last step carbonized fibers converted into boron carbide nanofibers by  $B_2O_2$  gas. X-Ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared spectrum (FTIR) were employed to study the crystal phase, morphology, stoichiometry and structure of the prepared nanofibers.

*P.S.A.61*

**TIME-DOMAIN PHOTOTHERMAL RESPONSE OF MEDIA WITH THERMAL  
MEMORY FOR VARIOUS SHAPES OF INCIDENT PULSES**

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Generalized model of time-domain photothermal response including thermal memory effects is derived. The influence of thermal memory to time-domain photothermal response for various shapes of incident pulses is analyzed. It is shown that photothermal pulse techniques have a great potential for determination of both material memory characteristics, thermal relaxation time and heat propagation speed.

*P.S.A.62*

**SMALL POLARON ELECTRICAL CONDUCTIVITY IN MACROMOLECULAR  
CHAINS**

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The temperature dependance of electrical conductivity of quazy one-dimensional crystal systems in which exists strong electron-phonon interaction is calculated in antiadiabatic limes. The calculation is based on previously developed model based on standard Holstein MCM model including the changes of phonon spectra due to small polaron effects. Obtained resultes show significant increase of electrical conductivity in the areas of low and medium temperature compared with standard Holstein model values. This can be very important for experimental verification of small polaron presence in examined structures.



P.S.A.63

**CHARACTERIZATION OF ORGANIC/METAL INTERFACES USING QUANTUM THEORY OF ATOMS IN MOLECULES: CORRELATION WITH EXPERIMENT**

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Herein the quantum theory of atoms in molecules (QTAIM) is fundamentally established as a valuable means of investigating the nature of the interactions between organic molecules and metallic surfaces from the physically justified (invariant) standpoints. The topological features of the electron density at the bond critical point (BCP), such as the Laplacian and ellipticity, associated with the relevant natural charges are shown to be a determinative factor of the nature of a specific interfacial interaction. A general methodology for the determination of the nature of the interfacial interactions is proposed by investigating the changes of the organic/metal BC parameters as consequences of both increasing the size and changing the shape of the metal surfaces. In particular, the adsorption of acrylonitrile (AN) on the model copper (Cu) clusters ( $\text{Cu}_n$ ,  $n = 9-14, 16, 18, 20$ ) simulating the actual Cu(100) surface is analyzed. Several statistical models with their goodness of fitting the data obtained by use of the topological analysis of the charge density at the AN/Cu<sub>n</sub> BCPs are reported. In this way the extrapolation of the nature of the AN/Cu(100)-bonded interaction becomes possible. The dipole moment, as a chemical descriptor arising directly from the electron density distribution in each of the model systems, is shown to be well-correlated with the experimentally determined electron affinities and ionization potentials of the Cu<sub>n</sub> clusters. Based on the experimental ionization potentials of some single atoms that are comparable to those of Cu<sub>n</sub> clusters, elucidation of the role of copper (100) surface in transferring charge to the AN organic molecule is given. One of the key beauties of this novel strategy essentially associated with the electronic properties and reactivity of various Cu<sub>n</sub> clusters is that, in getting these results, no reference to orbitals being pure theoretical constructs has been invoked. As the proposed methodology is independent of the scale and size of particular molecular components, its potential applications in changing and tuning the finest details of charge transfer taking place in the donor-acceptor complexes at the nanoscale is quite certain.

*P.S.A.64*

### **URANIUM (VI) ADSORPTION ON ACIDS MODIFIED ZEOLITIC TUFF**

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Acid modified natural zeolites are the prosperous materials for uranium (VI) removal from water solution. The modified zeolite samples were obtained by treatment of zeolite - clinoptilolite with acids: hydrochloric, oxalic and citric. Adsorption was investigated at different amounts of solid phase in suspension, different concentrations of uranium (VI) in solution, as well as at different pH values. Starting and modified zeolites were characterized by chemical analysis, XRPD analysis, thermal (DT/TG) analysis, IR spectroscopy, SEM and by determination of cation exchange capacity, while starting and nonadsorbed amounts of uranium (VI) ion were determined by fluorometric method. Modification of zeolitic tuff with acids significantly increased adsorption of uranium (VI). Uranium (VI) adsorption data for zeolite modified with hydrochloric acid was fitted to the Langmuir model.

*P.S.A.65*

### **BASIC OPTICAL MATERIALS OF FERRULE AND THEIR PERFORMANCE**

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In the early days of optical fiber jointing sophisticated manufacturing techniques were applied. Optical materials, such as alignment tool for securing of two fiber ends within metal tubes or ferrules, are increasingly popular nowadays, especially in the field of telecommunication and computer nets. Basic ferrule designs resorted to watch jewels made from synthetic ruby or sapphire which were inserted into tubes. These jeweled ferrules are still used for connecting to test equipment. Most fiber optic connectors comprise a ferrule which is responsible for control of fiber alignment. Nowadays, the ferrule is usually made of ceramic material, because it is accepted as being nearly as good. The particular ceramic is known as zirconium (zirconium dioxide  $ZrO_2$ ) chosen because its hardness and thermal coefficient of expansion is very similar to glass. It also polishes well. Material is usually tetragonal zirconium polycrystalline, which is zirconium and yttrium (yttrium oxide  $Y_2O_3$ ). This paper deals with the coupling properties of ferrules made of different materials and their junctions which produce various losses.

P.S.A.66

**CORRELATION BETWEEN ISOTHERMAL ANNEALING AND MAGNETIC SUSCEPTIBILITY RELATIVE CHANGE OF THE  $\text{Fe}_{89.8}\text{Ni}_{1.5}\text{Si}_{5.2}\text{B}_3\text{C}_{0.5}$  AMORPHOUS ALLOY**

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Structural changes of amorphous ribbon  $\text{Fe}_{89.8}\text{Ni}_{1.5}\text{Si}_{5.2}\text{B}_3\text{C}_{0.5}$ , causing its isothermal expansion, were investigated by sensitive dilatation method and X-ray analysis. The measurements were carried out concerning ribbon samples thermal expansion, having been exposed to constant strain degrees of  $\sigma_1 = 130$  MPa,  $\sigma_2 = 300$  MPa and  $\sigma_3 = 475$  MPa at temperatures  $T_1 = 653$  K,  $T_2 = 673$  K and  $T_3 = 693$  K. It has been determined that isothermal ribbon expansion is caused by the structural relaxation process. It has been shown that structural relaxation process occurs in two stages. The first stage is characterized by linear logarithmic dependence of isothermal ribbon expansion upon time ( $\ln(\Delta l) = f(\tau)$ ). It implies that the first stage of structural relaxation process is rapid kinetic process. The process time decreases with the increase in annealing temperature. The second stage of structural relaxation process is characterized by linear dependence of isothermal expansion upon the square root of process time ( $\Delta l = f(\tau^{1/2})$ ). Such time dependence of isothermal expansion shows that the second stage of structural relaxation process is a slow diffuse process. For both stages of structural relaxation process, for the ribbon sample exposed to strain degree of 475 MPa, rate constants were determined  $k_1' = 6,25 \cdot 10^{-3} \text{ s}^{-1}$ ,  $k_1'' = 9,56 \cdot 10^{-3} \text{ s}^{-1}$ ,  $k_1''' = 14,59 \cdot 10^{-3} \text{ s}^{-1}$ ,  $k_2' = 2,82 \cdot 10^{-4} \text{ s}^{-1}$ ,  $k_2'' = 6,11 \cdot 10^{-4} \text{ s}^{-1}$ ,  $k_2''' = 16,48 \cdot 10^{-4} \text{ s}^{-1}$  as well as activation energies  $E_1 = 79,72$  kJ/mol,  $E_2 = 165,80$  kJ/mol. The results of X-ray analysis show that during these processes the ribbon preserves its amorphous structure with reduced defects density and reduced internal strain.

Temperature dependence of the magnetic susceptibility relative change was investigated by the modified Faraday method in the temperature region from room temperature up to 900 K, in argon atmosphere.

*P.S.B.1*

**EXCITON STATES IN IRREGULAR TYPE-II QUANTUM-DOT SUPERLATTICES  
IN A MAGNETIC FIELD**

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The electronic structure and the optical properties of superlattices composed of quantum-dots of different size are computed. We analyze recently fabricated superlattices of ZnTe/ZnSe quantum dots, where the hole is confined inside the dot, while the electron is localized outside, and therefore allows for optical Aharonov-Bohm oscillations typical for type-II quantum dots. For the irregular stacks of quantum dots, composed of a wide quantum dot and a few smaller quantum dots in the period of the superlattice we find that the hole wavefunction is distributed in the matrix, close to the radial boundary of the smaller dots, and therefore the binding energy in these stacks is reduced with respect to those composed of equal-sized quantum dots.

*P.S.B.2*

**CORE-LEVEL AND VALENCE BAND STUDIES OF (GaMn)As WHISKERS**

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Following the recent discovery of the technique of growth of (GaMn)As whiskers by molecular beam epitaxy at a temperature in the range 300-350 °C, a detailed study of the core-level and valence bands of these structures has been made using synchrotron-based photoemission. A comparison has also been made between the results obtained for the whiskers to those reported previously for (GaMn)As films. The origin of these differences has been discussed.

P.S.B.3

### MODELLING THE INFLUENCE OF DIFFERENT PACKAGING ON RADFET RESPONSE TO PROTON IRRADIATION

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Radiation sensing MOSFETs (RADFETs) have found numerous applications in space, nuclear industry and research, and radiotherapy. Since protons contributions is an important part of the space radiation environment, numerical simulations of RADFET proton response has been studied in this paper. Speciality proton irradiation results of RADFETs indicate that the RADFET response is dependent on proton energy and the packaging effect. In this work, the proton transport Monte Carlo software SRNA-2KG has been adopted for determining the energy deposited in RADFET structure and dose distribution within microscopic dimensions of the dosimeter sensitive volume. The SRNA simulation method demonstrated the analysis of the influence of different packaging configurations on RADFET response to proton irradiation.

P.S.B.4

### COMPOSITION DEPENDENCE OF THE DC AND AC CONDUCTIVITY OF NON-CRYSTALLINE SEMICONDUCTORS OF $\text{Cu}_x[(\text{As}_2\text{Se}_3)_{0.9}(\text{AsI}_3)_{0.1}]_{100-x}$ TYPE

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Glasses based on the multicomponent pseudobinary system  $(\text{As}_2\text{Se}_3)-(\text{AsI}_3)$  with addition of copper were carefully characterized to establish the correlation between chemical composition and the magnitude and behaviour of electrical conductivity. The DC conductivity of the bulk samples measured as a function of temperature shows semiconducting behaviour of the Arrhenius-type. The AC conductivity has been measured in the range of  $10^2-10^6$  Hz at different temperatures and found to be proportional to  $\omega^s$ . The parameters like pre-exponential factor  $\sigma_0$  and activation energy  $E_\sigma$  or frequency exponent  $s$  were analyzed from the aspect of mechanism of conductivity. It was found, also, that addition of copper significantly increase the conductivity of investigated glasses.

P.S.B.5

## DEVELOPMENT OF FINE-GRAINED OXIDE CERAMICS USING PULSED COMPACTION OF LOW AGGLOMERATED NANOPOWDERS

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Institute of Electrophysics UD RAS develops the technologies and modern equipment for synthesis and consolidation of low agglomerated nanopowders with the aim of sintering fine-grained ceramics for construction and functional applications.

Currently, the installations for nanopowders synthesis by the methods of electrical explosion of wires (EEW) and pulsed CO<sub>2</sub> laser evaporation (PLE) are available. When the processes of electrical explosion of wires are realized in oxygen-containing media, nanopowders (20 nm – 1 μm) of a number of oxides, such as Al<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, ZrO<sub>2</sub>, CuO, NiO, MgAl<sub>2</sub>O<sub>4</sub>, etc., are obtained. The productivity of the EEW systems created is 40–200 g/h, depending on the wire material, at a power consumption less than 50 kW-h/kg.

For the production of weekly agglomerated nanopowders of complex composition, it was proposed to use a repetitively pulsed CO<sub>2</sub> laser that ensures evaporation of the target material followed by synthesis of nanoparticles in the stream of buffer gas. Technological modes have been determined in which the productivity of the system is 15–80 g/h with radiation power inputs of 8–30 kW-h/kg. Foundations were developed for the technology of synthesis of a number of nanopowders containing solid solutions of complex oxides: YSZ, SmDCe, GdDCe, Nd:YAG, Nd:Y<sub>2</sub>O<sub>3</sub>, and others. A distinctive feature of this type of powders is a small average particle size (10–15 nm) with a narrow size distribution: more than 98% of the particles are less than 40 nm in size.

Investigations have shown that Magnetic Pulsed Compaction (MPC) is an efficient method for pressing of a wide spectrum of powdered materials, especially on the nanometer particle size scale. MPC provides compacted powder states of increased density, promotes destruction of particle agglomerates, and favors structural transformations resulting in microdistortions of the lattice, defects, and phase transitions. Two types of equipment were developed which harness flat and cylindrically converging compression waves.

Sintering technologies have been developed for a number of oxide ceramics with fine nanosized structure, including those based on Al<sub>2</sub>O<sub>3</sub>, tetragonal and cubic YSZ, GDCe, TiO<sub>2</sub>, etc., which use MPC and subsequent sintering of weakly agglomerated nanopowders.

The nanostructured ceramics of YSZ and GDCe solid solutions shaped as thin-layered (10–500 μm) plates or tubes have been shown to be promising as electrolytes for solid-oxide fuel cells (SOFC's), the most important units in hydrogen power systems. Due to their fine structure, these materials feature improved oxygen-ion conductivity and allow formation of thin gas-tight layers, which are necessary for efficient operation of SOFC's at temperatures as low as 600–800°C.

The sintered submicron-structured ceramics based on Mg-doped Al<sub>2</sub>O<sub>3</sub> exhibits high hardness and resistance to abrasive wear and high-temperature corrosion. The efficiency of its application as a structural material under erosive and abrasive wear conditions has been demonstrated.

*P.S.B.6*

### SINGLE CRYSTAL ALLOYS. THERMAL FATIGUE AND CREEP

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Tests for creep and thermal fatigue of single crystal samples from a heat resisting nickel base alloy with different crystallographic orientations are carried out. Tests for creep were carried out by a standard technique down to destruction, test for thermal fatigue by a special technique with clamp flat sand-glass shaped test-pieces with the polished surface and to provide their cyclic heating by current conducting in vacuum. During tests were observed with use of a microscope  $\times 250$  processes of formation of lines of sliding and micro cracks. Are constructed isochrones curves of creep, the data on conditions of origin of micro cracks and destruction of samples with orientations 001, 011 and 111 without concentrators and with the concentrator as apertures in diameter of 0,5 mm are received at thermo cyclic loading. Tests for creep were carried out at 900 and 1000 °C, tests for thermal fatigue - with the maximal temperature of cycle  $T_{\max}=850, 900, 950, 1000$  and  $1000^{\circ}\text{C}$  with stay of 2 and 5 minutes and without stay at  $T_{\max}$ . Dependences of numbers of cycles before destruction from orientation,  $T_{\max}$ , time of stay, stress concentration are determined. It is established, that character of destruction at thermo cyclic loading (shear and cleavage) depends on a mode of test and crystallographic orientations; the stay at the maximal temperature of a cycle intensifies the ratcheting processes. Results of tests for creep are used for settlement definition of damages at thermo cyclic loading. The received data are supposed to be used for computation of life durability and safety factors of single crystal gas turbine blades.

*P.S.B.7*

### OPTICAL AND MAGNETIC PROPERTIES OF PbTe(Ni) SINGLE CRYSTALS

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Semimagnetic semiconductors have attracted a great deal of interest not only for their potential use in spintronics, but also because of the fundamental question of how a magnetic metal can be derived from a paramagnetic insulator. The most common method involves substitution of d-elements into a crystal structure of IV-VI semiconductors. In this paper we used X-ray, far-infrared reflectivity, magnetic susceptibility and Hall effect measurements to investigate transport, optical and magnetic properties of PbTe(Ni) single crystals. The Ni concentration in the samples used here were  $1 \cdot 10^{19}$  and  $2 \cdot 10^{19}$  at./cm<sup>3</sup>. Agreement between experimental results and models for phonon and magnetic structure, which predict existence of impurity atoms in different valence states, are very good.

*P.S.B.8*

### ELECTRON STRUCTURE AND LUMINESCENCE PROPERTIES OF $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$ GARNET CRYSTALS

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The crystals with garnet structure are prospective materials for scintillation detectors and solid state lasers. Their recent development has aroused interest in the investigation of their physical properties.

This paper reports on results of investigation of electronic structure and luminescence properties of  $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$  garnet crystals.

The  $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$  garnet crystals were grown by the Czochralski technique in a flow of dry oxygen using a platinum crucible. The edge of fundamental absorption of  $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$  garnet crystals is observed at  $\lambda \sim 240$  nm ( $T=80$  K). At 80 K the cathodoluminescence spectrum of undoped  $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$  besides the UV luminescence band with maxima near 360 nm, the bands due to luminescence of defects and bands characteristic to Cr or Mn microdoping are observed. The UV band can be excited at band to band and exciton absorption region, is not elementary and presents a superposition of at least two bands. The origin of UV luminescence is discussed.

X-ray photoelectron and emission spectroscopes have been used to study the electron structure of  $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$  garnet crystal. The experimental X - ray emissions spectra of components in  $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$  garnet crystals were matched (used core level energy) in unified energetic scale. X-ray emissions spectra Ga and Ge in  $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$  garnet crystals were obtained at 80K and 300K using a tube spectrometer equipped with an RKD-01 co-ordinate detector.

*P.S.B.9*

### REFRACTION IN 2D HEXAGONAL-LIKE PHOTONIC CRYSTALS

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We study refraction in 2D dielectric hexagonal-like photonic crystal Archimedean lattices. The tools which are used are the planewave method (for calculations of band structures and band maps) and FDTD simulations for calculation of electromagnetic propagation through these structures.



*P.S.B.10*

### **SYNTHESIS AND SANS STUDY OF POROUS ANODIC TiO<sub>2</sub> FILMS**

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Films of anodic titania are composed of nanotubes aligned perpendicular to the metallic substrate, which tend to self-organize into ordered structure. Diameter of the nanotubes depends on oxidation conditions and can be varied in wide range. Porous TiO<sub>2</sub> was obtained by anodization of metallic titanium foils in two-electrode cell in the solution of 0.5% NH<sub>4</sub>F in glycerol or in ethylene glycol (0.25% NH<sub>4</sub>F) with addition of natrium dodecyl sulfate. Small angle neutron scattering (SANS) allowed finding symmetry of local surrounding in the porous structure depending on anodization voltage. Values of interpore distance calculated from SANS data are in good agreement with SEM and TEM data. This work was supported by RFBR grants 06-08-01443-a and 06-03-89507-HHC\_a.

*P.S.B.11*

### **DYNAMIC OF THE PROFILE CHARGING IN TWO FREQUENCY PLASMA ETCHING OF SiO<sub>2</sub>**

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Etching submicron features in insulating material such as SiO<sub>2</sub> or other materials masked with insulators is accompanied by feature charging effects caused by differences in electron and ion angular distribution functions. In this paper we shall present some new results of our efforts to include charging effects in 3D level set etching profile evolution simulations, related to the temporal dynamic of the profile charging. PIC/MCC code will be employed for obtaining the energy and angular distribution functions of the charged particles in two-frequency plasma discharges. These data will be used as the boundary conditions for the calculations of ion fluxes incident on the profile surface. Finite difference method cannot be used when the geometry of the problem is irregular, as it is usual for the etching profiles, so the calculations of the electric field generated by the profile charge are performed by integrating of a finite element solver in our simulation framework.

P.S.B.12

**CRYSTAL STRUCTURE OF A AND B SITE Ce DOPED  $\text{CaMnO}_3$  PEROVSKITE**

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In the case of Ce substituted Ca-manganites the rare-earth element in the A site has multiple valence state and will be likely incorporated as 3+ on the A-site and as 4+ on the B site, and this can further increase the charge disorder in the Mn ( $\text{Mn}^{2+}$ ,  $\text{Mn}^{3+}$  and  $\text{Mn}^{4+}$ ) site. In cerium-doped manganites, it is possible for  $\text{Ce}^{3+}$  and  $\text{Ce}^{4+}$  species to coexist in the same compound, adding an extra source of structural disorder. The experimental data on cerium-doped manganites available in the literature are limited nowadays. There are few studies about these compounds, but none of the papers have taken the possibility of multiple valence states of Ce into account. Using modified glycine/nitrate procedure we synthesized Ce doped manganites with nominal compositions:  $\text{Ca}_{0.5}\text{Ce}_{0.5}\text{MnO}_3$  and  $\text{CaMn}_{0.5}\text{Ce}_{0.5}\text{O}_3$ . Using XRPD analysis we investigated possibility of incorporation of Ce ions in positions A and B of the perovskite structure. Influence of Ce ions on unit cell volume of the perovskite compound, occupation numbers and distances between atoms were analysed. Our study on the samples,  $\text{Ca}_{0.5}\text{Ce}_{0.5}\text{MnO}_3$  and  $\text{CaMn}_{0.5}\text{Ce}_{0.5}\text{O}_3$ , suggests that samples with these nominal compositions do not form single-phase compounds with perovskite structure. Instead, they form multi-phase mixtures comprising perovskite with Ce ions in the solid solution and free  $\text{CeO}_2$ . Amount of cerium added to form solid solution, overcomes solubility limit under the experimental conditions applied in this study. Microstructure size-strain analysis was performed as well as Raman spectroscopy investigations.

*P.S.B.13*

### PHONON CONTRIBUTION IN THERMODYNAMICS OF CRYSTALLINE QUANTUM WIRES

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Spectra of possible phonon states, as well as thermodynamic characteristics of quantum wire of simple cubic crystalline structure are analyzed in this paper, using the method of two-time dependent Green's functions. Internal energy of the system as well as thermal capacitance of quantum wire in low temperature region are found. The temperature behavior of quantum wire's specific heat is compared to that of corresponding bulk structure. It is shown that at extremely low temperatures thermal capacitance of quantum wire is considerably lower than the thermal capacitance of bulk sample. Consequences of this fact are discussed in detail and its influence to kinetic and thermodynamic properties of materials are estimated.

*P.S.B.14*

### STRUCTURAL DEFORMATION IN Hf<sub>2</sub>Ni OBSERVED BY TDPAC METHOD

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The electric quadrupole interaction in Hf<sub>2</sub>Ni was measured at <sup>181</sup>Ta probe using the time-differential perturbed angular correlation method (TDPAC) in the temperature range 78 to 1314 K. Analysis of the obtained spectra revealed the presence of a single nuclear quadrupole interaction (NQI) and its linear descending dependence with increasing temperature. In the region 1134 to 1314 K, the presence of structural deformation is evident from the coincidence spectra.

*P.S.B.15*

**THE EFFECTS OF POLARIZATIONAL BREMSSTRAHLUNG IN ELECTRON  
COLLISIONS WITH CLUSTERS**

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In this paper we consider the emission of photon in scattering of electrons with some clusters. Our calculations are investigated when the radiation of the clusters (atomic) electrons is significant and dominates in the whole spectrum. This is the case when the emitted photon frequency is comparable with the energy of the plasmon resonance in a cluster.

Using the many body treatment we present the theory of polarizational bremsstrahlung and the calculations of the cross sections of this process for some clusters. The obtained results are very important in the nano region, and significant for designing new materials.

P.S.B.16

## PREPARATION AND IR-SPECTROSCOPIC CHARACTERIZATION OF AURIVILIUS BI-LAYERED PEROVSKITE

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Several bismuth-layered crystal structures and their properties have been investigated in detail. However, a lot of aspects of the preparation and properties of barium bismuth titanate remain unexplored, whereas being promising candidate for memory applications.

In present work barium-bismuth titanate ( $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ ) was prepared from stoichiometric quantities of barium titanate and bismuth titanate obtained via mechanochemical synthesis. Barium titanate ( $\text{BaTiO}_3$ ) has been synthesised from mixture of  $\text{BaO}$  and  $\text{TiO}_2$  and bismuth titanate ( $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ ) was prepared starting from  $\text{Bi}_2\text{O}_3$  and  $\text{TiO}_2$ , commercially available. Mechanochemical synthesis in both cases was performed in air atmosphere in a planetary ball mill for time up to 720 min. Milling conditions were: zirconium oxide jars and zirconium oxide balls, ball-to-powder weight ration 20:1 and determined basic disc and disc with jars rotation speed. The powder mixture of  $\text{BaTiO}_3$  and  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  was homogenized for 60 min and after that sintered at 1100 °C. Separatly,  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  was sintered in region 875-1000 °C, in both cases without pre-calcination step and by conventional sintering technique.

The phase formation and crystal structure of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  and  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$  powders were analysed by XRD analysis revealing the existance of tetragonal phase. Also structures of these powders were investigated by IR spectroscopy. The characteristic bands of these powders were identified and analyzed. For this a deconvolution of each experimental spectrum was made using a Gaussian type function. The morfology of obtained powders was exhamined by SEM and TEM method. The microstructure development of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  and  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$  ceramics was followed by SEM. Microstructure of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  is in accordance with the view that  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  exhibits plate-like grains with thr average grain size increasing with the sintering temperature. It is evident that  $\text{Ba}^{2+}$  adition leads to the change in the microstructure development, particularly in the change of the average grain size and homogeneity of the grains of  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ .

*P.S.B.17*

**EVOLUTION OF STRUCTURE AND PROPERTIES OF Ti-Si-C COMPOSITES AT MECHANICAL SYNTHESIS AND HOT PRESSING**

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Composites of the ternary carbide  $Ti_3SiC_2$  received by mechanical synthesis of system Ti-Si-C in vacuum chamber are investigated. It is shown that at mechanical synthesis with the subsequent hot pressing the composite consisting from  $Ti_3SiC_2$  and TiC is formed. The samples sintered at 1400-1500 °C have a microporous structure at 85 % relative density. Hot pressing allows reaching 98-99 % relative density. The effect of decrease of Vicker's hardness in polycrystalline samples is found out at increase in the loading, caused by the area of contact of an indenter with a sample. Results of the analysis of structure and some physical-mechanical properties of a synthesized material are submitted. Polycrystalline  $Ti_3SiC_2$  at density of 98-99 % has crack resistance 11.4-12.6 MPa·m<sup>1/2</sup>.

*P.S.B.18*

**ANALYTICAL MODEL OF DRIFT REGION VOLTAGE IMPACT ON SiC DIMOSFET STRUCTURE CHARACTERISTICS**

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The present silicon technology is reaching the material's theoretical limits and cannot meet all the requirements of the modern electronics. The semiconductor silicon carbide (SiC) has been identified as a material with the potential to overcome silicon limitations, because of its superior material advantages such as large bandgap, high critical breakdown field and high thermal conductivity. SiC electron components are suitable for high-power, high-temperature and high-frequency applications. This paper presents new observations resulting from the investigation of the SiC based vertical Double Implanted Metal Oxide Semiconductor Field Effect Transistor (DIMOSFET). The observations are described and presented by the analytical model of the drift region voltage impact on SiC DIMOSFET structure characteristics. The drift region is divided into sections. For each of them, voltage analytical model across the corresponding section is developed. Drain to source voltage model is created from the mentioned partial voltages. Finally, current-voltage characteristic is obtained. Exposed model is based on the physics of the SiC DIMOSFET. In the model all relevant effects are taken into account. At the same time proposed model is relatively simple. By using developed model simulations were performed. Obtained results are in a very good agreement with already known ones, available in literature.

*P.S.B.19*

**ENERGY LOSS AND DEFLECTION OF FAST IONS MOVING PARALLEL TO THE GRAPHENE SHEET**

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We investigate the interactions of fast ions with graphene, describing the excitations of the electron gas in graphene by a two-dimensional hydrodynamic model. By linearizing the hydrodynamic equations, we derive general expressions for the induced potential, the stopping force and the image force for an ion moving parallel to the graphene sheet. Moreover, the Barkas effect on the stopping force and the analogous corrections to the induced potential and the image force are evaluated within the second-order perturbation approach to the hydrodynamic equations. The numerical results of the linear and nonlinear theories are obtained showing the influence of the ion position and its velocity on the stopping force and the image force.

*P.S.B.20*

**INVESTIGATION OF GAMMA-RAY INDUCED CHARGE IN SILICON DIOXIDE FILMS BASED ON A STOCHASTIC MODEL**

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A stochastic model based on Monte Carlo method was developed and used to investigate gamma-ray induced traps spatially distributed in silicon dioxide films. These traps can be charged positively and caused threshold voltage shift of MOS transistors. In this paper we are considered the influence of electric field applied on silicon dioxide film during irradiation on traps distribution. Also, we are analyzed corresponding threshold voltage shift of MOS transistors and its predicted statistical deviations calculated using predicted model. These results are compared with experimentally determined threshold voltage shift of MOS transistors with different voltage applied during irradiation versus gamma irradiation doses and satisfactory agreements are obtained.

*P.S.B.21*

**MATHEMATICAL MODELLING AND MULTICRITERIA DESIGN  
OPTIMIZATION OF A THIN-WALLED BEAM**

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One approach to the optimization of a thin-walled open section beam subjected to complex loads is considered. For given loads, material and geometrical characteristics the problem is reduced to the determination of minimum mass i.e. minimum cross-sectional area of thin-walled beam and minimum of safety factor for the given construction. A method is described to solve a nonlinear parameter optimization problem with several objective functions. In the present work, multicriteria optimization technique is introduced to extremise simultaneously several objective functions. For the defined multicriteria optimization model, a computer program based on interactive dialogue was developed. The graphical illustration of the above problem is presented in terms of objective functions.

*P.S.B.22*

**PARALLEL ANALYSIS OF HF MEASUREMENTS AND METHOD-OF-MOMENTS  
BASED ELECTROMAGNETIC SIMULATION OF LC EMI CHIP FILTERS**

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In this paper a parallel analysis of HF measurements and electromagnetic simulation of LC EMI chip filters is presented. Electromagnetic (EM) simulator used was method-of-moments based tool Microwave Office (MWO). Insertion loss S<sub>21</sub>(f) measurements were performed on T-type LC EMIFIL chips (CTC, Korea) realized by multilayer green sheet technology. Two different types of LC filters with peak insertion losses at 300 and 500 MHz respectively were evaluated by a network analyzer in the range from 0 to 3 GHz. After that a full equivalent electrical circuit of LC chip including parasitic components was fitted by MWO tool from the experimental data. The obtained values helped to model the parameters of internal structure of LC filters, which was finally simulated by MWO EM simulator. Obtained simulation results were compared with experimental results and validity of the adopted approach was verified. The paper presented here aims at establishing the quivalency between HF measurements and electromagnetic simulation results done on a particular commercially available LC EMI filter.



*P.S.B.23*

**MOLECULAR STRUCTURE IN CORRELATION WITH ELECTROCHEMICAL  
PROPERTIES OF MIXED-LIGAND COBALT COMPLEXES**

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Cobalt(III) and Cobalt(II) form numerous mixed ligand complexes. Some of them with nitrogen-based macrocyclic ligands could catalyze oxygen reduction. Besides, complexes with polar atoms like oxygen, sulphure or nitrogen could be corrosion inhibitors, etc. Their structural and electronic properties may simultaneously affect spectral assignments as well as potentials of possible reactions and catalytic features of the complexes. In our studies we examined some Co(III) complexes with tetraazamacrocyclic ligand and different heterocyclic dithiocarbamates as well as Co(II) complexes with octaazamacrocyclic and  $\beta$ -diketonato ligands on glassy carbon and iron in perchloric acid. Molecular structure of those compounds was formulated on the basis of spectral analysis and molecular modeling. Electrochemical properties like electrocatalysis and inhibiting effect were correlated with the molecular structure of those complexes.

*P.S.B.24*

**ANTIFERROMAGNETIC COUPLING OF COPPER(II) IONS VIA HYDROGEN  
BONDING IN Cu(II) COMPLEX WITH AN ARYLPYRAZOLE LIGAND**

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The study of magnetic properties of the novel Cu(II) complex with an arylpyrazole ligand was conducted by measuring temperature dependence of the magnetic susceptibility in the wide temperature range 2-300 K. The maximum in the susceptibility curve at 9 K with the steep decrease at lower temperatures together with the Curie-Weiss dependence in the high temperature region pointed to the antiferromagnetic coupling between Cu(II) ions. The low-temperature data were successfully fitted to the theoretical expression based on the antiferromagnetically coupled pair of Ising ions, and values of the exchange integral and magnetic moments were obtained. Measurements of the isothermal magnetization at 2 K of the complex under consideration in the wide range of magnetic fields ( $\pm 5$  T) additionally confirmed the antiferromagnetic coupling between Cu(II) ions. The crystal structure investigation of the title complex indicated that the coupling between copper ions was established via hydrogen bonding.

P.S.B.25

## UPWARD PENETRATION OF GRAINS THROUGH A GRANULAR MEDIUM

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Interparticle contact friction, packing density, and polydispersity are known to be major contributors to the macroscopic strength of granular systems, that is, their bulk resistance to deformation. For example, when a solid object penetrates a granular material, the penetration resistance increases with an increase in the degree of polydispersity, packing density and interparticle friction. In this paper, we study experimentally the penetration of guest (percolating) particles through a host granular packing. We investigate a two-dimensional (2D) granular medium, i.e., the motion of the grains is confined to a plane. This plane is tilted at an angle  $\varphi = 35^\circ$  or  $70^\circ$ . This way we control the confinement pressure inside the granular material by an effective gravity field  $g \sin \varphi$ . We prepare host granular packings of metallic cylinders of equal heights of 3 mm, by mixing small (diameter 4 mm) and big ones (diameter 6 mm) in order to avoid macroscopic crystallization. The guest grains are cylinders 5mm of diameter initially located in the narrow channel below the bottom wall of a bidimensional rectangular glass container. The forces applied to the guest grains are large enough to unjam a host packing but the driving is slow enough to stay in quasistatic flow regime. Experimentally, we focus our attention on the dependence of the microstructural properties of percolating grains (grain displacement, Voronoi volumes) on some parameters like the packing fraction of host medium, and the effective gravitational field. We show, using a novel experimental method, that the microscopic texture of the packing of guest grains is quite sensitive to the details of initial preparation of host granular packing such as mixture composition and initial packing fraction. Finally, for the case of polydispersity of percolating grains segregation occurs.

P.S.B.26

## ON THE PREPARATION OF OPEN-FRAMEWORK MANGANESE(II)- SUBSTITUTED ALUMINOPHOSPHATE

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The crystalline porous compounds constitute an important area of solid state science due to their sorption, molecular sieving and catalytic properties. Here we report on the synthesis of manganese(II)-substituted aluminophosphate (MnAPO) by 3-methylaminopropylamine. The synthesis was carried out hydrothermally in poly(tetrafluoroethylene)-lined stainless-steel autoclaves at 130-160 °C for 4-7 days in fluoride and fluoride-free reaction medium. The presence of fluoride ion affects the crystallization of obtained products. In the presence of fluoride ions a novel crystalline MnAPO was obtained whereas in the absence of fluoride ions only an AlPO solid crystallized. All products were characterized by XRD, ICP, SEM, FTIR and TG/DSC analyzes. The influence of fluoride ions on the crystallization was explained by ligand possibility of fluoride ions, which increase the dissolution of  $Al_2O_3$  in reaction mixture.

P.S.B.27

### SYNTHESIS AND PROPERTIES OF NANO-SPINELS

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This work deals with synthesis and properties of nano-spinels obtained by self propagation room temperature method (SPRT). Behavior of the nano-spinel powder during the heating process was monitored by thermal microscopy, X-ray powder diffraction (XRD), scanning electron microscopy (SEM) and differential thermal analysis (DTA). Sintering parameters such as shrinking, expansion, softening, melting as well as phase composition were determined. Behavior of sintered samples after thermal shock treatments was investigated. Thermal shock of the samples was measured using standard laboratory procedure, water quench test. Level of surface deterioration before and during quenching was monitoring by image analysis. Dynamic Young modulus of elasticity and strenght degradation were determined by ultrasonic measurements.

P.S.B.28

### MODIFICATION OF PILLARED CLAYS WITH COBALT FUNCTIONALITY. THEIR CATALYTIC PROPERTIES

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Al-pillared interlayered clays were doped with different mass % of  $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  (1-20). The starting material was natural bentonite which was pillared with Al-polynuclear cations following the procedure described previously. Co has been incorporated in clay by impregnation method starting from  $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  solutions. Equivalent counties of salt of Co have been dissolved in small amount of water and Al-pillared interlayer clays were impregnated with these solutions. After the impregnation the samples were dried (24 h at room temperature and 18h at 60°C) and calcinated (4 h, at 295°C). In the process of calcination and denitration incorporated cobalt metal nitrate salts are transformed in Co-oxide.

Physicochemical properties of obtained samples were studied by X Ray Powder Diffraction (XRPD), Fourier Transform Infra-Red spectroscopy (FTIR) and microscopic techniques. Catalytic effect of the samples of pillared clay containing different mass % of cobalt in the range between 1 and 20 mass %, was done. With increasing content of cobalt, the increased catalytic activity is obtained.

Partial oxidation of cyclohexane to cyclohexanol and cyclohexanone is extensively used as an important step in industrial processes for the production of polyamides, nylon 6.6, urethane foams, adipic acid, acidulant in baking powder, lubricating additives, etc.

P.S.B.29

## SELF-ORGANIZING PROCESSES IN CONDENSED NANO-SYSTEMS

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The occurrence in 1945 of the theoretical work by Ya. I. Frenkel "On viscous flow of solids" in which an idea of spontaneous densification of a porous body caused by a tendency to surface free energy decrease was developed may be considered as the origin of scientific principles of physics of baking.

Last decade, the main principles of the baking theory founded by Ya.I. Frenkel have got a new development due to qualitative passage from the consideration of integral characteristics of baking process to the theory taking into account non-linear fluctuation non-uniformities. This was stimulated considerably by the passage to nano-meter range of structural elements (grains, blocks) characteristic to modern high efficiency methods of material production. The gradual passage to ultra-small components of nano-meter range with non-linear fractal topology of boundaries resulted in increased role of non-linear fluctuations leading to manifestation of self-organizing processes under structure formation. The basis of self-organization process is the principle of submission that is when a system attains some critical state, its following behaviour is controlled by one or several variables named by order parameters.

So, in process of non-porous material production, the controlling parameters are pressure and temperature of preparation which determine bifurcation non-stability of previous state of the system relative to the follows one. The fractality of boundaries causes the occurrence of non-linearity in baking processes, and the state of boundary atoms with nano-size grains may be considered as quasi-equilibrium melt state.

Super-rapid quenching characteristic to condensation from high-energy ion-plasma fluxes is an effective way of structure milling and obtaining of the materials with cluster- and nano-structures. This is promoted by development of high strains peculiar to formation process of condensed materials under ion bombardment.

At characteristic sizes for nano-structural range from 1 to 50 nm, all the peculiarities of surface state are revealed because in this case, the meaning of volume is practically lost (i.e. fractal dimensionality of such structures becomes smaller than 3). This causes appearance of non-linear processes defining bifurcation nature of size effects that follows by changing the properties of condensed materials. In the basis of formation process of such structures, the phenomenon of self-organization in crystals with non-equilibrium imperfections (radiation defects) lays.

The theoretical models for description of such processes are proposed based on consideration of several stages of transformation in non-equilibrium systems, and in general, obeyed the existing ideas of synergetic.

*P.S.B.30*

### CHANGES IN THE MICROSTRUCTURE OF Fe-DOPPED $Gd_5Si_2Ge_2$

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$Gd_5Si_2Ge_2$ -based alloys can exhibit a giant magnetocaloric effect (MCE), which gives them the potential for use in cooling and refrigeration technologies. Cast alloys of this type have been reported to have a three-phase microstructure: the main phase has a composition close to  $Gd_5(Si_{1.95}Ge_{2.05})$ ; the secondary phases are  $Gd_1(Si,Ge)_1$  and  $Gd_5(Si,Ge)_3$ , with the latter reported to have linear features in the microstructure characteristic of a Widmanstätten pattern. In this investigation we have looked at the effect on the microstructure resulting from a substitution of Si by Fe, according to the formula  $Gd_5Si_{2-x}Fe_xGe_2$ , where x was varied between 0 and 1. Alloys with five different compositions were prepared using the arc-melting technique. All the samples and their microstructures were observed using an optical microscope (OM) and a nano-resolution field-emission-gun scanning electron microscope (FEG SEM). The microstructures were quantitatively analysed with energy-dispersive X-ray spectroscopy (EDS). The samples were also characterised using X-ray diffraction (XRD) and thermomagnetic measurements.

*P.S.B.31*

### INVESTIGATION OF THE BEHAVIOUR OF NANOSIZED FERROMAGNETIC SOLUTIONS IN THE ELECTROMAGNETIC FIELD

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The need in novel materials and products, combining a wide spectrum of necessary physical-mechanical, technological and specific properties with high competitive power eco-manufacturability and stability in a wide composition and exploitation range, becomes increasingly sharp. Wide perspectives for the realization of these purposes are opened for the nanosized materials on the base of space-orientated nanosized structures, nano-ceramics, carbon nano-tubes, ferromagnetic fluids, metal and nonmetal nanosized particles, borides, clusters, fullerenes and many others.

In the presented paper were investigated ferro-fluid nano-particles obtained in different ways. The results shown here are referring to structures with diameter ranging from 25 to 2000 nm. The temperature increment (infinitely little increase) depending on time is presented. The efficiency of magnetic heating (hyperthermia) is presented. The results relate to the specified conditions for use in the techniques and treatment of some diseases.

P.S.B.32

**IN-SITU INORGANIC NANOPARTICLE FORMATION IN SELF-ASSEMBLED  
POLYELECTROLYTE MULTILAYER FILMS**

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Inorganic nanoparticles have attracted much interest lately due to their unique size-dependent properties, stemming from their quantum-confinement effect and their large surface-to-volume ratio. The main problem in nanoparticle synthesis is their aggregation, which often prohibits tailoring of the particle size. One of the convenient methods for manipulating and processing nanoparticles in a technologically useful form is an "in-situ formation" of the nanoparticles in a polymer template, where the surrounding polymer prevents their aggregation and enables a homogeneous distribution of the nanoparticles within the film.

The polyelectrolyte multilayers (PEMs) of polyallylamine (PAH) and polyacrylic acid (PAA) were assembled on hydrophilic polystyrene tissue-cultured substrates and on surface-modified quartz substrates by the sequential deposition of polyanions and polycations from an aqueous solution at various pH values until the desired thickness of the PEMs was obtained. Since the linear charge density of PAA chains is controlled by adjusting the pH value of the PAA dipping solution, PEMs contain some free carboxylic acid groups that do not bind to the positively charged groups of PAH during the film assembly. These free acid groups are then used to bind the metal ions as the multilayer film is exposed to the metal salt solution at the nominally neutral pH. By subsequent chemical reaction of the metal ions, metallic or semiconducting nanoparticles are formed within the PEMs. Due to the regeneration of the carboxylic acid groups upon nanoparticle formation, the control over the volume fraction, the size and the concentration of the particles within the polymer film can be obtained by repeatedly cycling the synthesis process. The aim of this work was to control the size and concentration of the in-situ-formed inorganic nanoparticles by varying the synthesis conditions.

P.S.B.33

### MODELING AND SIMULATION OF THICK FILM NTC THERMISTORS BASED ON NANO-STRUCTURED MANGANITE -NiMn<sub>2</sub>O<sub>4</sub>

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Modeling and simulation of thick film resistivity of NTC thermistors, based on nano-structured manganite (Mn,Ni,Co,Fe)<sub>3</sub>O<sub>4</sub> was realized using total mathematical / physical model - TMFM. Prior to that thick film geometries such as segmented and interdigitated were screen printed by NTC thermistor paste and PdAg conductive paste and sintered in a furnace at 850 °C/10 min. After their electrical characterization TMFM was formed using equations for the electrode effect on volume resistivity, dependence of geometrical parameters, temperature dependence, and time response function. Measured data for the electrode effect and temperature dependence were fitted to determine parameters for mathematical equations. TMFM was applied to calculate (simulate) the dependence of the measured parameters and values and after that the results were matched to non measured parameters and values, extended to the technological limits and even over them. The simulated results were discussed as technologically and practically realizable or unrealizable.

P.S.B.34

### CHARACTERIZATION OF BARIUM TITANATE CERAMICS BY IMPEDANCE SPECTROSCOPY

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In this paper, we report the results of preparation and properties of barium titanate (BaTiO<sub>3</sub>) sintered ceramics. The ceramics were prepared from four different particle-sized BaTiO<sub>3</sub> powders, and sintered at 1370°C for 2h. The electrical properties of sintered ceramics were investigated by *ac* impedance spectroscopy over the ranges of 25-210°C and 1 Hz-100 KHz. Results are compared with those obtained from fixed frequency measurements, at 1 kHz. Impedance spectroscopic data obtained on solids are often interpreted in terms of serial equivalent circuit models. In these models each relaxation process in a spectrum is usually related to exactly one transport or relaxation process, i.e. to one sample region (e.g. bulk, grain boundary, and electrode) or reaction step. Here an impedance model for the grain boundary in BaTiO<sub>3</sub> ceramics is proposed. Also, a grain boundary capacitance is discussed. The grain boundary is ferroelectric, similar to the grains, but its impedance is modified by either air gaps or high-impedance electrical inhomogeneity in the region of the necks between the grains. Finally, the grain size of barium titanate ceramics was correlated to the ceramics electrical properties.

*P.S.B.35*

**ELECTROCHEMICALLY DEPOSITED CUPROUS OXIDE AND ZINC OXIDE FILMS  
FOR SOLAR APPLICATION**

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An electrochemical deposited layer of cuprous oxide ( $\text{Cu}_2\text{O}$ ) offers wider possibilities for application and producing low cost cells both in metal-semiconductor and hetero-junction cells structures. Also, zinc oxide ( $\text{ZnO}$ ) is at present often used as transparent conductive oxides (TCO) especially in thin film solar cells. Therefore, first wide band-gap semiconductor  $\text{ZnO}$  film was electrochemical deposited onto conducting glass coated with tin oxide ( $\text{SnO}_2$ ) prepared by spray pyrolysis method and then thin film of cuprous oxide has been grown over the zinc oxide film. To complete the systems as solar cells, thin layer of graphite was sprayed on the rear of the  $\text{Cu}_2\text{O}$ . Front wall cells were formed. This paper reports preparing of  $\text{ZnO}$  and  $\text{Cu}_2\text{O}$  films, some of their structural and morphological characteristics and some of the characteristics of the cells.

*P.S.B.36*

**ELECTROCHEMICALLY DEPOSITED ZnO THIN FILMS AND THE INFLUENCE  
OF HYDROGEN PLASMA ON THEIR TRANSMITTANCE**

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Electrochemical deposition is a suitable method for preparing thin films of metal oxides such as zinc oxide ( $\text{ZnO}$ ). Wide band-gap semiconductor  $\text{ZnO}$  films were deposited potentiostatically onto glass substrates coated with tin oxide ( $\text{SnO}_2$ ) as cathode. This paper reports preparing of  $\text{ZnO}$  thin films and some of their characteristics. The structure of the films was characterized by X-ray diffraction and Scanning Electron Microscopy. Also the optical transmission spectrum was recorded. After deposition, the films of  $\text{ZnO}$  were exposed to the hydrogen plasma influence. It was noticed significant decrease of their transmittance.



*P.S.B.37*

**ELECTRICAL RESISTANCE AND TERMOPHYSICAL PROPERTIES OF Sc AND Ca  
AT SHOCK-WAVE COMPRESSION**

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Last years in the physic of high pressures the unexpected tendency in a rank of polymorphic transitions of such metals as Li, K, Rb, Cs, Ca, Sr, Ba, Si, As, Sb, Bi, Sc has been found out. In a range 20-150 GPa polymorphic modification of these metals have special structures with low- density packing are so-called “host-guest” incommensurate crystal structures. These structures of metals have been found out and studied basically in conditions of static isothermal compression. Studying of physical properties of these structures in shock waves till now was not undertaken. In the given work it is measured electrical conductivity and also thermodynamic properties samples of high-purity scandium and calcium samples in a range of shock compression up to 90 GPa are investigated. In particular, experimental data on change of electrical resistance of high pressure phases of these metals are received at shock compression. It is shown, that at shock loading phases of low pressure to experience polymorphic transition to low simmetrical incommensurate phases.

Work is executed at financial support of the Russian foundation for basic research, the grant N 06-02-16552a and the program of the Presidium of Russian Academy of Sciences “Investigations of matter under extreme conditions”.

P.S.B.38

## CONDUCTIVITY OF C<sub>60</sub> AND C<sub>70</sub> FULLERENES UNDER DYNAMIC SHOCK COMPRESSION

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Electroconductivity is the one of the few physical properties of the substance that is accessible to direct measurements behind the front of a powerful shock wave in the area of high dynamic pressure. The achievable time resolution of such experiments at the moment allows us to make important conclusions not only about the nature of transformations of compressed substances, but also about their kinetic characteristics.

The scope of the present work is the ongoing study of the influence of carbon polymorphous modifications on electroconductivity variations under shock wave compression.

The behavior of the fullerenes C<sub>60</sub> and C<sub>70</sub> electric resistance under step shock wave loading up to 25 GPa was investigated. Maximum of fullerene C<sub>70</sub> conductivity was observed as well as at fullerene C<sub>60</sub>. That confirms the rule of strong reversible conductivity change that was discovered earlier for the case of compression of fullerene C<sub>60</sub> [1,2] up to 25 GPa. At the same time the maximum value of electric conductivity for fullerene C<sub>70</sub> is observed at the lesser pressures than for C<sub>60</sub>. Besides, the differences between electric response of the fullerene C<sub>60</sub> and the fullerene C<sub>70</sub> appear in release wave.

Work is executed at financial support of the Russian foundation for basic research, the grant N 06-02-16552A and the program of the Presidium of Russian Academy of Sciences "Investigations of matter under extreme conditions".

*P.S.B.39*

**INTRINSIC BULK CARRIER CONCENTRATION AND MOBILITY IN  
NANOSTRUCTURED MANGANITE AFTER POWDER ACTIVATION**

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Intrinsic bulk electron concentration and electron transport parameters of sintered nanostructured manganite samples (NTC thermistor grade) were determined by Hall effect measurements. Powder mixtures composed of MnO, NiO, with less than 0.25 % CoO and Fe<sub>2</sub>O<sub>3</sub> were free surface energy activated by milling to nanometer particle size in ultra fast planetary mills 5, 15,30,45,60 min at 320 rpm. NTC discs were dry powder pressed and sintered at 1200<sup>0</sup>C for 60 minutes. A full characterization of nanostructured manganite samples was done using SEM, EDS, XRD, and electrical measurements. Four point wire contacts on the sintered samples were made by conductive epoxy. The Hall effect was measured at 0.37 T at room temperature. An intrinsic bulk concentration of electrons, their mobility, resistivity / conductivity, U-I diagrams, and Hall coefficients were measured and mutually compared vs. activation time and sintering temperature. In that way intrinsic electron generation was correlated to structure development, and macroscopic parameters such as activation time and sintering temperature.

*P.S.B.40*

**REMOVAL OF ANTIBIOTIC DOXYCYCLINE FROM WASTE WATERS BY  
SURFACTANT-MODIFIED ZEOLITES**

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In recent years there is an increase in reports about presence of pharmacologically active compounds in the environment e.g. in watercourses, open ocean and soil indicating a need for removal of these materials from the environment. Surfactant-modified zeolites are recognized as improved materials for environmental application due to their excellent instantaneous pollutants adsorption. In this work we have studied the effective behavior of synthetic zeolites (FAU and ZSM-5) functionalized by cationic surfactant stearyl-dimethylbenzyl-ammonium (SDMBA) chloride, for the removal of antibiotic doxycycline from water solutions. Comparison with natural zeolite (Clinoptilolite) functionalized by the same cationic surfactant has been made. Amounts of SDMBA were varied in order to determine minimal coverage of zeolite surface which will still show significant adsorption of doxycycline with the aim to decrease the cost of the final material. The batchwise adsorption method was applied to obtain the adsorption isotherms. When equilibrium is attained, the suspension was centrifuged and concentration of solutes was determined spectrophotometrically by measuring UV absorbance at 272 nm and 343 nm characteristic for doxycycline. The adsorbed doxycycline was washed off the zeolites with methanol and liquid chromatography was performed on those solutions. Obtained results have shown that the adsorption efficiency of doxycycline depends on the zeolite type, being the highest in the case of clinoptilolite. Zeolites which were not modified with cationic surfactants were also tested, but they did not show any adsorption of doxycycline. In addition to experimental data, the calculated values of molecular sizes and dipole moments are relevant for achieving better understanding of the adsorption mechanism of large molecules. For these purposes we performed optimization of the doxycycline molecule with the B3LYP functional and 6-31+G(d,p) basis set.

P.S.B.41

**SYNTHESIS AND CHARACTERIZATION OF MESOPOROUS MATERIALS  
OBTAINED USING FAU ZEOLITE IN THE PRESENCE OF CITRIC ACID**

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Mesoporous materials have attracted much attention because of their possible applications as supports for catalysts, hosts for nanosized materials and especially in the environment protection systems. These materials are very attractive for removing BETX and pesticides from water. Therefore, a remarkable effort has been devoted to their preparation and a variety of synthetic procedures have been proposed that can lead to materials with different structural and catalytic properties. Many different precursors are employed for the synthesis of mesoporous materials. In this work we used FAU zeolite and citric acid in the presence of cationic surfactant as structure directing agent for simple preparation of mesoporous materials. Synthesized samples were characterized by X-Ray Powder diffraction (XRPD), Temperature Programmed Desorption coupled with Mass Spectrometry (TPD-MS) and BET method. Adsorption capacity and catalytic activity of synthesized samples were also tested.

P.S.B.42

**CRYSTAL STRUCTURES OF RARE-EARTH DOPED HEXACELSIANS**

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Materials with small or negative thermal expansion coefficients as well as good dielectric properties are of the great importance. Celsian phases with ideal chemical composition  $MA_2Si_2O_8$  (M=Ba, Sr) are one type of these materials. For potential applications, celsians phases doped with rare earth ions are especially interesting. In this work, Ba and Sr hexacelsians doped with Yb and Er ions were synthesized using LTA zeolite as initial material. High temperature transformation of LTA framework structure is promising procedure for synthesis of celsian phases doped with rare earth ions because it is possible to obtain homogeneous distribution of dopant ions through the bulk. In order to characterize structures and the short-range order of doped and non-doped samples, various characterization methods have been used: X-Ray Powder Diffraction, Infra-Red Spectroscopy, Differential Scanning Calorimetry and NMR measurements.

*P.S.B.43*

### CONDUCTING NANOSTRUCTURES OF POLYANILINE DOPED WITH SULFURIC ACID

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Polyaniline nanostructures, e.g. nanotubes or nanorods with an average diameter of 120 – 260 nm and a conductivity of  $10^{-2} - 10^{-1} \text{ S cm}^{-1}$ , were synthesized by a self-assembly falling pH method in the presence of sulfuric acid, using ammonium peroxydisulfate as an oxidant. It was found that the morphology and conductivity of the nanostructured polyanilines depend on the reaction time and temperature. Molecular structure of polymeric products was investigated by FTIR spectroscopy.

*P.S.B.44*

### SYNTHESIS OF NANOSTRUCTURED CONDUCTING POLYANILINE IN THE PRESENCE OF 3,5-DINITROSALICYLIC ACID

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Nanostructured polyanilines were synthesized by oxidation of aniline with ammonium peroxydisulfate in aqueous solution in the presence of 3,5-dinitrosalicylic acid. The influence of monomer to acid molar ratio (starting pH), reaction time, as well as monomer to oxidant molar ratio on the conductivity, molecular weight distribution, molecular and supramolecular structure of polyaniline was studied. The weight-average molecular weight and polydispersity index were determined by gel-permeation chromatography to be in the range 36400–54900 and 3.7–4.2, respectively. Scanning and transmission electron microscopies revealed the existence of nanorods with an average diameter of 45–280 nm. Conductivity of the polyaniline samples was  $1 \times 10^{-3} - 6 \times 10^{-2} \text{ S cm}^{-1}$ , in dependence on the reaction conditions. Molecular structure of polyaniline was investigated by FTIR and Raman spectroscopies.

P.S.B.45

### SYNTHESIS AND CHARACTERIZATION OF THE BENZOCAINE OLIGOMERS

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Oligobenzocaines have been synthesized by oxidation of the benzocaine, using ammonium peroxydisulfate as an oxidant, in acidic aqueous solution at room temperature. The oligomerization of benzocaine was exactly proved by gel-permeation chromatography. The weight-average and number-average molecular weights,  $M_w$  and  $M_n$ , were determined to amount 1370 and 820, respectively. The molecular structure of benzocaine oligomers was studied by FTIR and Raman spectroscopies. Theoretical study of the benzocaine oligomerization mechanism has been based on the AM1 and MNDO-PM3 semi-empirical quantum chemical computations of the heat of formation and ionization energy of the benzocaine, generated reactive species and reaction intermediates, taking into account influence of pH and solvation effects.

P.S.B.46

### CHEMICAL OXIDATIVE OLIGOMERIZATION OF THE ETHACRIDINE LACTATE

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Ethacridine lactate has been oxidized with ammonium peroxydisulfate in aqueous solution at room temperature. Gel-permeation chromatography profile of oxidation products evidenced chains of molecular weights up to ~4000, and revealed oligomers (6-mer to 10-mer) as predominant species. Semi-empirical quantum chemical study of the oxidative oligomerization of ethacridine has been based on the AM1 and MNDO-PM3 computations of thermodynamic, redox, and acid-base properties of reactive species and the intermediates, combined with the MM2 molecular mechanics force-field method and conductor-like screening model of solvation. The regioselectivity of the formation of ethacridine dimers is analyzed. The theoretically predicted structural features are confronted with the analysis of FTIR and Raman spectra of the ethacridine oligomers. The influence of oxidant to monomer molar ratio on the molecular weight distribution and molecular structure of oligoethacridines was studied.

P.S.B.47

### **RADICAL POLYMERISATION OF MONO-n-BUTYL ITACONATE**

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The kinetics of the bulk radical polymerisation of mono-n-butyl itaconate (MBI) were investigated at 50° and 60° C with  $\alpha,\alpha'$ -azobisisobutyronitrile (AIBN) as initiator. The polymerisations were taken to low yields not greater than 10%. The number-average mean molar masses of the polymer samples were determined by gel permeation chromatography (Waters 1500 Series instrument, PMMA standards) and by the results of viscometry measurements. The dependence of the rate of polymerisation on the initiator concentration was determined, as were the values of the transfer constant to monomer,  $C_M$ . The transfer constants to monomer for MBI,  $C_M \approx 10^4$ , were an order of magnitude lower than the corresponding values for the diester, di-n-butyl itaconate.

P.S.B.48

### **THE INFLUENCE OF RADIATION ON THERMAL STABILITY OF POLYIMIDES BASED ON N-[4-BENZOYL-2-(2,5-DIOXO-2,5-DIHYDRO-PYRROL-1-YL)-PHENYL]-ACETAMIDE**

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Different polyimide resins were synthesized using N-[4-benzoyl-2-(2,5-dioxo-2,5-dihydro-pyrrol-1-yl)-phenyl]-acetamide and the following compounds with terminal amino groups: urea, 4-[(4-aminophenyl)sulfonyl]aniline, thiourea, 2-aminoethylamine, and 4,4'-diaminodiphenylmethane. The thermal behaviour of the polyimide resins was studied by thermogravimetric measurements (TG) in nitrogen. Polyimide resins have been irradiated (500 kGy) and their radiation stability evaluated on the basis of thermal and thermooxidative behaviour of irradiated samples. The thermal degradation of examined polyimides are complex and occur in two phases. The structure of the diamine component has a greater effect on the thermal stability. All samples showed very good radiation stability, i.e. their stability was not significantly altered by radiation. There is almost no change in the first degradation step while the span of the peaks in the second step is narrowed and temperatures slightly shifted to lower indicating that the structure of the samples after irradiation becomes more similar, probably due to additional crosslinking.



*P.S.B.49*

**CALCULATIONS OF STRUCTURE, ELECTRONIC AND VIBRATIONAL SPECTRA  
OF DISILOXANE BISBENZOCYCLOBUTEN**

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Using molecular mechanics, semiempirical quantum mechanic and ab-initio, Linear Combination of Atomic Orbitals (LCAO) calculations, we investigated structure, electronic and vibrational properties of disiloxane bisbenzocyclobutene (BCB). That way, valuable informations about exact bond lengths, angles, electronic levels and charge distribution in BCB, which are missing, or highly incomplete, have been obtained. Together with the calculated vibrational spectra, which is compared to existing experimental data, these results enable a deep insight in properties of this material, extensively used in micro and optoelectronic, its behaviour under different treatments and conditions to which it is exposed in the realistic exploitation regimes.

*P.S.B.50*

## **EVALUATION OF MOLECULAR DYNAMICS IN ELASTOMER BLENDS BY MDSC MEASUREMENTS**

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Dynamical properties of polymer blends are of high importance from both, material application and theoretical point of view. Polymer blends are structural analogues of metal alloys in modern commercial polymer materials. For example all present high performance tire materials are based on elastomer blends, obtained by mixing two or more raw rubbers with different properties. Those properties are combined on synergetic principles and moreover improved by addition of active fillers to form vulcanizing compounds.

But, although blending is today a common process, there are numerous problems in further improvement of such materials. Some of them are of fundamental character because almost all high polymers are incompatible i.e. tend to separate to different phases in such compounds. That is an important barrier for many applications of elastomer materials and polymer materials in general. Fortunately, there are some additional degrees of freedom in structuring of elastomer materials as networking and structuring by active fillers that can be used to overcome the difficulties mentioned above. But, for better understanding of the influence of degrees of freedom mentioned, better insight to molecular dynamics of elastomer blends is necessary.

In this contribution, experimental and theoretical considerations of chain dynamics of commodity elastomer blends are presented. Results of Dynamical Mechanical Analyses (DMA) and Modulated Differential Scanning Calorimetry (MDSC) are presented and compared. Especially, are of interest results of MDSC as new techniques providing better insight to some features of elastomer network dynamics. The results obtained indicate new possibilities for modification of stress transfer and energy dissipation in such elastomer materials influenced by molecular dynamics in blend network transition regions

P.S.B.51

### ORGANOBENTONITE-SYNTHESIS AND CHARACTERIZATION

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The removal of color dyes from wastewater before they are released in natural waters is important since some dyes are highly toxic for environment. Although several traditional chemical and biological processes exist for dye removal, the application of these techniques has been restricted due to the essentially non-biodegradable nature of dyes. Some modified clays, may play a role of low cost sorbents suitable for dye removal. Since natural clays are hydrophilic and ineffective as sorbents for organic compounds it is necessary to modify their surface. Organoclays represent a family of materials with hydrophobic surfaces that are synthesized by modifying swelling clays with various surfactants. In this paper domestic bentonite clay was modified with quaternary ammonium cationic surfactant in order to obtain more efficient sorbents. Various techniques have been used in characterization of organobentonites, including X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR). Nitrogen adsorption-desorption isotherms at -196 °C were used to estimate the specific surface area, pore volume and pore size distribution in micro and mesoporous region, while mercury intrusion porosimetry was used for macropore and mesopore measurement. The comparison between structural and textural properties of raw and organobentonite, as well as the preliminary investigation of their dye sorption potential is presented.

*Acknowledgements:* This work was supported by the Ministry of Science & Environmental Protection of the Republic of Serbia (Project TR6712B).

P.S.B.52

### SINTERING OF SILICON NITRIDE WITH Mg-EXCHANGE ZEOLITE ADDITIVE

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The possibility of using Mg-exchanged zeolite (MAS) as additive for densification of Si<sub>3</sub>N<sub>4</sub> ceramic was studied. The zeolitic precursor was previously heated at 800 °C to obtain an amorphous powder with a composition corresponding to MgO·Al<sub>2</sub>O<sub>3</sub>·nSiO<sub>2</sub>. The powder was mixed with Si<sub>3</sub>N<sub>4</sub> and the sintering additive was homogenized by attrition milling in the presence of isopropanol and finally compacted by cold isostatic pressure. Pushrod dilatometry was used to measure the shrinkage behavior of green bodies under a nitrogen atmosphere from room temperature to 1500°C. The chemical reactions and phase evolution during pressureless sintering were also followed by means of X-ray and differential thermal analysis. Results show that the first liquid forms as low as 1000°C, resulting in a significant reduction of sintering temperature. XRD data reveal that phase transformation from α- to β-Si<sub>3</sub>N<sub>4</sub> takes place after the second phase has been completely converted into a glassy phase. The results show that the Mg-exchanged zeolite is a very effective low-temperature sintering additive for silicon nitride.

P.S.B.53

### PREPARATION OF SiALON POWDER USING DIATOMACIOUS EARTH

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In this paper the SiALON powder was prepared by carbothermal reduction and nitridation of diatomaceous earth. Different sources of carbon were used for carbothermal reduction: active coal, carbon cryogel and sucrose. The aim was to investigate the potential use of diatomaceous earth as a main precursor for low-cost SiALONs by in situ carbothermal reduction-nitridation reactions. Also the influence of different sources of carbon on synthesis and properties of low-cost SiALONs is studied. The powders were characterized by X-ray and SEM investigations.

P.S.B.54

### PREPARATION OF HIGHLY POROUS SiC CERAMICS

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This paper deals with a new method for producing non-oxide ceramic using wood as a template. Highly porous silicon carbide (SiC) ceramic with woodlike microstructure has been prepared by carbothermal reduction reactions of Cornus mas wood/TEOS composite at 1600 °C. Wood specimens were carbonized at 1000 °C in Ar atmosphere for 2 hour. The porous carbon preform was infiltrated with TEOS (Si(OC<sub>2</sub>H<sub>5</sub>)<sub>4</sub>), as a source of silica, without pressure at 25 °C. The infiltration/annealing process was repeated up to five times to increase the SiO<sub>2</sub> content in the biomorphic samples. The morphology of resulting porous SiC ceramics, as well as the conversion mechanism of wood to porous SiC ceramics, have been investigated by mean of scanning electron microscopy (SEM/EDX) and X-ray diffraction analysis (XRD). Experimental results show that the biomorphic cellular structure of wood remained in the porous SiC ceramics. Obtained SiC ceramics consists of β-SiC with traces of α-SiC.

*P.S.B.55*

**COMPUTER SIMULATION OF SiO<sub>2</sub>  
DISSOLUTION IN NaOH AQUEOUS SOLUTION**

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A computer simulation of batch dissolution kinetics of SiO<sub>2</sub> particles in aqueous NaOH, according to the ratio SiO<sub>2</sub>/Na<sub>2</sub>O=2, at elevated temperatures and high pressure has been composed. The developed mathematical model is of mayor importance for prediction of dynamical response of process parameters. A few mathematical models were developed, within this work, and afterwards compared with experimental results. The influences of SiO<sub>2</sub> particle diameter, working temperature and hydroxide ion molality on dissolving kinetics were investigated, and illustrative both 2d and 3d graphics were drawn. The developed models are sufficiently correct, in engineering sense, and can be used for dynamical prediction of process parameters. Also, it is certain that these models can be used to correlate the experimental data on dissolution and for prediction of process parameters.

*P.S.B.56*

**NEW OPTIMAL TECHNOLOGY FOR SMALL SECTIONS OF HSS  
AND SOFTWARE FOR DOCUMENTATION PROCESSING**

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Characteristics of ESR technology for larger HSS tools is shortly presented from rich industrial experience and new optimal ESRR /ESRR-CC technology, recently developed by INTECO – special melting technologies and industrially tested at leading world producers of HSS tools have been successfully proposed for smaller sections of high speed tool steels. Comparative priorities of such sort of HSS steels have been presented and background of characteristic quality clearly explained from scientific and practical point of view. For producers of HS-steels and HSS-tools the ESRR-CC could be an option of greatest interest in the development trend. Shortly presented is also the specially adjusted software package INTECO-ACCESS for literature processing which is of great importance in such R&D program.

*P.S.B.57*

### **AGEING EFFECT ON THE PSEUDOELASTICITY CHARACTERISTICS OF Ti-RICH TiNi SHAPE MEMORY ALLOY**

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This paper presents the findings of an experimental study of how ageing temperature affects the pseudoelasticity (PE) and its phase transformation temperatures. These have been examined by means of tensile testing machine and differential scanning calorimetry (DSC). By increasing the ageing temperature (constant ageing time) from 350°C to 550°C critical stress for martensite formation and pseudo-elastic elongation increased. However, specimen aged at 650°C showed a decrease in the critical stress for martensite formation and pseudo-elastic elongation. After second and third sequence of loading and unloading, The critical stress shifted towards higher side was observed, The DSC measurement revealed that phase transformation was taking place in two-way transformation, i.e., during heating martensite (B<sub>19'</sub>) transformed to austenite (B<sub>2</sub>) while cooling the austenite (B<sub>2</sub>) transformed back to martensite (B<sub>19'</sub>). Martensite and Austenite start and finish temperatures decreased with increasing ageing temperature. On the other hand peak temperatures decreased and hysteresis temperature steadily increased with ageing temperature. Metallographic characterizations were carried out by scanning electron microscope and image analyzer.

*P.S.B.58*

### **HIGH TEMPERATURE LOW CYCLE FATIGUE OF SUPERALLOY INCONEL 738LC**

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Cylindrical specimens of cast polycrystalline nickel base superalloy Inconel 738LC were cyclically strained under total strain control at 23, 500, 700 and 800 °C to fracture. Cyclic hardening/softening curves, cyclic stress-strain curves, and fatigue life curves were obtained at four temperatures. Surface relief was studied in specimens fatigued to failure using scanning electron microscopy. Cyclic hardening/softening behaviour depends both on temperature and strain amplitude. Low amplitude straining was characterised by saturation of the stress amplitude. In high amplitude straining a pronounced hardening was found which was followed by saturation at room temperature or tendency to it at 700 and by cyclic softening at 800 °C. The cyclic stress-strain curves can be fitted by power law. They are shifted to lower stresses with increasing temperature. Fatigue life curves can be approximated by the Manson-Coffin and Basquin laws. Slip markings were detected on specimen surface at all test temperatures. When temperature increases the density of slip markings decreases and the Manson-Coffin and Basquin curves are shifted to lower lives.

P.S.B.59

**DESTRUCTIVE AND NON-DESTRUCTIVE TECHNIQUES APPLIED TO THE CHARACTERIZATION OF AS-CAST MODEL STEELS WITH PARAMETRIC VARIATION OF Ni, Mn, Si AND Cr CONTENT**

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The present work is aimed to investigate the role and influence of certain elements as Cr, Ni, Mn and Si on the radiation stability of reactor pressure vessel steels.

The 12 ferritic steels with basic typical composition of WWER-1000 and PWR reactor pressure vessel materials were manufactured and submitted to Charpy impact and magnetic Barkhausen Noise testing.

Results of Charpy impact test show, that DBTT values are independent on the tested steels composition and are ranging between -150 and -104 °C. Only two steels show extremely high DBTT (-16 and -42 °C); the mentioned steels contain low concentration of Ni and high concentration of Cr and vice versa. For those materials an additional heat treatment is designed in order to increase the DBTT values to values more near to those of the other steels

The results of MBN measurements show that the amount of Cr plays an important role: an increase of Cr content in model steels leads to an increase of RMS values independently on Mn and Si contents. The percentage of Ni has also significant influence i.e. low Ni content is responsible for lower RMS values.

By comparing the RMS and DBTT values of the 12 model steels it is not possible to find a general conclusion. However, most of the model steels combine high values of RMS with low values of DBTT.

The next step will be the neutron irradiation of such model steels in the HFR-LYRA irradiation facility up to accumulated neutron fluence in the order of  $10^{19}$  n.cm<sup>-2</sup> and the further comparison of material properties before and after irradiation.

P.S.B.60

### NUMERICAL MODELLING OF DUCTILE FRACTURE INITIATION IN PRESSURE VESSEL STEEL

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The problem encountered in exploitation of pressure vessels is assessment of the location of crack initiation in structural material. Considering the operating conditions of the vessels, experimental and numerical analysis was conducted under static conditions of external loading. Standard smooth specimens and compact tension (CT) specimens with fatigue pre-crack were used. Low-alloyed ferritic steel for pressure vessels 22 Ni MoCr 3 7 (DIN designation) was tested. The Gurson-Tvergaard-Needleman (GTN) model and micromechanical criterion for crack initiation were applied. Elastic-plastic finite element (FE) computations were carried out using embedded GTN yield criterion. Numerical procedure was used for computation of void-volume fraction growth,  $f_{growth}$ , ahead of the crack tip. The problem of the effect of FE size in that zone was solved by applying the quantitative microstructural analysis. It was demonstrated that the computations with FE size corresponding to the mean free path,  $\lambda$ , between the inclusions in tested steel provided adequate prediction of ductile crack initiation.

P.S.B.61

### THE ANALYSIS OF MICROSTRUCTURE AND MECHANICAL PROPERTIES OF WELDED JOINTS OBTAINED WITH TWO TYPES OF CORED FILLER WIRES

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In this paper, the results of mechanical properties and microstructural tests of welded joints made with flux cored activated wire under CO<sub>2</sub> protective atmosphere and with full wire under protective atmosphere of CO<sub>2</sub> and a mixture of (Ar + CO<sub>2</sub> + O<sub>2</sub>) on samples of boiler sheet of P265GH grade have been presented. A comparative analysis of the results obtained by microstructural testing of weld metal and HAZ and mechanical and technological properties of welded joints made using the two above specified metallurgical qualities of electrode wire has been conducted. Based on microstructural analysis and determined mechanical properties of welded joints the correlation between qualities of filler metal was established. The improvement of quality of welded joints made with filled-cored electrode wire demonstrated.



*P.S.B.62*

### **MECHANICAL AND MICROSTRUCTURAL PROPERTIES OF HIGH-CARBON STEEL SURFACE WELDED LAYER**

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Damaged components of high-carbon steel could be surface welded, in spite of their poor weldability, and with proper choice of filler material and welding technology, it is possible to get surface welded layer better properties than base metal. In this paper are shown microstructural and mechanical properties of high-carbon steel surface welded layer, obtained with self-shielded flux cored wire. The testing results of tensile characteristics, hardness, toughness via instrumented Charpy pendulum, microstructural analysis and fatigue crack growth resistance of all characteristic zones are shown in details. Acquired results indicate superior properties of repaired welded layers, due to their similarity to the new generation of bainitic steel, i.e., due to change of microstructure from original pearlitic structure to final bainitic structure. Finally, fatigue crack growth parameters have shown that deposit layer is safer place for future crack initiation, what provides reliably exploitation.

*P.S.B.63*

### **THE APPLICATION OF MODERN TECHNIQUES IN SUPER ALLOYS INVESTIGATION**

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Since superalloys of Fe, Co and Ni represent significant materials for construction parts working in the most demanding conditions, the detailed investigations of these alloys using modern techniques have to be performed.

The referred data about great number of superalloys from the chemical point of view (content), various thermal processing, the applications of vacuum and laser techniques, optical and electron microscopies, give the analytical approach to the complex problems in material structures.

The investigation of super alloys from the Hastelloy group is performed. The modern methods applied, which were presented in previously published papers, represent significant results which enable to explanation of complex material performances in the practical application and exploitation.

*P.S.B.64*

**STUDY OF THE SIMULATED HAZ OF CREEP RESISTANT 9-12% ADVANCED CHROMIUM STEEL**

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Global warming has had impact on worldwide increase of research and development attempts for reduction of CO<sub>2</sub> emission. Therefore, in the energy supply sector, a special focus has been directed to further development of steels that can endure the ultra supercritical steam conditions. Our paper presents the basic study on weldability of the advanced 9-12% chromium steels applying the thermo-mechanical simulation of the heat affected zone (HAZ). The changes of microstructures and material properties of HAZ before and after postweld heat treatment (PWHT) have been analyzed and compared by light microscopy, scanning electron microscopy (SEM), hardness measurements and impact toughness testing. Microstructures at representative points during typical welding cycle and PWHT were studied in details.

*P.S.B.65*

**USE OF IN-SITU SEM OBSERVATIONS FOR THE CHARACTERISATION OF FRACTURE PROCESS IN Al-Zn-Mg-Cu ALLOYS**

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New techniques, as in-situ observation of the fracture process, appear as powerful tools to determine the precise mechanisms of complex fracture Al-Zn-Mg-Cu alloys. In-situ SEM tensile test has been used to investigate fracture behaviours such as initiation and propagation and fracture in high-alloyed Al-Zn-Mg-Cu alloys of different purity. In order to get better insight of the mechanical behaviour and description of fracture process additional testing of tensile properties by actual in-situ method have been made. The in-situ observations demonstrate that three phenomena preceding ductile rupture of the material: void nucleation, growth, and coalescence. Nucleation of voids originate around particles of intermetallic (IM) phases by fracture of the particle itself and decohesion of boundary surface between particle and matrix. Crack grows, in all investigated alloys, by shear mechanisms of decohesion in the direction of maximal stresses, which produces deformation. However, crack propagates at different rates. A strong interaction of crack front with the particles of IM phases in least pure of the alloy is shown, resulting in a tortuous crack path, and consequently reduces its propagation rate.

*P.S.B.66*

**PERFORMANCE OF ALUMINOTHERMIC RAILS WELDING TECHNOLOGY**

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It is well known that rails are very important part of railway traffic so their quality must be satisfactory, especially their welding joints. This work describes aluminothermic welding of rail using aluminothermic mixtures which are produced in our country. The work also contains proper testing of achieved level of quality in welding joints, in rails types: 700 and 900-VIC 860V. Quality of rails joints that were welded with aluminothermic welding was examinee with: visually, chemical analysis, ultrasonic testing, determination of strength properties, determination of toughness, determination of hardness and microstructure testing. The quality of domestic produced aluminothermic mixtures improved rail welding and also assured the railway traffic safety.

*P.S.C.1*

**SIZE DEPENDENT INTRABAND ABSORPTION IN P-TYPE DOPED  
SELF-ASSEMBLED NANODOTS**

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The intraband absorption in p-type cylindrical InAs/GaAs self-assembled nanodots is computed by the six-band k.p model, and the variation of the transition matrix elements with the dot height is explored. The absorption spectra are computed for *x* and *z* polarized light. The transition matrix elements are found to vary considerably with the dot-height. Decrease of the thickness brings about an increase of the absorption for z-polarized light, while the absorption of x-polarized light is not too much sensitive on the height of the quantum dot. We found that the pillar-like geometry favors intraband absorption in THz range.

*P.S.C.2*

**VIBRATIONAL SPECTROSCOPY OF CdTe/ZnTe QUANTUM DOT SUPERLATTICES**

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In this paper we present far-infrared (FIR) and Raman scattering results on superlattices with CdTe quantum islands embedded between ZnTe barriers. The samples were grown by molecular beam epitaxy on (100)-oriented GaAs substrate followed by several micrometers thick CdTe buffer layer. Then, superlattices consisting of 200 periods of 2-nm-thick CdTe layers separated by ZnTe spacers (3 to 12 nm) were grown. The FIR spectra were measured in the spectral range of 50-650 cm<sup>-1</sup>. Analyses of the spectra were made by a fitting procedure, while the optical properties are described by the complex dielectric function that depends on 3D distribution of constituents. Multiphonon resonant Raman scattering has been registered. Overtones up to 8<sup>th</sup> order for the ZnTe longitudinal-optical (LO) phonons were observed.

*P.S.C.3*

**ELECTRON -ELECTRON SCATTERING IN THE ACTIVE REGION OF GaAs/AlGaAs  
QUANTUM CASCADE LASER IN MAGNETIC FIELD**

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The quantum cascade laser (QCL) has undergone tremendous development in the past decade, and has proven to be efficient and powerful light source in the mid- and far infrared spectral range. The output properties of this device can be suitably tailored and even optimized for particular applications. In numerical modeling, it is essential to include all the relevant scattering processes that might influence the optical gain of the lasers. So far, electron – phonon interaction have been considered dominant when solving a set of rate equations for a structure placed in magnetic field. The aim of this work is to calculate electron – electron contribution to the total scattering rates in three (the conventional triple quantum well) and four-level (the double-longitudinal optical phonon structure) QCL, in strong magnetic field, and assess its relative importance compared to previously obtained electron – phonon relaxation rates. The numerical results indicate that this additional type of scattering cannot be neglected in calculations of optical gain and should be therefore incorporated into the rate equations.

*P.S.C.4*

**EELS/HRTEM CHARACTERIZATION OF PHASES OBTAINED DURING THE  
HYDROTHERMAL SYNTHESIS OF CaTiO<sub>3</sub>**

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In order to understand the formation of nanostructured perovskite CaTiO<sub>3</sub> obtained by a hydrothermal synthesis, different intermediate phases were characterized. For that purpose we used combined techniques of High-Resolution Transmission Electron Microscopy (HRTEM) and Electron Energy-Loss Spectroscopy (EELS). We found that investigated phases were different by their morphology, crystal structure and composition. Morphologically the most interesting phase was formed in the shape of single-crystalline nanowires with an aspect ratio and a diameter of 100 and 10 nm, respectively. Second phase was represented by perfectly crystalline sheets with a thickness of 35 nm and dimensions of about 500x500 nm. According to the composition and the crystal structure parameters obtained from the HRTEM and electron diffraction analysis this phase is closely associated with the existing layered structure corresponding to either kassite (CaTi<sub>2</sub>O<sub>4</sub>(OH)<sub>2</sub>) or cafetite (Ca[Ti<sub>2</sub>O<sub>5</sub>](H<sub>2</sub>O)) phase. Our future goal is to employ these phases as template precursors for the synthesis of CaTiO<sub>3</sub> perovskite in the final form of nanowires or thin crystalline sheets.

P.S.C.5

### SYNTHESIS OF CdSe/MESOPOROUS SiO<sub>2</sub> COMPOSITES WITH NARROW PARTICLE SIZE DISTRIBUTION

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Semiconductor nanoparticles exhibit unique optical properties due to quantum confinement effects, however their properties are very size-sensitive and thus their application often requires precise size tuning. In the present work we use mesoporous silica molecular sieves with different pore diameters for size selective absorption of CdSe colloidal particles. According to TEM data CdSe particles penetrate to mesoporous channels, however it leads to stretching of amorphous silica walls. Besides, it was found that the particles exhibit red shift of band gap (2.4-2.3 eV) and photoluminescence (562-572 nm) peaks with increasing of silica sieves pore diameter, which corresponds to increasing of average particle size. Thus, one can propose this technique to tune particle distribution using mesoporous silica sieves. This work is supported by RFBR (06-03-33136).

P.S.C.6

### SYNTHESIS AND CHARACTERIZATION OF BaTiO<sub>3</sub> NANORODS

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In our work we present the synthesis of BaTiO<sub>3</sub> nanorods by sol-gel electrophoretic deposition into template membranes. The growth of the nanorods occurred at a working electrode of aluminum, on which we attached a polycarbonate membrane. Pt mesh was used as the counter electrode. The track-etched hydrophilic polycarbonate (PC) membranes were used as template membranes, with pore diameters of 200 nm and a thickness of 10 μm. For the electrophoretic growth the potentials of 2 V and 30 V was applied between the electrodes, and this was maintained for 30 min. After the deposition, the samples were annealed at elevated temperatures. This heating procedure was done in order to burn off the polycarbonate membrane and to make the nanorods dense and crystalline. The samples were then characterized by X-ray diffraction (XRD), scanning (SEM) and transmission electron microscopy (TEM). XRD analysis confirmed that nanorods consist of cubic BaTiO<sub>3</sub>. By using SEM we found that the BaTiO<sub>3</sub> nanorods grown in a PC membrane have a uniform diameter throughout their entire length. We also observed that higher potential leads to a layered formation of BaTiO<sub>3</sub> on the membrane surface after the pores are filled. By using TEM and electron diffraction analysis, we found that these nanorods are dense and polycrystalline BaTiO<sub>3</sub>, with the grain size ranging between 25 up to 50 nm and with a diameter of an individual nanorod in the range of 100 to 180 nm.

*P.S.C.7*

### **THE $W_{18}O_{49}$ NANOWIRES USED FOR SYNTHESIS OF THE $WS_2$ NANOTUBES**

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The  $W_{18}O_{49}$  nanowires up to several millimetres in length were synthesized by a chemical transport reaction using iodine as a transport agent. The morphology of the wires can be controlled by the ratio between starting materials and by the growth conditions. By optimisation we could gain pure purple  $W_{18}O_{49}$  phase with crystals several hundred nanometers wide or blue nanowire  $W_{18}O_{49}$  phase with wideness bellow 200 nm. The  $W_{18}O_{49}$  nanowires have been used as precursors for synthesis of the  $WS_2$  nanotubes by sulphurization in the mixture of 1%  $H_2$ , 1%  $H_2S$  and argon. The diameter of the tubes is smaller than the wideness of precursor nanowires revealing an exfoliation of the precursors. Beside nanotubes, also  $WS_2$  fullerenes grow simultaneously. Characterization of nanowires and nanotubes will be presented based on the results of transmission electron microscopy, electron diffraction, ultra high vacuum atomic force microscopy, scanning tunnelling microscopy and scanning tunnelling spectroscopy.

*P.S.C.8*

### **SCANNING PROBE MICROSCOPY OF ATOMIC AND NANO STRUCTURES**

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Here we present our results of various scanning probe microscopy techniques applied on nanostructured systems. They consist of ultra high vacuum atomic force/scanning tunneling microscopy (UHV AFM/STM) measurements and scanning near-field optical microscopy (SNOM) of Si (111), highly oriented pyrolytic graphite (HOPG), porous alumina and carbon nanotubes. As tools we used Omicron Variable Temperature AFM and TwinSNOM systems to perform contact, non-contact and needle sensor AFM, shear-force SNOM and STM measurements.

*P.S.C.9*

**SYNTHESIS AND CHARACTERIZATION OF SHAPED ZnS NANOCRYSTALS IN WATER IN OIL MICROEMULSIONS**

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Shaped zinc sulfide nanocrystals were synthesized in W/O microemulsions by using cyclohexane/Triton X-100/n-pentanol system. Under different synthetic conditions appearance of two distinct morphologies of ZnS nanocrystals, either cubes or nano-wires, was proven by transmission electron microscopy. The ZnS cubes have average size of about 40 nm, while the ZnS nano-wires have 25 Å diameter and length ranging from several hundred nanometers up to a few microns. The X-ray diffraction analysis revealed formation of ZnS with cubic crystal structure. Due to two dimensional confinements the exciton of ZnS nano-wires is blue shifted compared to the bulk material. Four well-resolved photoluminescence bands in visible spectral region were observed upon excitation of cubic ZnS particles, while in the case of ZnS nano-wires emission band was observed at 450 nm. The origin of photoluminescence bands was discussed in details.

*P.S.C.10*

**LOW TEMPERATURE SYNTHESIS OF DISODIUM DIMOLYBDATE**

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A new method for the synthesis of disodium dimolybdate in the process of ultrasonic spray pyrolysis using acidified aqueous solutions of thermodynamically stable molybdenum (VI) oxide clusters as precursor is described. Disodium dimolybdate particles were collected in alcohols (2-propanol and ethanol) and ultra-centrifugation was employed to isolate solid material from solution. The scanning electron microscopy revealed formation of uniform spherical disodium dimolybdate particles with average diameter of about 0.25 µm. The X-ray diffraction analysis confirmed formation of orthorhombic disodium dimolybdate for samples synthesized at temperature as low as 300 °C.



*P.S.C.11*

**RADIOLYTIC SYNTHESIS AND CHARACTERIZATION OF PVA HIDROGEL –Au NANOCOMPOSITES**

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The radiolytic formation of Au nanoparticles in PVA hidrogel (obtained by gamma irradiation) was investigated. The reduction of Au<sup>3+</sup> ions was performed using strongly reducing species such as hydrated electrons, 2-propanol and PVA radicals. Absorption spectra of PVA hidrogel–Au nanocomposites revealed the presence of surface plasmon absorption band around 520 nm which indicated formation of Au nanoparticles. In xerogel, position of peak maxima is shifted towards longer wavelength compared to that in hidrogel due to change of the dielectric permittivity of the environment. Molecular and supermolecular structure, as well as interaction between nanoparticles and polymer matrix, were investigated by IR spectroscopy. Surface morphology of nanocomposites and the size of nanoparticles were investigated by appropriate microscopy techniques. Thermooxidative degradation of nanocomposites was compared to the degradation in nitrogen atmosphere using TG analysis.

*P.S.C.12*

**CHARACTERIZATION OF Au NANOPARTICLES DISPERSED IN WATER AND POLYMER MATRIX**

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Gold nanoparticles were synthesized in water using citrate as reducing agent. Absorption spectra of the obtained colloidal solutions had prominent surface plasmon absorption band peaking at 530 nm, which match well with literature data for Au particles of about 20 nm in diameter. Diameter of Au nanoparticles was precisely determined by using TEM. The gold nanoparticles were incorporated in hydrophilic polymer polyvinyl alcohol. Influence of the polymer matrix on the optical properties of Au nanoparticles as well as influence of Au nanoparticles on the thermal properties of the polymer matrix was investigated.

*P.S.C.13*

### NANOSIZED SILICALITE-1 CRYSTALLIZATION – INFLUENCE OF TPA<sup>+</sup>

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Tetrapropylammonium bromide (TPABr) was used as templating agent in the starting systems TPA<sup>+</sup>-Na<sup>+</sup>-SiO<sub>2</sub>-H<sub>2</sub>O in a low temperature (358 K) synthesis of silicalite-1 (ZSM-5 zeolite structure). Precipitated silica is used as silica source, and silicalite-1 phase of high crystallinity arises inside of the nanosized particles, which were agglomerated in the wide scale of size. Role of template in synthesis is of a great interest for better understanding and optimization of the process. TPA<sup>+</sup>/SiO<sub>2</sub> ratio was changed in the wide range up to 0.23. Solid phase transformation was investigated. Period of nucleation and crystallinity of the solid phase at the end of the process of crystallization are affected by TPA<sup>+</sup>/SiO<sub>2</sub> ratio. The powder was investigated using FTIR spectroscopy with KBr pellet technique, X-ray diffraction with monochromatic CuK<sub>α</sub> radiation, TG-DTA analysis and SEM analysis with magnifications in the range up to 300,000x.

*P.S.C.14*

### INVESTIGATION OF NANOSIZED SILICALITE-1 BY FTIR SPECTROSCOPY

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Compactly agglomerated nanosized silicalite-1 crystal phase (ZSM-5 zeolite structure) was investigated by FTIR spectroscopy. Especially, the dependence of the ratio of absorptions of the bands on the position of 550 cm<sup>-1</sup>, assigned to vibrations of double five-membered rings of TO<sub>4</sub> tetrahedra (T=Si or Al) as secondary building units of silicalite-1 phase, and on the position of 450 cm<sup>-1</sup>, assigned to internal vibrations of the TO<sub>4</sub> tetrahedra (T=Si or Al), upon mass fraction of the silicalite-1 phase in an amorphous silica matrix was investigated. Absorption assigned to TO<sub>4</sub> tetrahedra (T=Si or Al) is originated from silicalite-1 crystal phase or from amorphous silica phase where Si/Al→∞. The powder was investigated using FTIR spectroscopy with KBr pellet technique, X-ray diffraction with monochromatic CuK<sub>α</sub> radiation, TG-DTA analysis and SEM analysis with magnifications in the range up to 300,000x.

P.S.C.15

**SYNTHESIS AND CHARACTERIZATION OF SILVER NANOPARTICLES AND  
COMPLEX IT'S WITH LYSINE AND ANTIBODY OF PSA AND THEIR  
APPLICATION IN PRODUCING DIAGNOSTIC PROSTATE CANCER KIT**

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For synthesis of Silver Nanoparticles we used Silver Nitrate ( $\text{AgNO}_3$ ), Hydrazine ( $\text{N}_2\text{H}_4$ ), PVP (Poly Vinyl Pyrrolidone) Ethylene Glycol and *Poly Process* method. Silver nanoparticles have been prepared by a soft solution technique from the aqueous solution of silver nitrate and poly (vinyl pyrrolidone) (PVP) in the presence of ethanol used as a reducing agent. The resultant silver nanoparticles were characterized by using scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD). It was found that the well-defined silver nanoparticles which had the 15-50nm. After preparation and characterization of nanoparticles and confirmation of their size, they were reacted with Lysine and were conjugated with antibody of prostate specific antigen (PSA) (Due to the present of free amine groups). This complex (silver nanoparticle-Lysine-antibody of PSA) would be used in production of diagnostic cancer kit.

P.S.C.16

**CHARACTERIZATION OF Eu-DOPED  $\text{Zn}_2\text{SiO}_4$  POWDERS OBTAINED BY  
POLYMER INDUCED SOL-GEL SYNTHESIS**

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In the present work we explored the possibility of obtaining nanocrystalline powders of Eu-doped  $\text{Zn}_2\text{SiO}_4$ , using polymer induced sol-gel synthesis. With this novel synthetic route we were able to obtain nanopowders at lower temperature than needed for classical, solid state methods. The synthesis started from TEOS as alkoxide precursor while PEG with different average molecular weights (200, 4000 and 20000) was used as fuel. Our experiments were aimed to observe the influence of different polymer fuels on structural, morphological and optical properties of  $\text{Zn}_2\text{SiO}_4$  samples. The resulting powders were fired in two ways: in normal furnace and in microwave, and then thermally treated in furnace at 1180°C for 1h. Samples were characterized with X-ray diffraction for phase identification and line broadening analysis, and electron microscopy for morphological investigation. XRD measurements indicated as better material the one treated in microwave, i.e. of pure zinc silicate phase (less ZnO remained). Optical properties of synthesized powder were investigated using emission and excitation fluorescence. Typical emission spectra of europium trivalent ion, with lines that corresponds to  $^5\text{D}_0 \rightarrow ^7\text{F}_j$  are found, and the emission decays are investigated.

P.S.C.17

### SYNTHESIS AND STRUCTURE OF FERRITE POLYMER NANOCOMPOSITES

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Magnetic nanoparticles and their unique properties make them attractive, both from the scientific value of understanding their properties and the technological significance of enhancing the performance of the existing materials. Therefore synthesis and application of magnetic nanoparticles is a subject of intense research. Our interest is in developing a convenient method to incorporate ferrite nanoparticles in polymer matrix in order to evaluate their structure and magnetic behavior. In this paper, a procedure for the incorporation of nanocrystalline In-doped  $ZnFe_2O_4$  in polystyrene (PS) matrix via in situ polymerization will be presented. The structure of ferrite-PS nanocomposite will be characterized by differential scanning calorimetry (DSC), X-ray diffraction, scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

P.S.C.18

### STUDY OF STRUCTURAL AND OPTICAL BEHAVIORS OF $TiO_2:Eu$ , Pd THIN FILMS

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Incorporation of different dopants into  $TiO_2$  matrix could modify its properties. For example, Eu dopant can be applied to change the optical properties of  $TiO_2$  thin films. Pd dopant can be used for changing the electrical properties of  $TiO_2$  from dielectric oxide to semiconducting oxide.

This work refers optical and structural characterization of europium and palladium doped titanium dioxide thin films prepared by modified magnetron sputtering. The metallic Eu and Pd dopants have been co-sputtered from a base Ti target (mosaic target) and deposited on  $SiO_2$ . In this sputtering process a low pressure of pure oxygen as a working gas and additionally heated target (hot target) were employed. After the deposition, some selected samples were additionally annealed in air ambient for 2 hours at the temperature of 470 K, 670 K, 870 K and 1070 K. Structural properties of  $TiO_2: (Eu,Pd)$  thin films were examined by X-ray diffraction (XRD) and atomic force microscopy (AFM). XRD patterns were recorded after each of thermal treatment and showed the rutile phase, independently on the temperature of annealing. Heat treatment results in an increase of average size of rutile grains from few to several nanometers. Optical properties of prepared  $TiO_2 (Eu,Pd)$  thin films were studied by means of optical transmission and photoluminescence (PL) spectroscopy.

It was found that Pd doping shifts the fundamental absorption edge of  $TiO_2$  in the longer wavelength range. Simultaneously doping with Eu, results in a strong red luminescence upon ultraviolet (UV) radiation at 300 nm. That makes prepared nanocrystalline  $TiO_2 (Eu,Pd)$  thin films optically active in UV-visible range.

P.S.C.19

### TEMPERATURE DEPENDENCE OF OXYGEN REDUCTION KINETICS ON CARBON SUPPORTED Pt NANOPARTICLES

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The temperature dependence of oxygen reduction reaction (ORR) was studied on highly dispersed Pt nanoparticles supported on carbon cryogel. The specific surface area of the support was  $517 \text{ m}^2 \text{ g}^{-1}$ , the Pt particles diameter was about 2.7 nm and the loading of the catalyst was 20 wt.%. ORR kinetics at Pt/C electrode was examined in  $0.5 \text{ mol dm}^{-3} \text{ HClO}_4$  solution in the temperature range from 274 to 318 K. At all temperatures, two distinct  $E$ -log  $j$  regions were observed: at low current densities with the slope of  $-2.3RT/F$  and at high current densities with the slope of  $-2.3 \cdot 2RT/F$ . In order to confirm the mechanism for oxygen reduction previously suggested at polycrystalline Pt and Pt/Ebonex nanostructured electrodes, the apparent enthalpies of activation at the selected potentials vs. reversible hydrogen electrode were calculated in both current density regions. Although  $\Delta H_{a,l}^\ddagger > \Delta H_{a,h}^\ddagger$ , it was revealed that the enthalpies of activation at the zero Galvani potential difference were the same, and concluded that the rate determining step of ORR was the same in both current density regions. The synthesized Pt/C catalyst showed a small enhancement in the catalytic activity for ORR in comparison to the polycrystalline Pt, but no change in the mechanism of the reaction.

P.S.C.20

### SYNTHESIS AND PROPERTIES OF POLYSTYRENE-CO-MALEIC ACID/Cd<sub>1-x</sub>Mn<sub>x</sub>S NANOCOMPOSITES

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Cd<sub>1-x</sub>Mn<sub>x</sub>S diluted magnetic semiconductor samples were synthesized as nanoparticles confined in a polystyrene-co-maleic acid (PS-co-MAC). Acid groups of the co-polymer is used to control the aggregation of the nanoparticles and form a composite. Concentration of Mn was  $x = 0.01, 0.02$  and  $0.05$ . UV-Vis measurements showed that the average particle size was  $\sim 4$  nm. Fourier transform infrared, UV-vis, X-ray diffraction, electron paramagnetic resonance and magnetic susceptibility measurements were employed to study the size, optical and magnetic properties of the Cd<sub>1-x</sub>Mn<sub>x</sub>S nanocrystals in the copolymer matrix.

P.S.C.21

### STRUCTURAL PROPERTIES OF EUROPIUM-DOPED YTTRIA OBTAINED VIA AEROSOL SYNTHESIS

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Eu-doped yttrium oxide, a well-known red phosphor, is employed in modern high-resolution display devices. Utilization in such devices requires particles with spherical shape, narrow size distribution and non-aggregation characteristics since they ensure required resolution and brightness. In this work cubic yttrium oxide doped with 5 at% and 10 at% of europium was synthesized by spray pyrolysis at 900°C. Higher crystallinity of the as-prepared samples was achieved through additional thermal treatment. The effects of different doping concentrations and synthesis parameters were monitored. The  $Y_2O_3:Eu^{3+}$  phosphor was synthesized by ultrasonic atomizing (1.3 MHz) of aqueous yttrium nitrate/europium nitrate precursor solution, directed by an air flow into the tubular flow reactor consisted out of three heating zones. Solvent evaporation, drying, solute precipitation and chemical decomposition occurred successively on a droplet level, leading to the formation of the final powder particles that were characterized by XRD, SEM/EDS and TEM. Microstructural refinement was carried out by using Rietveld based program Fullprof and the average crystallite size was calculated by Scherrer method and program Profit. It was shown that the as prepared particles are submicronic, spherical and non-agglomerated with crystallite size around 20nm. The determined morphological characteristic persists in samples after their thermal treatment, while thermally induced growth of primary crystallites affects the particle surface roughness.

P.S.C.22

### OPTICAL AND ELECTRICAL PROPERTIES OF INDIUM DOPED NANOCRYSTAL ZINC OXIDE PREPARED BY SPRAY PYROLYSIS METHOD

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Thin films of indium-doped zinc oxide have been prepared by spray pyrolysis from the zinc acetate methanol solution on heated substrates. As prepared films show hexagonal wurtzite nanocrystal structure with grain size of 11 nm and 14 nm, for films thickness of 600 nm and 1.2 μm, respectively. The transmission of the films is nearly 90 % for wavelength greater than 550 nm, regardless on the doping concentration. The films thickness was estimated from the interference fringes on the transmission spectra. It was found that the conductivity of the films depends from the indium doping concentration. As deposited ZnO: In films by 3.5 % of indium, showed conductivity  $1.3 \times 10^{-5} \Omega^{-1} \text{cm}^{-1}$ . Optical band gap showed dependence from indium-doped of the films.

P.S.C.23

### THE INFLUENCE OF THE CONCENTRATION AND KIND OF MODIFICATION OF MONTMORILLONITE ON PROPERTIES OF NANOCOMPOSITE COATINGS

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Natural or chemically modified montmorillonite (MMT) dispersed in water was added into the reaction mixture forming hybrid organic – inorganic (O-I) nanocomposite coating. Final properties depend not only on the concentration and kind of MMT used but also on the inner constitution of the O-I matrix. Already 1 wt. % of natural MMT influences considerably surface and mechanical properties, while the effect of chemically modified MMT is not so pronounced. This can be due to the worst dispersion of chemically modified MMT within the matrix compared with natural one: while natural MMT is partially intercalated, partially exfoliated in the product, substantial amount of original, unaffected MMT clusters was found there. Solid state NMR spectroscopy i.a., confirmed the interaction of MMT platelets with the O-I matrix.

Acknowledgements: The authors wish to thank the Grant Agency of the Academy of Sciences of the Czech Republic (grant A400500505) for financial support.

P.S.C.24

### STRUCTURE PARTICULATES OF NANOSTRUCTURED CONDENSATES OF QUASIBINARY

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The possibility of studying the different stages of concentration-and-structure ordering in nano-crystalline condensates of solid solutions is shown. It was found that in magnetron sputtered model Ti-W-B condensates, the concentration-and-structure ordering with modulation period  $a_m \approx 4\text{nm}$  took place at deposition temperature lower than 970K. Intensity of the process depends on deposition temperature and stress state of the condensates. Analysis of the electron microscope results as well as the data of small-angle X-ray scattering has shown that as a result of the ordering, cell-like structure with non-uniform cell volume distribution of solid solution atoms was formed. Based on diffusion mechanism of the concentration-and-structure ordering leading to modulated structure formation in nano-crystalline condensates, perspective of small-angle method for studying the beginning stage kinetics of the process is shown.

P.S.C.25

**CORRELATION BETWEEN THE CHANGE OF ELECTRON DENSITY STATES ON THE FERMI LEVEL AND THE RELATIVE CHANGE OF THE MAGNETIC PERMEABILITY OF THE  $\text{Fe}_{81}\text{B}_{13}\text{Si}_4\text{C}_2$  AMORPHOUS ALLOY**

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Analysis of X-ray diffractograms enabled following of structural changes of the  $\text{Fe}_{81}\text{B}_{13}\text{Si}_4\text{C}_2$  amorphous alloy in the form of a tape 30  $\mu\text{m}$  thick after multiple annealing at temperatures of 200, 300, 400, 440 and 460°C for 60 min. The structural relaxation process was investigated by measuring the thermo-electromotor (TEMS) of a thermocouple made by joining a copper conductor and the investigated amorphous alloy in non-isothermal and isothermal conditions at temperatures of 400, 440 and 460°C.

The relative change of electron density states on the Fermi level in the amorphous alloy was determined from changes of the temperature coefficient of the TEMS after each

annealing as  $\frac{\Delta n_1}{n} = 3,53\%$  ;  $\frac{\Delta n_2}{n} = 5,33\%$  and  $\frac{\Delta n_3}{n} = 7,81\%$  .

Analysis of the results of isothermal TEMS measurements showed that the structural relaxation process occurred in two stages. The first stage is characterized by a linear logarithmic dependence of TEMS on time for a constant temperature. The second stage of structural relaxation is characterized by a linear dependence of the isothermal change of TEMS on the square root of time. These results lead to the conclusion that the first stage is a fast kinetic process, while the second stage is a slow diffusion process.

By the thermo-magnetic measurements in non-isothermal conditions, both before and after annealing, was found an expressed correlation between a change of electron density state on Fermi level and a change of magnetic properties.



*P.S.D.1*

### **SYNTHESIS AND MECHANICAL PROPERTIES OF BIOMORPHIC C/SiC COMPOSITES**

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Cornelian cherry dogwood (cornus mas), and white poplar (populus alba) were transformed by pyrolysis into carbon preforms which were subsequently converted into biomorphic C/SiC composites by infiltration technique of resorcinol-formaldehyde (RF) cryogel, and TEOS. In situ reaction between silica and carbon template took place in the cellular wall at high temperature. The morphology of resulting C/SiC biomorphous composites has been investigated by scanning electron microscopy (SEM/EDX) and X-ray diffraction (XRD). Mechanical characterization such as strength (3-point flexure tests) and micro hardness measurements was followed. The influence of different morphology on mechanical properties of resulting biomorphous C/SiC composites was discussed.

*P.S.D.2*

### **DETERMINATIONS OF MECHANICAL PROPERTIES OF PARTIALLY CARBONIZED CARBON FIBRES AND THEIR CARBON-CARBON COMPOSITES**

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Mechanical characteristics of carbon fibres represent very important indication of their quality. Polyacrylonitril (PAN) fibers were used as raw for getting partially carbonized fibers (PCF). The process of making PCF consist from two phases, stabilization of initial PAN fibers and partially carbonization of stability fibers in range 400-1000 °C in inert atmosphere. The stabilization were carried out continually on experimental plant which was constructed and modified in INN «Vinča». Partially carbonized fibers were impregnated in one step with thermosetting phenol-formaldehyde resin, type resol. Mechanical properties of carbon-carbon composites (strength and modulus) were determined in three points bending test. Aim of this paper was examination a possibility to use PCF as reinforced materials instead of carbon fibers in production of carbon-carbon composites.

*P.S.D.3*

**THE INFLUENCE OF CARBON BLACK AND SILICA FILLER ON THE PROPERTIES OF ACRYLONITRILE-BUTADIENE/ ETHYLENE-PROPYLENE-ETHYLIDENENORBORNENE RUBBER BLENDS**

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In this applicative investigation the reinforced elastomers based on acrylonitrile-butadiene/ ethylene-propylene-ethylidenenorbornene rubber blends (NBR/EPDM) were studied. The influence of filler nano-sized particles on the mechanical properties and ageing resistance was estimated. The rubber compounds with different content of furnace carbon black (46 nm) and precipitated silica (22 nm) were prepared in a laboratory mixing roll mill. The vulcanization characteristics of samples were determined by oscillating disk rheometer. The vulcanizates were prepared at 150 °C using an electrical press. Hardness of crosslinked materials was measured using an indentation hardness tester. The stress-strain experiments were performed before and after ageing the specimens in an air-circulating oven. Morphology of fractured surface was studied by scanning electron microscopy (SEM).

*P.S.D.4*

**THE INFLUENCE OF CARBON BLACK AND WOOD FLOUR ON HIGH ENERGY RADIATION RESISTANCE OF COMPOSITES BASED ON NR/CSM RUBBER BLEND**

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In this applicative contribution the effect of carbon black (average particle size 26nm) and wood flour (particle size from 300 to 400 µm) on thermal ageing and γ-radiation resistance of natural rubber/chlorosulphonated polyethylene rubber blend (NR/CSM) was studied. The compounds with different filler loading (from 10 to 50 phr) were prepared in a two-roll mill. The samples were crosslinked by sulphure at 150°C to optimum cure time (obtained by Monsanto rheometer). The tensile strength of the aged samples was determined, after conditioning at 70°C during 72h. For radiation, the samples were kept in a gamma chamber, for the required time. The radiation exposure of samples was performed at two doses: 212 and 400 kGy. At high filler loadings the rubber blend composites showed better resistance to ageing.

P.S.D.5

**POSSIBILITIES OF APPLICATION OF CARBON STEEL-SiC CAST IN CARBIDE  
COMPOSITES AS WEAR RESISTANCE MATERIAL**

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In the paper was studied the possibilities of applying *Cast-in-Carbide* composites based on carbon steel and SiC, for production of wear resistance machine parts like mill hammers, excavator teets, etc. *Cast-in-Carbide* (CIC) technology offers new opportunities to improve wear resistance, prolong life time of the parts and increase productivity. Optimized content of SiC in low carbon steel, combine extreme hardness and wear resistance of casting surface, rich on SiC, with high strength and toughness of metal base. In order to effectively protect the surface of the parts against wear, it is necessary to know what types of wear the parts might be subjected to. Solid body abrasion, adhesion wear, and impact– fatigue wear are possible types of wear. In most cases, combination of two types of wears comes together, and due to that, the wear mechanism is extremely complex. The decisive factors for forming of successful wear resistance surface are: quantity, size, shape and distribution of SiC particles in the composite. It is very important to make possible those SiC particles, which density is much lower then steel, to concentrate in upper layer of casting and form composite structure. Upper parts of the castings, which contain high concentration of SiC particles, will have extreme hardness, and lower parts will have high strength and excellent toughness. These properties, extreme hardness in combination with high toughness guarantied exceptional wear resistance of *Cast-in-Carbide* SiC–Steel composite castings.

*P.S.D.6*

### **COMPUTER MODEL OF HEAT AND MASS TRANSFER DURING HEAT TREATMENT OF WOOD**

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During the heat treatment process, the heat and mass transfer takes place between the solid and the drying medium, and the moisture evaporation occurs within the solid due to the capillarity action and diffusion. In this work, the three-dimensional Navier–Stokes equations along with the energy and concentration equations for the fluid coupled with the energy and mass conservation equations for the solid (wood) are solved to study the conjugate heat treatment behaviour. Whitaker's continuum approach has been used to obtain the equations for the liquid and vapour migration within the solid. Three moisture phases are accounted for: free water, bound water, and water vapour. The model equations are solved numerically for the temperature and moisture content histories under different treatment conditions. The model validation is carried out via a comparison between the predicted values with those obtained experimentally. The comparison of the numerical and experimental results shows good agreement, implying that the proposed numerical algorithm can be used as a useful tool in designing high-temperature wood treatment processes.

*P.S.D.7*

### **MODELLING OF AIRFLOW THROUGH A WOOD-DRYING KILN**

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A two-dimensional pore-scale model is used to predict air flow through a wood drying stack for which both the interstitial and the average flow can be considered as two-dimensional. Timber-drying kilns consist of two parts, a centre region and staggered end sections, each with different flow characteristics. In the centre region the flow resembles flow through a duct and empirical models from literature were used for the evaluation of the pressure loss across the timber stack. The staggered ends, resulting from the stacking method, were analyzed by considering them as porous media. A unified modelling theory for the prediction of the pressure drop of crossflow in a prismatic structure was proposed. The model was derived by volumetrically averaging the equations of motion over an arbitrary two-phase system of stationary solids and a traversing fluid. Closure was obtained by using a formerly introduced rectangular representation of the pore space morphology. The predicted results compared favourably to the test results.

*P.S.D.8*

**EXPERIMENTAL INVESTIGATION OF A SOLAR DRYER  
WITH NATURAL CONVECTIVE HEAT FLOW**

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A direct type natural convection solar dryer mathematical model is developed and afterwards tested with acquired experimental data in fruit drying. This study relates mainly kinetics and establishment of drying heat balances. The influence of significant parameters governing heat and mass transfers, such as solar incident radiation, drying air mass flow and effectiveness, is analyzed in order to evaluate its thermal performances. Experimental data can be represented by empirical correlations of the form for representation of drying process. The resolution of these drying equations makes possible to predict total drying time of each product. Moreover, this drying process allows reducing the moisture content of fruit approximately to 80% in 19 and 22 h, respectively to reach the safety threshold value. This value permits the conservation of these products about one year without deterioration. The determination of parameters, like ambient temperature, drying chamber temperature, drying air mass flow and incident heat fluxes, allow predicting the drying effectiveness for modeling and refining the dimensioning of the elaborate prototype.

*P.S.D.9*

**MODELLING OF FRICTION PAIR CONTACT CHARACTERISTICS BY MEANS OF  
ARTIFICIAL NEURAL NETWORKS**

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The complex and highly nonlinear phenomena are involved in the contact of brake's friction pair. These contact phenomena are primarily caused by the third body generating in the contact of friction pair. The properties of the third body are mostly affected by friction material characteristics. The third body characteristics are influenced by complex structure of composite material which may contain over to 20 different ingredients. Synergetic effects of all these ingredients determine the contact situation of friction pair i.e. the third body characteristics. Moreover, the same composition of friction material can be differently affected by manufacturing conditions of dry mixing, pre-forming, hot moulding, and heat treatment (post curing). That is why very little is known about the complex and highly nonlinear phenomena that are involved in the contact of brake's friction pair. The improvement of friction material performance and prediction of the friction pair contact influences on the brake's performance requires accurate modelling the friction pair behaviour during braking. An artificial neural network technique was used in this paper to develop a neural model of friction pair behaviour during braking. The neural model has been developed to establish functional relationship between 26 input parameters and one output parameter (coefficient of the friction). The input parameters have been defined by the whole composition of brake lining (18 parameters), its manufacturing conditions (5 parameters), and testing conditions (3 parameters).

*P.S.D.10*

### NONWOVEN GEOTEXTILE COMPOSITES WITH BENTONITE

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Commercial geotextile composites that contain bentonite as a sorption layer are made by binding dry bentonite in powder or granular form between two woven and/or nonwoven (NW) layers. Binding can be performed by sandwiching bentonite between textile layers by needling and/or stitching or adhering bentonite layers to textile surfaces by water-based adhesive. In this paper, the possibility of synthesizing composite by embedding bentonite particles into NW structures was investigated. The composites were synthesized from commercial needlepunched polypropylene and polyester NW and domestic bentonite clays with previously defined physical-chemical and textural properties. Bentonite was applied on NW in the form of suspensions in water solution of adhesive based on modified cellulose soluble in water. Suspensions of bentonite with particle size less than 75 µm were used in synthesis. Composite structure was microscopically examined and image analysis was performed. The absorption capacity and liquid retention ability of starting NW and final composites were measured according to EDANA (European Disposables and Nonwovens Association) recommendations. The mechanical properties of obtained composites were tested according to JUS regulations. The composite materials have improved mechanical properties in comparison with starting nonwovens.

*Acknowledgements:* This work was supported by the Ministry of Science & Environmental Protection of the Republic of Serbia (Project TR6712B).

*P.S.D.11*

### ELECTRODEPOSITION OF NiMo ALLOY COATINGS AND THEIR CHARACTERIZATION AS CATHODES FOR HYDROGEN EVOLUTION IN SODIUM HYDROXIDE SOLUTION

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The hydrogen evolution reaction on electrodeposited NiMo alloy coatings, as well as their electrochemical properties in NaOH solutions have been investigated by polarization measurements, cyclic voltammetry and EIS technique. It is shown that NiMo alloy coatings electrodeposited from pyrophosphate-sodium bicarbonate bath possess high catalytic activity for hydrogen evolution in NaOH solutions. Their stability in 1M NaOH at 25 °C under the condition of reverse polarization is shown to be very good, while in 33% NaOH at 85°C (conditions of industrial electrolysis) electrodeposited NiMo alloy coatings exhibit also high catalytic activity, but low stability, as a consequence of massive dissolution of alloy coatings under the condition of reverse polarization.

*P.S.D.12*

**AN AUSTEMPERING STUDY OF DUCTILE IRON ALLOYED WITH COPPER AND NICKEL**

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Austempered ductile iron (ADI) is an alloyed and heat treated ductile cast iron which has a good combination of mechanical properties: high strength, ductility and toughness are combined with good wear resistance and machinability.

An investigation has been conducted on the austempered ductile irons (ADI) alloyed with copper and nickel, austenitized at 900°C and austempered at 300°C and 350 °C. This paper describes the results of an investigation the austempering of ADI alloyed with 1,6% copper and 1,5% nickel for a range of times and temperatures are reported.

The microstructure and fracture mode developed throughout these treatments have been identified by means of light and scanning electron microscopy (SEM) and X-ray diffraction analysis. The impact energy measurements were performed on un-notched Charpy specimens.

It was shown that the strength, elongation and impact energy strongly depend on the amounts of bainitic ferrite and retained austenite. Based on these results, optimal processing window was established.

*P.S.D.13*

**APPLICATION ON DESIGN AND CONSTRUCTION OF GLASS REINFORCED PLASTIC BOAT**

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This paper presents the results of a project focused on design, construction and built of glass reinforced plastic boat. In the shipbuilding industry, a construction branch which produces light weight structures that operate in relatively unfavorable environmental conditions and where a failure may cause a lot of human loses, composite materials found an excellent application. Besides the applications in large variety of ship types and other naval applications of F.R.P. (landing crafts, fast patrol boats and submersibles), this material found its widest range of applicability in the construction of small crafts etc. These applications in our country are in the beginning. Marine Faculty, as the only scientific institution, aims at influencing on the improvement of the design techniques in this shipyard.



*P.S.D.14*

**APPLICATIONS OF REPRODUCTION METHOD WITH SOLDERING OF MASSIVE  
DETAILS IN ALBANIAN SEA PORTS**

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The usage of the reproductive method with soldering of massive details with high productive cost such as: axes, other body machineries is a contemporary technologic process.

Due to the right choice work parameters are provided almost the same with new produced details and reduction of industrial waste increasing the level of materials' exploitation. In the course study comparing soldering methods is concluded that.

The automatic soldering with arch and over melting with homogeneous and vesicle sub layers as well as over melting with vibrating arch in liquid current compose the most efficient and qualifying methods for reproduction.

The study through fulfilling experiments brings optimal calculating and applied regimes. It enables the ways and the possible measurements to avoid tensions caused by controlling cooling speed, pre cooling and start of soldering and over melting process.

There are given arguments experimentally that the reduction of melting deepness base metal is practically left out, in the cases of the middle over melting doesn't change its composition. It enable the reduction of rising interior tensions and deformations fulfilling an entire over melting without crack.

*P.S.D.15*

**RELIABILITY ASSESSMENT OF A BI-MATERIAL WEDGE: STRAIN ENERGY  
DENSITY APPROACH**

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Joints of different materials have many applications in structural engineering and microelectronics. In the present contribution the joint is modeled as a bi-material wedge. The singular character of the stress field near the wedge tip is investigated. Depending on the geometry of the wedge and the selection of the materials, the stress field can have two singularities. Correspondingly the singular stress field is expressed as a sum of two singular terms with different stress singularity exponents. It is shown that to study the problem of a crack onset at the wedge, both two terms have to be taken into account. First, the angle of the direction of potential crack initiation is determined. Then a criterion for crack nucleation and propagation in the selected direction is formulated. These two steps utilize knowledge of the strain energy density distribution in a bi-material wedge vicinity.

P.S.E.1

### MECHANOCHEMICAL SYNTHESIS OF ANTIMICROBIAL MATERIALS BASED ON Ag-APATITES

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In recent years there has been increasing interest in antimicrobial materials doped with silver ions because of their wide application in medicine, cosmetics, fabrics, etc. Antimicrobial activity of hydroxyapatite (HAP) containing silver ion that was synthesized using sol-gel and wet methods has previously been reported. In this work we applied the mechanochemical method for synthesis of HAP/Ag materials from oxides and hydroxide. Starting powders of Ca(OH)<sub>2</sub>, P<sub>2</sub>O<sub>5</sub> and Ag<sub>2</sub>O were milled using a planetary ball mill for different time intervals. Formation of crystallized HAP/Ag was confirmed after 300 min. of milling time by X-ray diffraction analysis (XRD) and FTIR spectroscopy. Partial amorphization was observed after 420 min. of milling time. The obtained results indicate that a simple mechanochemical technique can be used for synthesis of Ag-apatite materials.

P.S.E.2

### SONOCHEMICAL PREPARATION OF HYDROXYAPATITE / POLY (DL-LACTIDE- CO-GLYCOLIDE) COMPOSITE

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In recent years there have been many attempts in the direction of developing materials and techniques to impart suitable biological and mechanical properties to synthetic composites to be used in the replacement and reconstruction of the human hard tissue. The objective of this study was to evaluate actual ultrasonication concept for the production of ceramic/polymer composite. Ceramic part of this composite was hydroxyapatite (HAP) - the main constituent of the bone tissue and polymeric part was poly (lactide-co-glycolide) - component which retains useful bioactive properties as well as enhancement in mechanical properties. Composite was made in two steps- HAP ultrasonic synthesis and its encapsulation in polymeric matrix. Influence of the polymer/ceramics molar ratio, ultrasonic synthetic parameters and concentration of stabilizers (PVA and SDS) on the morphology and size of products were analyzed. Characterization methods were X-ray diffraction (XRD), infrared spectroscopy (IR) and scanning electron microscopy (SEM).

P.S.E.3

### **pH SENSITIVE HYDROGELS BASED ON METHACRYLATES**

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Novel copolymeric hydrogels based on methacrylates were prepared by chemical radical copolymerization of poly(alkylene glycol) methacrylates (BIS) and 2-hydroxyethyl methacrylate (HEMA) in a mixture of water/ethanol as solvent. These hydrogels were characterized in terms of swelling in conditions similar to the biological fluids (buffers pH range of 2.2-7.4), compression-strain measurements and thermal properties. The influence of the Bisomer type on swelling and mechanical properties, as well as on thermal behavior of the resulting hydrogels, were investigated. The prepared copolymeric hydrogels with non-ionizable groups in compositions showed an interesting pH-sensitivity in the pH range of 2.2-7.4. The mechanical properties, as well as the thermal behavior of the prepared copolymeric hydrogels based on methacrylates are satisfactory that these polymeric biomaterials possess a potential for drug carriers, dressings and other medical devices.

P.S.E.4

### **SYNTHESIS AND CHARACTERIZATION OF Cu(II), Cd(II), Pt(II) AND Pd(II) COMPLEXES WITH CONDENSATION DERIVATIVE OF PYRIDINE-2-CARBOXALDEHYDE AND ETHYL HYDRAZINOACETATE**

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In search for agents that might show less negative side effects and overcome the resistance to cisplatin, in this work a series of complexes of Cd(II), Cu(II), Pd(II) and Pt(II) with the condensation product of pyridine-2-carboxaldehyde and ethyl hydrazinoacetate were synthesized. All four complexes were obtained by template synthesis. Elemental analysis, molar conductivity, magnetic susceptibility (with Cu(II) complex), IR, <sup>1</sup>H NMR and <sup>13</sup>C NMR spectral data showed that all the obtained complexes had a coordination number four. In the neutral square planar Pt(II), Pd(II) and Cd(II) complexes, the organic ligand is coordinated as a bidentate *via* pyridine and hydrazone nitrogen atoms, the remaining two coordination sites being occupied by chloride ion. In Cu(II) complex the ligand is coordinated as a tridentate, with chloride in the fourth coordination site, so that the geometry is tetrahedral, and the complex is 1 : 1 electrolyte.

P.S.E.5

### **IN VITRO CYTOTOXIC ACTIVITY OF WATER-SOLUBLE CARBOXYFULLERENES DERIVATIVES**

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Carboxyfullerenes are water-soluble carboxylic acid derivatives of a fullerene C<sub>60</sub>. The chemical and physical properties of these compounds are discussed in an interdisciplinary manner, with emphasis on biological properties and biomedical applications. It is known that they act as free radical scavengers and have been investigated as protective agents against oxidative stress *in vivo* and *in vitro*. Toxic effects of carboxyfullerenes derivatives *in vitro* are not well defined. In our investigation, we were monitored potential cytotoxicity of these compounds on two human cell lines, as well as differences in surviving between normal and malignant cells. The synthesized carboxyfullerenes derivatives were tested in MRC-5 human fibroblasts cell line and in MCF-7 human breast carcinoma cell line using SRB and MTT assays for cytotoxicity.

P.S.E.6

### **BIOMOLECULAR-TISSUE CONFORMATION AND ELECTRICAL PROPERTIES CHANGES: BASE FOR EARLY DIAGNOSIS OF SKIN CANCER AND MELANOMA**

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It is well known that biomolecular conformation change of skin tissue has consequence on electrical and other properties of tissue. Skin resistance *in-vivo* is widely variable depending primary upon the state of hydration of the stratum corneum, secondary of stratum granulosum and tertiary from stratum spinosum. Tissue hydration may be happened adding water from outside or during water synthesis through metabolism. Experimentally it was observed that skin tumor contains 21% more water than normal contra lateral tissue. Consequence of tissue degradation as a violation of normal conformation state of biomolecules is gathering water molecules in skin tumor. Bearing in mind that electrical property of tissue is sensitive to water, we develop original method for imaging tissue based on its electrical conductivity. Experimental results of normal and skin lesion regions (mole, tumor, and melanoma) showed that this method, together with dermoscopy may be very beneficial tool for early diagnosis of skin cancer and melanoma.

P.S.E.7

**MEDICINE APPLICATION OF LIQUID CRYSTAL AND FULLERENE-DOPED MATERIALS**

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Some aspects of pure and fullerene-doped liquid crystals have been discussed in order to visualize, orient and testify human erythrocytes. The possible mechanism responsible for the interaction between liquid crystal dipoles and erythrocytes has been considered.

P.S.E.8

**FLUORIDE CONTENT, RECHARGE ABILITY AND REMINERALISATION POTENTIAL OF GLASS-IONOMER CEMENT**

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The aim of this *in vitro* study was to assess the fluoride content of glass-ionomer, Fuji VII (GC, Tokyo), stored in different media, to investigate its recharge ability and the potential to interact with the dental tissues using scanning electron microscopic and energy dispersive spectroscopic techniques. The sample consisted of 20 cured cement disks (10x1.5mm), 5 teeth in which glass ionomer was used as a sealant, and 5 teeth in which it was used as a restorative material. Cement disks were divided into 4 experimental groups according to storage media (distilled water, saline, acid solution pH=5.5, NaF (c=500/10<sup>6</sup>)) and 6 sections of each tooth were analysed. The results were analysed using the chi square test. SEM/EDS revealed fluoride content of Fuji VII reaching 20 mass%, depending on the storage media (p<0.05), recharge ability in the presence of fluoride ions, and the zone of interaction between the glass ionomer and dental tissues. Glass-ionomers, biocompatible materials demonstrate satisfactory anticariogenic potential.

P.S.E.9

**PDLLA MICROPARTICLES CONTAINING BSA: EFFECT OF FORMULATION VARIABLES ON SIZE DISTRIBUTION**

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Worldwide, there is currently considerable care for the development of biodegradable microspheres as systems for controlled release of medicaments. The major disadvantage of traditional administration routes of medicaments is the need for frequent repetition. Encapsulation has been proven to be an effective vehicle for the controlled delivery of various medicaments. The encapsulation efficiency and release kinetics of the medicaments have been found to be dependent upon the size of the microspheres synthesized. The aim of this study was to formulate microparticles from poly-dl-lactide (PDLLA) by modified precipitation method. Bovine serum albumin (BSA) was used as a model protein for encapsulation. The surfactant polyvinyl alcohol (PVA) was incorporated to increase encapsulation efficiency and to achieve PDLLA spheres with desired size. The main focus was to study the effect of co-solvent selection (methanol or ethanol), PVA concentration, chloroform-to-water ratio, the speed and time of homogenization and solvent removal rate on the properties of microparticles. The average size and morphology of microparticles varied substantially among these preparation conditions. An increase in stirring rate and time of homogenization and concentration of stabilizer agent were found to reduce moderately the size of microparticles. Other process parameters had limited influence on particle size.

*P.S.E.10*

**NEURAL MODELLING OF PLLA POLYMER IN H/A<sub>p</sub>/PLLA BIOCOSMITE  
MATERIAL BEHAVIOUR DURING NANOINDENTATION**

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Knowing the PLLA polymer in hydroxyapatite (HAp)/poly-L-lactide composite behaviour is important from the mechanical point of view especially when it is used as load carrying elements. Contrary to the ceramics (HAp) material behaviour, the thermoplastic polymers (PLLA) mechanical properties in the solid state are strongly affected by processing conditions (hot pressing). That is why nanoindentation is recently introduced for the precise characterization of biomedical materials regarding the mechanical properties of polymer matrix phase. In this paper, the mechanical properties of polymer matrix phase (modulus of elasticity, yield stress, work-hardening rate) have been modelled using artificial neural networks. The approach of neural modelling has been employed for functional approximating of the nanoindentation load-displacement curves. The data obtained from finite element analyses has been used for artificial neural networks training and validating. The neural model of polymer matrix phase of PLLA polymer in hydroxyapatite (HAp)/poly-L-lactide mechanical behaviour has been tested versus unknown data related to the load-displacement curves that were not been used during neural networks training. Based on this neural model, the nanoindentation matrix phase properties of PLLA polymer in hydroxyapatite (HAp)/poly-L-lactide composite can be predicted providing preconditions for optimizing its mechanical characteristics.

P.S.E.11

### IMMOBILIZATION OF *SACCHAROMYCES ELLIPSOIDEUS* CELLS FOR BIOETHANOL PRODUCTION

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Bioethanol can be produced by fermentation of sugars from waste agricultural materials. Whichever system for bioethanol production is chosen, the attention must be paid to the overall economics and energy consumption.

The aim of present study was to investigate the immobilization of *Saccharomyces ellipsoideus* yeast cells for bioethanol production from corn meal hydrolyzates. For this purpose the biocompatible polymers such as: PVA and Ca-alginate were assessed. The conditions of ethanol fermentation, such as initial glucose and inoculum concentration and time required for the efficient ethanol production were optimized for both immobilized and free cells. In experiments with immobilized *S. ellipsoideus*, high ethanol concentration of 10% and the yield of more than 90% of the theoretical were achieved. These experiments have also shown that the immobilized cells have higher tolerance to ethanol and can endure higher initial glucose concentration in corn meal hydrolyzate than the free cells.

P.S.E.12

### INVESTIGATION OF ANTIMICROBIAL ACTIVITY OF ESSENTIAL OILS AND MICROBIAL METABOLITS FROM LACTIC ACID BACTERIA FOR IMPREGNATION IN MEDICAL TEXTILE

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Textile materials with antimicrobial properties, which are used in prophylaxis – prevention of occurrences and spreading of infections, have a broad use in medicine. Essential oils of *Rosmarinus officinalis*, *Abies sibirica* and antimicrobial products of metabolism from lactic acid bacteria *Lactobacillus rhamnosus* A71 are natural compounds with broad spectrum of antimicrobial activity. Antimicrobial activity of those natural compounds was detected using indicators strains *Staphylococcus aureus* ATCC 25923, *Escherichia coli* ATCC 25922 and *Candida albicans* ATCC 24433, respectively.

Detection of antimicrobial activity of essential oils and antimicrobial products of metabolism from lactic acid bacteria, respectively, was monitored in their free condition and attached to the textile materials. Also, the release of essential oils and microbial metabolites attached on textile materials was followed by determination of viable bacterial cells during a seven-day incubation these textile materials in saline. The most susceptibility for all applied textile materials showed *Candida albicans* ATCC 24433, with percentage of inhibition between 70-100% after five days of incubation.



P.S.E.13

**SURFACE MODIFICATION AND CHARACTERIZATION OF METHACRYLATE  
POLYMER NETWORKS FOR TISSUE ENGINEERING**

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Synthetic hydrogels have been known to fulfil most of the requirements for artificial tissue properties. Our contribution is part of a complex tissue engineering project dealing with a development of universal bioactive support for cell cultivation. To incorporate the biologically active molecule, avidin was immobilized onto the polymer surface by non-specific interactions, electrostatic forces or covalently using reactive groups in the polymer. To control the physical-chemical properties of materials, different monomers based on methacrylic acid were copolymerized and chemical modification of the polymer surface was employed. The way and the quantity of immobilized avidin depending on various polymer supports were investigated.

P.S.E.14

**CHROMATOGRAPHIC STATIONARY PHASES FOR SEPARATION OF BIOACTIVE  
COMPOUNDS - CORRELATION OF MORPHOLOGY AND SEPARATION  
PROPERTIES**

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One of the promising techniques for separation of bioactive compounds is chromatography on the molecularly imprinted stationary phases. Comonomers of ethylene glycol dimethacrylate and methacrylic acid were polymerized in the presence of various porogenic mixtures. *In situ* polymerization was carried out under the various conditions. The morphology of prepared monoliths was investigated by electron microscopy, mercury porosimetry and surface area measurements. From chromatographic point of view, columns were tested by separations of standard hydrophobic solutes and enantiomers of imprinted compounds. The influence of polymerization conditions on morphology and subsequent chromatographic behaviour was evaluated.

*P.S.E.15*

**THE INFLUENCE OF THE STERILIZATION PROCESS BY GAMMA RAYS  
IRRADIATION ON THE ACTIVATED CARBON CLOTH PROPERTIES AS A  
DRESSING MATERIAL**

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The activated carbon cloth was tested as a dressing material for wound care, but without drugs. For this purpose the sterilization process is very important and was performed by gamma rays irradiation. The adsorption characteristics of the activated carbon cloth as well as the surface chemistry before and after sterilization process were examined. The activated carbon cloth is nanoporous and contains surface oxygen structures. The sterilization process by gamma rays irradiation influenced retain of adsorbate in the material, also, changed the surface chemistry quantitatively, but not qualitatively and last for several years. The activated carbon cloth dressing was clinically tested on dogs that have lacerations. The assumption was that the biocompatibility, sterility and adsorption characteristics of activated carbon material were enough to achieve wound healing.

*P.S.E.16*

**HEPATOPROTECTIVE ROLE OF TUNGSTATES**

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Tungstates and polyoxotungstates are known to be bioactive compounds for long time. Our consideration of them as nontoxic compounds in adequate doses, according to literature data, emphasize to wondering if they may have some health beneficial effects. In that aim, the seven weeks lasted experiment on rats was performed, with sodium tungstate-ST and 12-tungstophosphoric acid-TPA for pretreatment in chemically induced acute liver necrosis. The effects were evaluated by the activity of serum enzymes, oxidative stress parameters, antioxidative defense markers, and histopathology in Wistar rats. The obtained results are promising and suggest that treatment with ST and TPA for 7 weeks before the induction of liver necrosis could be useful for the prevention of hepatic injury in rats.

*P.S.E.17*

**ADDITIONAL ENZYME CATALYTIC EFFECTS TO DEGRADATION OF SMART  
POLYMER BIOMATERIALS**

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Selfregulated behavior of some polymer materials adapting to their environment conditions, especially when applied as biomaterials is very attractive for biomedical application. It has been stressed also with their popular name: "intelligent" or smart biomaterials. From practical point of view such material properties provide a wide variety of applications, both for replacement of body tissues or temporarily overtaking some tissue functions during healing of different organs or tissue damages.

From molecular point of view mechanisms dominating the present smart material application are related to dynamics of polymer molecules and intermolecular structures and to chain degradation processes as well. It is common opinion that enzyme contribution to smart material behavior is dominantly related to degradation of their structure in a body. Such degradation opens a new space for growing tissue during healing of damaged organs and in that way helps to the new tissue to take over a part of body load from the implant. But, in many cases the process is much more complex. Besides the different degradation processes, enzymes influence the chain structure changes as the first by configurational and than conformational changes.

In this contribution are considered conformational properties of alginates in relation to energy changes produced by enzyme conversion of epimer D-manuronic acid residues to L-guluronic residues. In particular different radii of gyration obtained experimentally and persistent length are related to both, conformational models of alginate chains with different M/G blocks and models of gel structure

*P.S.E.18*

## **RHEOLOGICAL ASPECTS OF STRUCTURED-GEL IMPLANT APPLICATIONS**

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Polymers in gel state exhibit numerous attractive and unique properties. For bio-medical application are of especial interest hydrogels that resemble natural tissue more than any other class of synthetic biomaterials. Hydrogels are three-dimensional hydrophilic polymeric networks, capable of absorbing large amounts of water or body liquids. It makes them soft in contact with other body parts but, at the same time polymer network provides material integrity and elasticity under load. These gels exhibit a thermodynamic compatibility with water, which allows them to swell in aqueous media while polymer structure provides biocompatibility or at least bioinertness. Moreover there are numerous possibilities for design gel structure of such kind from both, chemical and physical point of view. All attractive features mentioned above have raised high interest for gel applications in biomedicine last years. Starting from standpoints of very different scientific and technical disciplines, various authors use gels in a broad spectrum of purposes and often with quite new and unexpected effects produced. In biomedicine for example, it is used from simple elastomer tissue extensions up to "intelligent" selfassembling materials.

But, the new and pragmatic approach to such multidisciplinary field sometimes overshadow some serious problems, important in long term application of such materials, especially for medical purposes. One of the issues is the anomalous time-temperature relation of some gels during long term application. Unfortunately such simplifications lead to misinterpretations of gel properties by some authors that are not from polymer field, although the issues are stressed already in the first theories on polymer gel structure, formulated by P.J. Flory, and coworkers and later in papers of L. Onsager, Lord Todd, A. Isihara and others.

In this contribution is analyzed just the part of the problem, which is related to its energetic aspects, using internal variable method. The viscoelastic properties of the material are considered not in terms of classical rheological models, but using approach of fractional derivatives. Examined was first the reproducibility level of experimental results obtained for living systems by such method and later the generality of application for systems of different gel constitution. Obtained results are in good agreement with experiments.

*P.S.E.19*

**STUDY OF THE RELEASE OF THE HEAVY METALS FROM VARIOUS FIXED DENTURES (APPLIANCES) INTO SYNTHETIC SALIVA, USING ELECTROCHEMICAL STRIPPING ANALYSIS**

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In dental-prosthetic praxis, various kinds of fixed dentures, crowns and bridges, very often were used in order to replace natural teeth and to respond to all health and esthetic needs. For the creation of these appliances many high purity dental ceramic materials, acrylics, composites and metallic compounds were used. Stability of the fixed dentures depends on material characteristics and the level of management, as well as on characteristics of environment where they are situated. Because of the natural contact of saliva and the denture, influence of oral liquids on fixed dentures and the status (releasing and incorporating) of heavy metal ion (Pb, Cd, Cu) is of high importance. Depending on the various liquids and food passing through the mouth, this influence can be more or less expressed.

For a heavy metal migration characteristic analyses, 3 types of crowns were used: Co-Cr-Mo total crowns, metal-ceramic and facet crowns. For process of cementing Zn-phosphate, poly-carboxylate and glassionomer cement were used. Also, the influence of saliva medium on natural human teeth was observed. In order to analyze the influence of time period of contact on these processes, samples (natural teeth and dentures) have been exposed to the synthetic saliva solution for 24 hours, and for 40 days.

The study confirmed that synthetic saliva does not have any significant influence on heavy metal ion migration from the natural teeth, but from the fixed dentures (artificial teeth) there was migration of some observed toxic heavy metal ions in low doses.

P.S.E.20

**APPLICATION ANALYSIS OF MICRO AND NANO COMPOSITES IN RESTORING  
OF BONE TISSUE OF THE JAW**

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Application of synthetic polymer biomaterials is very often used in biomedicine and dentistry. That's why the need for creating the new polymer biomaterials is more and more obvious. Hydroxy-apatite, as a natural constituent of bone, has been already used for many years in all segments of dentistry. In order to develop better properties, hydroxy-apatite is combined with polymers. In this research, application of micro and nano composite biomaterials in reconstruction of osteoporosis damaged alveolar bone of rats is analyzed. Evaluation of regeneration of restored osteoporosis damaged alveolar bone of rats was done by histopathological analyses. The optimal results were after 24 weeks after implantation of calcium-phosphate/poly-D, L-lactide-co-glycolide (CP/DLPLG) composite biomaterials nano particles in comparison to micro particles. Regeneration and reparation of damaged alveolar bone with creation of new bone tissue which is very similar to mature bone, are much better on the place of nano CP/DLPLG implantation. Because of its very good osteoconductive effect, applied nano CP/DLPLG composite can totally renew lost bone tissue, so it can be the material of choice for the alveolar bone defect rehabilitation.

*P.S.E.21*

**EVALUATION OF GLASSIONOMER CEMENT APPLICATION FOR PERMANENT  
BINDING OF PROSTHETIC DENTURES**

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Fixed dentures are created in order to rehabilitate the function of orofacial system, to correct disordered interdental relation, as well as the relation between jaws and to do esthetic correction. Binding of fixed dentures to the teeth carriers is done with a layer of binding biomaterials from the group of dental cements. Cement as the choice of dental biomaterials has to be the best cement for the most frequent, routine management for these type of works and most frequently used materials – metal, acrylate, ceramics. Cement must be safe to use with patients. Ideally, it must have longtime advantages such as to be for various uses, to find the right balance between results and simplicity of application, which are the most important for routine management. There are many types of cement. In this study, Zn-phosphate and glassionomer cement were used. In modern dental technology, production of cement is well developed and the most concerns are about non-toxicity, biocompatibility, bioinertness, biofunction. In some cases acidic balance disorder of saliva medium can bring to release of low doses of heavy metal ions after the reaction of cement and heavy metal ions from dental compounds. In this study, the best results were achieved with glassionomer cement, because the lowest percent of released heavy metal ions in saliva medium was noticed after cementing of fixed dentures by glassionomer cement. Because of its characteristics, glassionomer cement can be the choice material for permanent cementing of fixed prosthetic dentures.

*P.S.E.22*

**BOVINE SERUM ALBUMIN (BSA) ION INTERACTION FOLLOWED BY ITC**

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Interaction between Bovine Serum Albumin (BSA) and several biological metal ions ( $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Na}^+$ ) have been studied by Isothermal Titration Calorimetry (ITC). Thermodynamical parameters (H - enthalpy of binding, K - binding constant and N - number of binding sites) of protein/ion interaction were obtained. Possibility of BSA usage, as potential ion delivery agent, in protein drug delivery system was discussed.

*P.S.E.23*

### **THIN FILMS AND IMPLANT MATERIALS**

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In this paper presents analysis of thin films in implant materials. On the basis of preliminary results, it can be concluded that thin polymer films between bone and implant achieve bio-compatibility. In addition, analysis will be conducted for other characteristics, such as bio-inertness and bio-functionality.

*P.S.E.24*

### **EFFECT OF HYDROGELS BASED ON 2-HYDROXYETHYL METHACRYLATES TO ERYTHROCYTE RESISTANCE TO HEMOLYSIS**

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In this study hemolytic activity of hydrogels different chemical construction and synthesized under different conditions was examined. The hydrogels are synthesized by radiation and chemical polymerization of 2-hydroxyethyl methacrylate (HEMA), copolymerization of HEMA with itaconic acid (IA), and copolymerization of HEMA, IA with poly (alkylene glycol) (met) acrylates - Bisomers. In this purpose we used hemolytic test on rat erythrocytes. Materials with the same area show different hemolytic activity. According to given hemolysis, all of tested materials can be considered nonhemolytic.



*P.S.E.25*

**EFFECT OF HYDROGELS BASED ON 2-HYDROXYETHYL METHACRYLATES TO VIABILITY AND OXIDATIVE ABILITY OF RAT PERITONEAL MACROPHAGES**

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The aim of this study was to examine the effect of hydrogels different chemical construction and synthesized under different conditions to viability and oxidative ability of macrophages. The hydrogels are synthesized by radiation and chemical polymerization of 2-hydroxyethyl methacrylate (HEMA), copolymerization of HEMA with itaconic acid (IA), and copolymerization of HEMA, IA with poly (alkylene glycol) (met) acrylates - Bisomers. We used the cytotoxicity test to exam the viability and the chemiluminescent test by which was measurement the oxidative ability of rat macrophages. The oxidative ability of macrophages decreases in the presence of hydrogels. All of tested materials reduce the viability of macrophages. Degree of reduction of rat peritoneal macrophages viability is proportional with concentration of tested material.

*P.S.E.26*

**OSTEOGENIC ACTIVITY IN A MICE SUBCUTANEOUS IMPLANT OF POROUS HYDROXYAPATITE/POLY-L-LACTIDE LOADED WITH BONE MARROW CELLS**

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Hydroxyapatite (HAp) is biomaterial widely used in the regeneration of bone tissue. Addition of osteogenic cells to HAp implants may accelerate the bone repair process. The aim of this study was to investigate how the bone marrow cells (BMCs) loading of porous hydroxyapatite/poly-L-lactide (HAp/PLLA) act to ectopic osteogenesis. In this purpose HAp/PLLA with and without BMCs was subcutaneously implanted into BALB/c mice. As a control served implants from both types which weren't implanted. Three weeks after implantation, histological analysis of implants was done. It was observed significant resorption and induction of collagenogenesis in implanted biomaterials. The structure of new bone was seen in implants loaded with bone marrow cells.

*P.S.E.27*

**DESIGNING OF THE ALGINATE HYDRO GEL BEADS MORPHOLOGY USING  
ULTRASONIC SPRAY GELLING METHOD**

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Alginate is biopolymer, which is due to its biocompatibility and biodegradability widely used for immobilization of enzymes, cells and drugs and their encapsulation. The basic method for producing alginate beads is electrostatic extrusion. In this work, to our best knowledge, this is the first attempt of using ultrasonic spray gelling method for the same purposes. Produced beads by electrostatic extrusion are usually in spherical form. It is shown, that ultrasonic spray gelling method, provides to get them in various shapes and sizes, by using ionic species of different ionic strength. This may have influence to the activity of cells and enzymes and drug release rate encapsulated in these beads.

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ISBN 978-86-80321-11-0



CIP – Каталогизација у публикацији  
Народна библиотека Србије, Београд

66.017/.018(048)

YUGOSLAV Materials Research Society  
(Beograd). Conference (9 ; 2007 ; Herceg  
Novi)

Programme and the Book of Abstracts /  
Ninth Annual Conference of the Yugoslav  
Materials Research Society YUCOMAT 2007,  
Herceg Novi, September 10-14, 2007 ;  
organized by Yugoslav Materials Research  
Society, Faculty of Metallurgy and Tehnology,  
Podgorica and Institute of Technical Sciences  
of the Serbian Academy of Sciences and Arts,  
Belgrade ; [editor Dragan R. Uskoković]. -  
Belgrade : Institute of Technical Sciences  
of SASA, 2007 (Belgrade : Čigoja). - LI,  
202 str. : tabele ; 30 cm

Tiraž 300. - Registar.

ISBN 978-86-80321-11-0

1. Yugoslav Materials Research Society  
(Beograd) 2. Faculty of Metallurgy and  
Tehnology (Podgorica) 3. Institute of  
Technical Sciences of SASA (Beograd)  
а) Наука о материјалима - Апстракти б)  
Технички материјали - Апстракти  
COBISS.SR-ID 141931788

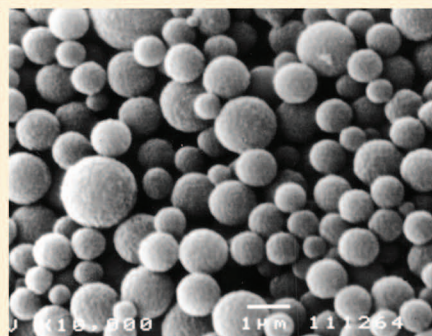


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