

Programme & The Book of Abstracts

Twentieth Annual Conference

YUCOMAT 2018

Herceg Novi, Montenegro, September 3–7, 2018

Organised by



endorsed by



TWENTIETH ANNUAL CONFERENCE

YUCOMAT 2018

Hunguest Hotel Sun Resort Herceg Novi, Montenegro,
September 3-7, 2018
<http://www.mrs-serbia.org.rs>

Programme and The Book of Abstracts

Organised by:
Materials Research Society of Serbia

Endorsed by:
**Materials Research Society,
European Materials Research Society
and
Federation of European Material Societies**

Title: THE TWENTIETH ANNUAL CONFERENCE
YUCOMAT 2018
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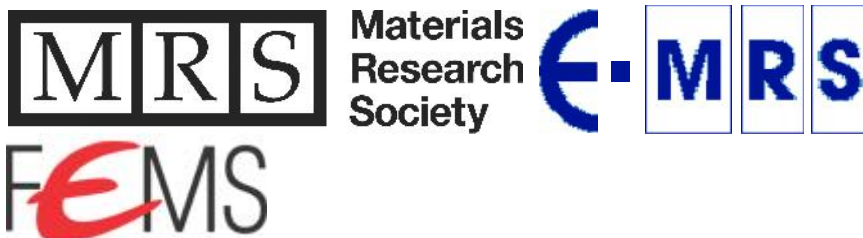
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Acknowledgments: This conference is celebrating 20 years of YUCOMAT



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WELCOME SPEECH BY THE PRESIDENT OF MRS-SERBIA:

Dear Attendees,



It is my pleasure to welcome you to the 20th anniversary YUCOMAT. We started off in 1995 and have made great strides since then, having transformed a small national conference that the 1st YUCOMAT was into an international and world-renowned meeting of today. Crème de la crème of the field of materials science and engineering gathers here every year and none of us, including the four founders of the MRS-Serbia (Drs. Milonji , Radmilovi , Rakovi and myself), could have foreseen the eminent levels that YUCOMAT would reach when we organized it for the

first time, 23 years ago.

This particular, 20th anniversary YUCOMAT is above all the others based on some measures, one of which is the total duration of oral presentations. It is to be blamed for the minimal free time in-between the talks this year and I know that some participants will not forgive this to me so easily. We have 33 plenary lectures, 2 satellite symposia with around 12 talks each and 44 regular oral presentations, along with 63 posters, and I will let these numbers alone speak about the continuous rising track that YUCOMAT has been on since its inception. Out of 170 works that are to be presented, eighty percent are international in origin, whereas one-third will be presented by scientists affiliated with national institutions. As for the international participants, the most numerous delegation is that of the United States, with 15 presenters. It is followed by South Korea with 13 participants, Taiwan with 12 and then by Poland, Czech Republic, Germany and other countries. Serbian researchers are very well represented too, with 38 presentations in total, as well as the researchers from the region of the former Yugoslavia.

This YUCOMAT is the fourth one in a row at which we give out the award of the MRS-Serbia for a lasting and outstanding contribution to materials science and engineering. After Ivan Božovi , Gordana Vunjak-Novakovi and Velimir Radmilovi , the winner of this award for 2018 is Laszlo Forro, a professor of the physics of complex matter at the École polytechnique fédérale de Lausanne (EPFL), for his immense contribution to the field of engineering of new materials, including inorganic and organic, as well as biomaterials. Dr. Forro is recognized not only for his scientific contribution, but also for the effort to unify the community of former Yugoslavian scientists working domestically and abroad, which is one of the important missions of our MRS. Dr. Forro is the member of Croatian, Hungarian and Serbian academic

institutions, which is a transnational accomplishment that a very small number of scientists from this region can pride themselves on. All of us are delighted that Laszlo Forro is here with us today and that he will present some of his most significant research as a part of the Opening Ceremony.

Two years ago we organized the seminal satellite symposium dedicated to presentations by Korean researchers working in the field of hybrid materials. The positive impressions they received here have brought them back to YUCOMAT this year for the satellite symposium on Hybrid Interphase Materials. All Korean experts this year participate through solicitation by the Director of the National Core Research Center for Hybrid Solutions of Busan University, Prof. Kwang-Ho Kim and the renowned Fellow of the Korea Institute of Science and Technology (KIST), Prof. Kyung-Ho Shin. At the symposium, which will be held on Wednesday, twelve Korean distinguished researchers will present their newest discoveries on this subject. Positive impressions are passed around within the materials science community and following the success with this satellite symposium two years ago, another one held this year is organized by Prof. Feng-Huei Lin, the Director of the National Health Research Institute (NHRI) in Taipei, Taiwan, and its title is Advanced Materials for Biomedical Engineering. In this exciting symposium, professors and students from Taiwan will present their most recent research in the field of advanced materials for various applications in biomedical engineering. Specifically, six Taiwanese professors will present orally on Wednesday morning as well as seven PhD students, who will give shorter talks and will additionally have the opportunity to present posters at the third and the final poster session, which will be held on Thursday evening.

Like the last year, this year's diamond sponsors of YUCOMAT are Thermo Fisher Scientific and the International Journal of Nanomedicine. We are incredibly indebted to them for lightening up the financial burdens that have been troubling our society in the past years. The members of our International Advisory Board, specifically its President Bob Sinclair and its distinguished member, Hamish Fraser, should also be acknowledged for initiating the idea of voluntary registration fee self-coverage by the invited lecturers traditionally freed of that obligation. Another thing we achieved with the voluntary help of the members of our MRS is the expansion of the current database of potential participants up to 11,000 names, which makes it twice larger than the previous list. It gives us hopes that informing a greater number of people from the materials science community about YUCOMAT would directly correspond to a greater number of participants in the years that follow. Also, for the first time in its history, YUCOMAT is financially supported by the gold and the silver sponsors too, the names of which could be found on the list of sponsors in the Book of Abstracts.

One of the central goals of MRS-Serbia is the promotion of science through support of young scientists. The lecture hall, for those who have not noticed, is filled with young

people who are members of various organizational committees at YUCOMAT. In addition, from the first to the present YUCOMAT, we have engaged in the effort to inspire and motivate young researchers through rewarding the best oral and poster presenters and the best doctoral theses defended in the timespan between the two successive conferences. The same practice was adopted at our conferences for young researchers held at the Serbian Academy of Sciences and Arts in Belgrade every December. As of two years ago, we have also begun to subsidize these prospective young scientists' participations at EUROMAT Junior conferences.

Many of you might notice that YUCOMAT has traditionally attracted scientists from academic institutions, but the conference has not been as popular among scientists coming from industry. Materials science and engineering is a highly applicative field and a number of technologies presented at this conference are directly translatable to marketable applications. On top of this, we could wonder if the economy of a country could ever grow beyond a certain level if its basic science and industry remain as disconnected as they are in today's Serbia and most other countries of this region. Oh well, but how do we simultaneously promote state-of-the-art basic materials science, whose applications may be decades ahead, and industrial research, which in this particular setting would feed best on more modest concepts, some of you might ask and there is no easy answer. Aside from learning from some of the best examples, including the Korean and the Taiwanese success, which we will hear about in the respective satellite symposia, palpable ideas are needed on how to bridge this gap between basic science and industry in the region with many of the limitations and challenges that are no longer relevant in the developed world.

As we do succeed in bridging this gap, there will be, as ever, other challenges to cope with and some of them stem from today's rather ambiguous relationship between science and money. When I began my scientific career 50 years ago, science was a place attracting true aficionados of knowledge, who paid no heed to finance, but this is not so anymore in the developed world. There, science has become a lucrative business to many and being indifferent to money is these days, sadly, a secure way out of the scientific profession. The general opinion of youth in science today, especially in this region of the world, where funding is meager, is that lots more money would solve all their problems. It would enable better and more numerous experiments to be conducted, thus increasing the quality of science, and it would also bring about the comfort of professional and private lives to the scientists. However, the other side of the coin is often overlooked. In the United States, for example, the country I visit often, I witness firsthand the extent to which money spoils this very science that it helps grow. How? One reason is that scientific institutions, increasingly adopting aggressive business models, have begun to prioritize the acquisition of funds over the creation of new knowledge. This flawed prioritization has been creating negative selection, especially at

the level of junior scientists; namely, those who are very smart and cunning when it comes to acquisition of funds, knowing how to sell their ideas well, even when they are not so inventive, push out of the scientific pyramid those who are not so skilled at selling their science. Like in the business world, the quality of packaging and marketing has taken over the quality of the product. As science evolves on top of these flawed premises, it becomes a cutthroat business where not the most benevolent and inventive are retained, but rather those who are the most talented entrepreneurs. The latter model, very often, feeds on an exploitative environment, careless mentorship and, perhaps most critically of all, superficially conducted science. For, science conducted on the premise that material wealth and prolific resources are all that matter sooner or later becomes akin to a conveyer belt, a factory that inertly produces knowledge with not even a zest of creativeness. What I urge the young scientists in this region of the world and abroad to do is to be aware of this rampant materialism and the dehumanization of science that it bears and take a stand against it when their time to change the science policies for better comes. As far as this region is concerned, inertly following in the footsteps of the developed world when it comes to creation of these policies is an error and every country should find a model that is suited to it, uniquely. It should also watch out for inevitable mistakes committed by the more developed countries and, like a frog, leap over them, thus accelerating its progress and, one day, maybe even transcending those who are way ahead of them right now. After all, if this region of the world has been historically known for something, it is the ability to rebuff imperialism while showing that the power of the mind rules over matter and that ideas should drive technologies and not the other way around. What better time to elicit this bold stance in the sphere of materials science and science in general than today?

This is all to say that in spite of the enjoyable times spent at YUCOMAT, we should be aware that all of us are assigned the task to do something creative to ameliorate the existing imbalances and promote welfare for the future generations of humanity, both locally and globally, to the best of our capacities. No greater gift could be left to them than relishing in the joys of scientific exploration of the world. Therefore, I wish this to be yet another YUCOMAT that brings the joy of science and friendship to us all. Let us enjoy in all good that materials science and we, its stewards and spokespersons, have to offer!

Sincerely Yours,

Dragan Uskokovi
MRS-Serbia, President

2018 MRS-SERBIA AWARD FOR A LASTING AND OUTSTANDING CONTRIBUTION TO MATERIALS SCIENCE AND ENGINEERING

We are pleased to announce that the laureate of the 2018 MRS-Serbia Award for a Lasting and Outstanding Contribution to Materials Science and Engineering is Prof. Dr. László Forró of the Ecole Polytechnique Fédérale de Lausanne, Laboratory of Physics of Complex Matter. He is awarded for his achievements in the engineering of new materials, including inorganic and organic materials, as well as biomaterials.



This is the decision of the MRS-Serbia Executive Board:

The Executive Board of the MRS-Serbia Presidency, at their meeting on April 10, 2018, considered the submitted nominations for the MRS-Serbia's 2018 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering and concluded that the procedure was conducted in accordance with the Awarding Rulebook, that the Call was announced on the MRS-Serbia's website on January 1, 2018, and that in the stipulated period of 45 days only one nomination was submitted, that for Prof. László Forró, by Prof.

Dr. Davor Pavuna (Ecole Polytechnique Fédérale de Lausanne, Switzerland). The nomination was strongly supported by five members of the Presidency of the MRS Serbia: Academician Zoran Popovi , Academician Zoran Petrovi , Academician Slavko Mentus, Prof. Milenko Plavši and Prof. Dr. Miodrag Zlatanovi .

Having received the opinion from the Expert Committee members, Prof. Dragan Uskokovi (President of MRS-Serbia), Prof. Robert Sinclair (Chair of YUCOMAT Conferences International Advisory Board), Dr. Slobodan Milonji (Vice-President of MRS-Serbia), Prof. Danilo Suvorov (Member of YUCOMAT Conferences International Advisory Board), Prof. Dejan Rakovi (Vice-President of MRS-Serbia) and Prof. Dr. Ivan Božovi (2015 Laureate), Prof. Dr. Gordana Vunjak-Novakovi (2016 Laureate), and Prof. Dr. Velimir Radmilovi (2017 Laureate), the Executive Board of the MRS-Serbia Presidency took the decision that Prof. Dr. László Forró be granted MRS-Serbia's 2018 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering.

Prof. Dr. László Forró's invited plenary lecture "Organo-metallic lead iodide perovskites: a material science approach" will be presented during the Opening Ceremony of the 20th Materials Research Society of Serbia Annual Conference YUCOMAT 2018 on September 3, 2018.

President of MRS-Serbia, Prof. Dr. Dragan Uskokovi
Vice-President of MRS-Serbia, Dr. Slobodan Milonji
Vice-President of MRS-Serbia, Prof. Dr. Dejan Rakovi

MRS-Serbia

President: Dragan Uskokovi

Vice-presidents: Slobodan Milonji , Velimir Radmilovi , Dejan Rakovi

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Conference Organising Committee

Chairperson: Dragana Jugovi , or e Veljovi

Members: Ljiljana Damjanovi , Veljko oki , Branko Matovi , Željka Nikitovi , Irena Nikoli , Bojana Obradovi , Nebojša Rom evi , Mira Vuk evi

Conference Manager: Sava Stoislavljevi

Conference Technical Committee

Ivana Dini , Veljko oki , Sonja Jovanovi , Zoran Jovanovi , Petar Lauševi , Željko Mravik, Milica Ševkuši

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 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 and, similar to other MR societies in the world, the programme was made and objectives

determined. 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. Until 2003, Conferences were held every second year and then they grew into Annual Conferences that were traditionally held in Herceg Novi in September of every year. Following the political separation between Serbia and Montenegro, in 2007 Yu-MRS formed two new MRS: MRS-Serbia (official successor of Yu-MRS) and MRS-Montenegro (in founding). In 2008 MRS-Serbia became a member of FEMS (Federation of European Materials Societies).

GENERAL INFORMATION

DATE AND VENUE: The conference will be held on September 3-7, 2018, at the Hunguest Hotel Sun Resort, in Herceg Novi, Montenegro. Participants will also be accommodated there. The conference will begin on Monday, September 3th, at 09.00 and end on Friday, September 7th, 2018, 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 2, and Monday, September 3, from 8.00 to 19.00, on Tuesday, Wednesday and Thursday 8.00-13.00 and 19.00-20.00, and on Friday from 8.00 to 12.00. At registration, the participants are requested to submit a proof of their advance registration fee payment.

INSTRUCTION FOR AUTHORS: The conference will feature plenary sessions, oral sessions, poster sessions, and an Exhibition of synthesis and characterization equipment.

Time of papers' presentations to be given in ORAL SESSIONS is limited. Time available for delivery is 30 min for plenary and 15 min for other papers, including discussion. Video-beam is available. PowerPoint presentations, recorded on CD or USB flash-memory, should be given at registration, specifying the name of the speaker and the day and session number.

In POSTER SESSIONS, the authors are requested to display their posters minimum one hour before the session and to be present beside their posters during the session. Poster sessions' venue will be open from Tuesday to Thursday, from 20.00-22.00.

CONFERENCE AWARDS: Materials Research Society of Serbia 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 theses defended between two conferences. Awarded researchers are granted free registration at the next YUCOMAT Conference.

ADDITIONAL ACTIVITIES: An Exhibition of synthesis and characterization equipment will be held during the Conference. Traditional Cocktail Party on Monday evening and excursion on Thursday afternoon (boat trip around Boka Kotorska Bay) will be organized again.

Programme

GENERAL CONFERENCE PROGRAMME

Sunday, September 2 2018

08⁰⁰-19⁰⁰ **Registration**

Monday, September 3, 2018

08⁰⁰-19⁰⁰ **Registration**
09⁰⁰-10⁰⁰ **OPENING CEREMONY**
- Introduction and Welcome
Main Conference Hall

10³⁰-13⁰⁰ **First Plenary Session**, Main Conference Hall
13⁰⁰ **Photo Session**
14³⁰-19⁰⁰ **Second Plenary Session**, Main Conference Hall
19³⁰-21⁰⁰ **Cocktail Party**

Tuesday, September 4, 2018

08³⁰-13⁰⁰ **Third Plenary Session**, Main Conference Hall
14³⁰-20⁰⁰ **Fourth Plenary Session**, Main Conference Hall
20⁰⁰-22⁰⁰ **Poster Session I** (Symposium A and B1), Villa MIMOZA

Wednesday, September 5, 2018

09⁰⁰-13⁰⁰ **Symposium F**, Main Conference Hall
15⁰⁰-19⁰⁰ **Symposium G**, Main Conference Hall
20⁰⁰-22⁰⁰ **Poster Session II** (Symposium B2, C and D), Villa MIMOZA

Thursday, September 6, 2018

09⁰⁰-12⁴⁵ **First Oral Session**, Main Conference Hall
09⁰⁰-12¹⁵ **Second Oral Session**, Small Conference Hall
14⁰⁰-19⁰⁰ **Boat-trip around Boka Kotorska Bay**
20⁰⁰-22⁰⁰ **Poster Session III** (Symposiums E), Villa MIMOZA

Friday, September 7, 2018

09⁰⁰-12¹⁵ **Third Oral Session**, Main Conference Hall
09⁰⁰-12⁰⁰ **Fourth Oral Session**, Small Conference Hall
12³⁰-13⁰⁰ **Awards and Closing of the Conference**

SYMPOSIUM A: Advanced Methods in Synthesis and Processing of Materials
SYMPOSIUM B: Advanced Materials for High-Technology Application
SYMPOSIUM C: Nanostructured Materials
SYMPOSIUM D: Eco-materials and Eco-technologies
SYMPOSIUM E: Biomaterials
SYMPOSIUM F: Advanced Materials for Biomedical Applications
SYMPOSIUM G: Hybrid Interface Materials

OPENING CEREMONY

Monday, September 3, 2018

Main Conference Hall

09⁰⁰-10⁰⁰

Welcome Speech

Dragan Uskokovi , President of MRS-Serbia, Belgrade, Serbia

Welcome Address

Robert Sinclair, Chair of International Advisory Board

Presentation of YUCOMAT 2017 Awards

Slobodan Milonji , Vice President of MRS-Serbia, Belgrade, Serbia

**MRS-Serbia 2018 Award for a Lasting and Outstanding Contribution to
Materials Science and Engineering**

Organo-metallic lead iodide perovskites: a material science approach

László Forró

Laboratory of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne,
Switzerland

Break: 10⁰⁰-10³⁰

FIRST PLENARY SESSION

Main Conference Hall

Session I: 10³⁰-13⁰⁰

Chairpersons: Yury Gogotsi and Joseph T. Hupp

10³⁰-11⁰⁰ Synthesis and properties of two-dimensional carbides and nitrides (MXenes)

Yury Gogotsi

Department of Materials Science and Engineering, and A. J. Drexel Nanomaterials Institute, Drexel University, Philadelphia, PA 19104, USA

11⁰⁰-11³⁰ AIM-ing for single-atom precision for heterogeneous catalysts

Joseph T. Hupp

Northwestern University Department of Chemistry Evanston, IL 60208, USA

11³⁰-12⁰⁰ Applying chemistry to make today's best tunable millimeter wave dielectric even better

Darrell G. Schlom

Department of Materials Science and Engineering, Cornell University, USA

12⁰⁰-12³⁰ Ultra-high resolution study by aberration-corrected TEM of pyrochlore BZN supplying information on displacive atom-site disorder

Knut W. Urban^{1,2}, Chun-Lin Jia^{1,2}, Hong Wang²

¹PGI-5 and Ernst Ruska Center, Research Center Juelich, Juelich/Germany; ²School of Electronic and Information Engineering and State Key Laboratory for Mechanical Behaviour of Materials, Xi'an Jiaotong University, Xi'an, China

12³⁰-13⁰⁰ Electric field control of magnetism

Ramamoorthy Ramesh

Department of Physics and Department of Materials Science and Engineering

Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720, USA

13⁰⁰-13³⁰ Photo session

Break: 13³⁰-14³⁰

SECOND PLENARY SESSION

Main Conference Hall

Session I: 14³⁰-16³⁰

Chairpersons: Knut W. Urban and Rolf Erni

- 14³⁰-15⁰⁰ **Correction of aberrations – past – present – and future perspectives**
Harald Rose
Ulm University, Ulm, Germany
- 15⁰⁰-15³⁰ **Prospects and challenges for high-resolution transmission electron microscopy**
Rafal E. Dunin-Borkowski, Lei Jin, András Kovács, Andreas Thust
Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter
Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany
- 15³⁰-16⁰⁰ **High precision STEM studies of spatial strain distribution in nanostructures with correlation to properties**
Eva Olsson
Chalmers University of Technology, Eva Olsson Group, Gothenburg, Sweden
- 16⁰⁰-16³⁰ **Unconventional imaging by scanning transmission electron microscopy**
Rolf Erni, Trond Henninen, Feng Wang, Marta Bon, Debora Keller, Nabeel Ahmad,
Marta D. Rossell, Marco Campanini
Electron Microscopy Center, Empa, Swiss Federal Laboratories for Materials Science
and Technology, 8600 Dübendorf, Switzerland

Break: 16³⁰-17⁰⁰

Session II: 17⁰⁰-19⁰⁰

Chairpersons: Eva Olsson and Rafal E. Dunin-Borkowski

- 17⁰⁰-17³⁰ **Growth of wide bandgap semiconducting layers: a transmission electron microscopy study**
Bela Pecz
Institute for Technical Physics and Materials Science, Centre for Energy Research,
Hungarian Academy of Sciences, MTA EK MFA, 1121 Budapest, Konkoly-Thege M.
u. 29-33, Hungary
- 17³⁰-18⁰⁰ **The role of interface complexions on processing ceramic matrix nanocomposites**
Ruth Moshe, Rachel Marder, Wayne D. Kaplan
Department of Materials Science and Engineering, Technion - Israel Institute of
Technology, Haifa, Israel

- 18⁰⁰-18³⁰ **Sub 30 meV in a monochromated Themis Z**
Anil Yalcin
Thermo Fisher Scientific, Eindhoven, Netherlands
- 18³⁰-19⁰⁰ **High-resolution 3D crack visualization in multi-component materials and structures during mechanical loading – A novel application of X-ray microscopy**
Ehrenfried Zschech, Sven Niese¹, Kristina Kutukova, Juergen Gluch
Fraunhofer IKTS Dresden, Germany
¹now with AXO Dresden GmbH, Dresden, Germany

THIRD PLENARY SESSION

Tuesday, September 4, 2018

Main Conference Hall

Session I: 08³⁰-10³⁰

Chairpersons: Vladimir Torchilin and Robert Sinclair

- 08³⁰-09⁰⁰ **An update on advanced electron microscopy for cancer nanotechnology research**
Robert Sinclair^{1,2}, Yitian Zeng^{1,2}, Steven J. Madsen^{1,2}, Ai L. Koh¹
¹Stanford University, Department of Materials Science and Engineering, Stanford, USA; ²Stanford University, Center for Cancer Nanotechnology Excellence, Stanford, USA
- 09⁰⁰-09³⁰ **Recent developments in combination nanopreparations against cancer**
Vladimir Torchilin
Center for Pharmaceutical Biotechnology and Nanomedicine, Northeastern University, Boston, MA 02115, USA
- 09³⁰-10⁰⁰ **The future of medicine: implantable nanosensors**
Thomas J. Webster
Department Chemical Engineering; Northeastern University; USA
- 10⁰⁰-10³⁰ **Ceramic nanoparticles for advanced biomedical applications: from bone to brain**
Vuk Uskokovi
University of Illinois at Chicago, USA

Break: 10³⁰-11⁰⁰

Session II: 11⁰⁰-13⁰⁰

Chairperons: Danilo Suvorov and Paul V. Braun

- 11⁰⁰-11³⁰ **Solid-state oxygen abstraction from stable oxides for energy storage materials**
Mamoru Senna
Keio University, Yokohama, Japan Faculty of Science and Technology, Hiyoshi,
Yokohama 223-8522, Japan
- 11³⁰-12⁰⁰ **High energy density electrodeposited Li and Na-ion battery electrodes**
Paul V. Braun
University of Illinois at Urbana-Champaign, Urbana, USA
- 12⁰⁰-12³⁰ **(Early actinoid metal)-boron-carbon systems: phase equilibria, crystal structures and physical properties**
Peter Rogl¹, Raimund Podloucky², Henri Noel³, Gerald Giester⁴
¹Institute of Materials Chemistry & Research, University of Vienna, A-1090 Vienna, Austria; ²Institute of Physical Chemistry, University of Vienna, A-1090 Vienna, Austria; ³Laboratoire de Chimie du Solide et Materiaux, UMR-CNRS 6226, Université de Rennes I, F-35042 Rennes, France; ⁴Institute of Mineralogy and Crystallography, University of Vienna, A-1090 Vienna, Austria
- 12³⁰-13⁰⁰ **Solid-state synthesis of lead-free (K/Na)_{0.5}Bi_{0.5}TiO₃ piezoceramics: peculiarities and their influence on the electrical properties**
Danilo Suvorov, Jakob König, Matjaž Spreitzer
Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia

Break: 13⁰⁰-14³⁰

FOURTH PLENARY SESSION

Main Conference Hall

Session I: 14³⁰-17⁰⁰

Chairpersons: Richard W. Siegel and Hamish L. Fraser

- 14³⁰-15⁰⁰ **A unified computational approach for dislocation-based plasticity**
Richard LeSar, John Graham, Laurent Capolungo
Iowa State University, Department of Materials Science and Engineering, Ames, IA, USA; Ames Laboratory, Ames, IA, USA; Los Alamos National Laboratory, Los Alamos, NM, USA

- 15⁰⁰-15³⁰ **Materials characterization and integrated computational materials engineering: providing solutions for near-net shape manufacturing**
Hamish L. Fraser
Center for the Accelerated Maturation of Materials, The Ohio State University,
Columbus, USA
- 15³⁰-16⁰⁰ **On the nucleation of planar faults in single crystal Ni-base superalloys**
Gunther Eggeler
Bochum University, Ruhr, Germany
- 16⁰⁰-16³⁰ **Quo vadis quantum matter?!**
Davor Pavuna
Complex Matter Laboratory - Institute of Physics, Ecole Polytechnique Federale de
Lausanne, CH-1015 Lausanne, Switzerland
- 16³⁰-17⁰⁰ **Ultimate atom resolution**
Richard W. Siegel
Materials Science and Engineering Department, Rensselaer Polytechnic Institute,
Troy, New York 12180, USA

Break: 17⁰⁰-17³⁰

Session II: 17³⁰-20⁰⁰

Chairperson: Toshiaki Makabe and Vikram Jayaram

- 17³⁰-18⁰⁰ **Probing mechanical behaviour at small length scales: from spatially resolved toughness in Pt-Ni-Al bond coats on superalloys to small scale cantilever creep for residual life assessment**
Vikram Jayaram
Indian Institute of Science, Department of Materials Engineering, Bangalore 560012,
India
- 18⁰⁰-18³⁰ **NV centers in diamond: potentials and limitations for quantum metrology**
Karoly Holczer¹, Jason Cleveland²
¹UCLA, Department of Physics & Astronomy 475 Portola Plaza, Los Angeles, CA
90095-1547, USA; ²SomaLogic Inc. 2945 Wilderness Place Boulder, CO 80301, USA
- 18³⁰-19⁰⁰ **Metastable-watching for the structure and property of low-temperature plasmas**
Toshiaki Makabe
Keio University, Japan

19⁰⁰-19³⁰ **On the origin of high glass forming ability in metallic systems**
Emil Babi¹, Ramir Risti², Ignacio A. Figueroa³, Damir Paji¹, Željko Skoko¹, Krešo Zadro¹

¹Department of Physics, Faculty of Science, University of Zagreb, Zagreb, HR 10000, Croatia; ²Department of Physics, University of Osijek, Osijek, HR 31000, Croatia; ³Institute of Materials Research-UNAM, Universitaria Coyoacan, C. P. 04510 Mexico, Mexico

19³⁰-20⁰⁰ **Fundamental aspects of the use of metal hydrides in hydrogen energy and chemical current sources**

Yuriy Solonin, Valentin Dobrovolsky, Olga Ershova, Oleg Khyzhun
Institute for Problems of Materials Sciences National Academy of Sciences of Ukraine, Ukraine

SYMPOSIUM F: ADVANCED MATERIALS FOR BIOMEDICAL APPLICATIONS

Wednesday, September 5, 2018

Main Conference Hall

Session I: 09⁰⁰-10³⁰

Chairpersons: Feng-Huei Lin and Ching-Li Tseng

09⁰⁰-09³⁰ **The preparation of injectable angiogenic bone cement for femoral head avascular necrosis**

Feng-Huei Lin

Institute of Biomed Eng & Nanomed., National Health Research Institutes, Taiwan ;
Institute of Biomed Eng., National Taiwan University, Taipei, Taiwan

09³⁰-10⁰⁰ **Gelatin nanoparticles with anti-inflammatory/anti-angiogenesis agent loading for ocular disease treatment**

Ching-Li Tseng

Graduate Institute of Biomedical Materials & Tissue Engineering, College of Biomedical Engineering; Taipei Medical University, Taipei, Taiwan, ROC

10⁰⁰-10¹⁵ **High throughput generation of alginate-gelatin capsules for human osteoblast-like cells (MG63) long-term cultivation**

Jia-En Yang¹, Yi-Chia Hsieh¹, Ching-Yun Chen², Kai-Fa Teo¹, Chun-Hsu Yao^{3,4},
Cherng-Jyh Ke^{1,4}

¹China Medical University, College of Biopharmaceutical and Food Sciences, Department of Biological Science and Technology, Taichung, Taiwan; ²National Health Research Institutes, Institute of Biomedical Engineering and Nanomedicine, Miaoli, Taiwan; ³China Medical University Hospital, Biomaterial Translational Research Center, Taichung, Taiwan; ⁴China Medical University, College of Medicine, Department of Biomedical Imaging and Radiological Science, Taichung, Taiwan

10¹⁵-10³⁰ **Using continuous bioreactor system to cultivate human bone-like tissues for bone tissue engineering**

Ching-Yun Chen¹, Cherng-Jyh Ke^{2,3}, Jui-Sheng Sun^{4,5}, Feng-Huei Lin^{1,6}

¹Institute of Biomedical Engineering and Nanomedicine (I-BEN), NHRI, Taiwan; ²Biomaterials Translational Research Center, China Medical University Hospital, Taiwan; ³Department of Biological Science and Technology, China Medical University, Taiwan; ⁴Department of Orthopedics, College of Medicine, NTU, Taiwan; ⁵Department of Orthopedic Surgery, NTUH, Taiwan ; ⁶Institute of Biomedical Engineering, College of Medicine and College of Engineering, NTU, Taiwan

- 10³⁰-10⁴⁵ **Fabrication of multilayered gold/silica/gadolinium compound core-shell particles and their properties of X-ray imaging and MRI**
Yuta Shindo¹, Tomoya Inose, Takahiro Oikawa¹, Masayuki Tokunaga², Yohsuke Kubota², Kohsuke Gonda³, Yoshio Kobayashi¹
¹Ibaraki University, College of Engineering, Department of Materials Science and Engineering, Hitachi, Japan; ²Tohoku University, Graduate School of Medicine, Department of Gastroenterological Surgery, Sendai, Japan; ³Tohoku University, Graduate School of Medicine, Department of Medical Physics, Sendai, Japan

Break: 10⁴⁵-11¹⁵

Session II: 11¹⁵-13⁰⁰

Chairperson: Chien-Chung Chen and How Tseng

- 11⁴⁵-12¹⁵ **The self-assembled, microtube array membranes (MTAM) and their applications for cancer translation**
Chien-Chung Chen^{1,2,3,7}, Chee-Ho Chew¹, Wan-Ting Huang⁷, Kang-Yan Lee⁴, Po-Li Wei^{5,6}, Shih-Shin Tu^{5,6}
¹Grad Inst. Biomedical Materials and Tissue Engineering, College of Biomedical Engineering, Taipei Medical University, Taipei, Taiwan; ²Ph.D Program in Biotechnology Research and Development, Taipei Medical University, Taipei, Taiwan; ³International Ph.D. Program for Cell Therapy and Regenerative Medicine, Taipei Medical University, Taipei, Taiwan; ⁴Division of Thoracic Medicine, Taipei Medical University Shuang Ho Hospital, Taipei Medical University, Taipei, Taiwan; ⁵Division of General Surgery, Taipei Medical University Hospital, Taipei Medical University, Taipei, Taiwan; ⁶TMU Research Center of Cancer Translational Medicine, Taipei Medical University Hospital, Taipei Medical University, Taipei, Taiwan; ⁷Research & Development Dept. MTAM Tech Inc. Taipei, Taiwan
- 12¹⁵-12³⁰ **Cornea epithelium reconstruction by a new way to engineer cell sheet**
How Tseng, Chein-Cheng Tai, Yuan-Yi WU, Kun-De Lin
Taipei Medical University, Medical School, Department of Biochemistry and Molecular Cell Biology, Taipei 11031, Taiwan
- 12³⁰-12³⁵ **Addition of porogens improved the characteristics of biodegradable implants made of poly(-caprolactone)/calcium phosphate ceramic composites**
Chang-Chin Wu^{1,2}, Kai-Chiang Yang^{3,4}, Feng-Huei Lin⁵
¹Department of Orthopedics, En Chu Kong Hospital, New Taipei City, Taiwan; ²Department of Orthopedics, National Taiwan University Hospital, College of Medicine, National Taiwan University, Taipei, Taiwan; ³Department of Organ Reconstruction, Institute for Frontier Medical Sciences, Kyoto University, Kyoto, Japan; ⁴School of Dental Technology, College of Oral Medicine, Taipei Medical

University, Taipei, Taiwan; ⁵Ins. of Biomed. Eng., National Taiwan University, Taiwan

12³⁵-12⁴⁰ **The application of hydroxyapatite as the *Bletilla striata* polysaccharide carrier for sarcopenia treatment**

Ya-Jyun Liang¹, Jia-Yu Hong¹, Chun-Han Hou², Feng-Huei Lin¹

¹National Taiwan University, Institute of Biomedical Engineering, Taipei, Taiwan; National ²Taiwan University Hospital, Department of orthopedic surgery, Taipei, Taiwan

12⁴⁰-12⁴⁵ **Hydroxyapatite/gelatin particles embedding stromal cell-derived factor-1 for bone tissue engineering**

Chih Hsiang Fang¹, Yi Wen Lin¹, Jui Sheng Sun², Feng Huei Lin^{1,3}

¹Institute of Biomedical Engineering, College of Medicine and College of Engineering, National Taiwan University, Taipei 100, Taiwan; ²Department of Orthopedic Surgery, National Taiwan University Hospital, Taiwan; ³Division of Biomedical Engineering and Nanomedicine Research, National Health Research Institutes, Miaoli 350, Taiwan

12⁴⁵-12⁵⁰ **A novel multilayer capsule as desensitizing agent for dental hypersensitivity**

Kuo-Hui Chiu¹, Hsiu-Min Chen¹, Yuan-Yu Hsia¹, Ting-Ru Chung², Chih-Yu Shu³, Chia-Yung Lin⁴, Cherng-Jyh Ke^{1,3}

¹China Medical University, College of Biopharmaceutical and Food Sciences, Department of Biological Science and Technology, Taichung, Taiwan; ²China Medical University, College of Medicine, Department of Biomedical Imaging and Radiological Science, Taichung, Taiwan; ³China Medical University Hospital, Biomaterial Translational Research Center, Taichung, Taiwan; ⁴Taichung Hospital, Ministry of Health and Welfare, Department of Dentistry, Taichung, Taiwan

12⁵⁰-12⁵⁵ **Electrospun silk fibroin composite scaffold for tendon repair**

Yi-You Huang

Institute of Biomedical Engineering, National Taiwan University, Taipei, Taiwan.

12⁵⁵-13⁰⁰ **BMP-2 and insulin delivered from plasma synthesis of carbon-based nanocarriers for bone regeneration**

Yi Wen Lin¹, Chih Hsiang Fang¹, Jui Sheng Sun², Feng Huei Lin^{1,3}

¹Institute of Biomedical Engineering, College of Medicine and College of Engineering, National Taiwan University, Taipei 100, Taiwan; ²Department of Orthopedic Surgery, National Taiwan University Hospital, Taiwan; ³Division of Biomedical Engineering and Nanomedicine Research, National Health Research Institutes, Miaoli 350, Taiwan

Break: 13⁰⁰-15⁰⁰

SYMPOSIUM G: HYBRID INTERFACE MATERIALS

Wednesday, September 5, 2018

Main Conference Hall

Session I: 15⁰⁰-16⁴⁵

Chairpersons: Kwang Ho Kim and Yeon Sik Jung

15⁰⁰-15³⁰ **Vertical alignment of BaTiO₃ nanoparticles for enhanced piezoelectric performance**

Je Moon Yun¹, Kwang Ho Kim^{1,2}

¹Global Frontier R&D Center for Hybrid Interface Materials (GFHIM), Republic of Korea; ²School of Materials Science and Engineering, Pusan National University, Republic of Korea.

15³⁰-15⁴⁵ **High performance photodetector using graphene barristor**

Byoung Hun Lee

Center for emerging electronic devices and systems (CEEDS), Korea; School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), Republic of Korea.

15⁴⁵-16⁰⁰ **High performance Al alloys development by simultaneous increasing strength and its trade-off properties**

Seung Zeon Han¹, Kwang Ho Kim^{2,3}

¹Computational materials department, Korea Institute of Materials Science (KIMS), Korea; ²Global Frontier R&D Center for Hybrid Interface Materials (GFHIM), Republic of Korea; ³School of Materials Science and Engineering, Pusan National University, School of Materials Science and Engineering, Korea

16⁰⁰-16¹⁵ **Improving the mechanical properties and wettability of metals by control interfacial characteristics: Study based on first-principles**

Eun-Ae Choi

Computational materials department, Korea Institute of Materials Science (KIMS), Korea

16¹⁵-16³⁰ **Hybrid materials imaging initiative: past, present and future**

Seungbum Hong

Dept. of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea

16³⁰-16⁴⁵ **Circular double-patterning lithography using a block-copolymer template and tomic layer deposition**

Se-Hun Kwon, Kyung Mox Cho

School of Materials Science and Engineering, Pusan National University, Korea

Break: 16⁴⁵-17¹⁵

Session II: 17¹⁵-19⁰⁰

Chairpersons: Kyung Ho Shin and Se-Hun Kwon

17¹⁵-17⁴⁵ Various nanoarchitectural hybrid materials for high-performance supercapacitors

Kyung Ho Shin¹, Kwang Ho Kim^{2,3}, Je Moon Yun²

¹Technology Business Division, Korea Institute of Science and Technology (KIST), Republic of Korea; ²Global Frontier R&D Center for Hybrid Interface Materials (GFHIM), Republic of Korea; ³School of Materials Science and Engineering, Pusan National University, Republic of Korea

17⁴⁵-18⁰⁰ High-performance hybrid energy storages enabling ultrafast charging and high energy density along with robust cycle life

Jeung Ku Kang

Dept. of KAIST, 373-1 Guseong Dong, Yuseong Gu, Daejeon (305-701), Republic of Korea

18⁰⁰-18¹⁵ Thermal management by electrochemical process: thermoelectric and radiative cooling materials

Jae-Hong Lim

Department of Electrochemistry, Korea Institute of Material Science, Korea

18¹⁵-18³⁰ Solution plasma synthesized carbon-supported hybrid catalysts for energy converting systems

Oi Lun (Helena) Li

School of Materials Science and Engineering, Pusan National University, Korea

18³⁰-18⁴⁵ 3-dimensional hybrid nanostructures: novel fabrication strategies and applications

Yeon Sik Jung

Dept. of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea

18⁴⁵-19⁰⁰ Virus: the next generation material

Jin-Woo Oh

Dept. of Nanoenergy Engineering, Pusan National University
Busan, Republic of Korea, 609-735

FIRST ORAL SESSION

Thursday, September 6, 2018

Main Conference Hall

Session I: 09⁰⁰-10⁴⁵

Chairpersons: Branko Z. Matovi and Zoran Jovanovi

- 09⁰⁰-09¹⁵ **Anion-mediated photophysical behaviour in a C₆₀ fullerene [3] rotaxane shuttle**
Timothy A. Barendt¹, Ilija Rašovi², Maria A. Lebedeva², George A. Farrow³,
Alexander Auty³, Dimitri Chekulaev³, Igor V. Sazanovich⁴, Julia A. Weinstein³,
Kyriakos Porfyrakis², Paul D. Beer¹
¹University of Oxford, Chemistry Research Laboratory, Department of Chemistry,
Oxford, United Kingdom; ²University of Oxford, Department of Materials, Oxford,
United Kingdom; ³University of Sheffield, Department of Chemistry, Sheffield,
United Kingdom; ⁴Research Complex at Harwell, Laser for Science Facility,
Rutherford Appleton Laboratory, Didcot, United Kingdom
- 09¹⁵-09³⁰ **Synthesis and densification of monolithic nanocrystalline SiC ceramics**
Branko Z. Matovi
Belgrade University, Institute for nuclear sciences Vinca, Cextreme Lab, Serbia
- 09³⁰-09⁴⁵ **First principles investigations of structural, electronic, elastic and mechanical properties of barium sulfide from standard to extreme high pressures**
Dejan Zagorac^{1,2}, Jelena Zagorac^{1,2}, Dragana Jordanov¹, Milena Rosi¹, Maria ebel¹,
Jelena Lukovi^{1,2}, Branko Matovi^{1,2}
¹Institute of Nuclear Sciences Vin a, Materials Science Laboratory, Belgrade
University, Belgrade, Serbia; ²Center for synthesis, processing and characterization of
materials for application in the extreme conditions-CextremeLab, Belgrade, Serbia
- 09⁴⁵-10⁰⁰ **Tuning of the stoichiometry of PLD grown SrO thin films via fluency optimization**
Zoran Jovanovi^{1,2}, Matjaž Spreitzer¹, Anže Založnik³, Danilo Suvorov¹
¹Advanced Materials Department, Jožef Stefan Institute, Jamova 39, 1000 Ljubljana,
Slovenia; ²Laboratory of Physics, Vin a Institute of Nuclear Sciences, University of
Belgrade, P.O. Box 522, 11001 Belgrade, Serbia; ³Department of Low and
Intermediate Energy Physics, Jožef Stefan Institute, Jamova 39, 1000 Ljubljana,
Slovenia

10⁰⁰-10¹⁵ Conduction in calcium containing LaAlO₃ solid solutions prepared via ball milling

Martin Fabián¹, Aleksey Yaremchenko², Hristo Kolev³, Mária Kauchová⁴, Jaroslav Brian in¹

¹Institute of Geotechnics, Slovak Academy of Sciences, 040 01 Kosice, Slovak Republic; ²Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal; ³Institute of Catalysis, Bulgarian Academy of Sciences, Acad. G. Bonchev St., Bldg. 11, 1113 Sofia, Bulgaria; ⁴Technical University of Košice, Letná 9, 04200 Košice, Slovakia

10¹⁵-10³⁰ Novel reactive infiltration process for production of fine grained Fe-Al intermetallics

Sr an Milenkovi, Anna Hynowska
IMDEA Materials Institute, Madrid, Spain

10³⁰-10⁴⁵ Properties of composite parts manufactured with help of LATP technology

Samoil Samak¹, Svetlana Risteska², Dijana Cvetkoska¹, Julija Gogu², Stefanija Acevska¹

¹Mikrosam A.D.

²Institute for Advanced Composites and Robotics (IACR) Prilep, Macedonia

Break: 10⁴⁵-11¹⁵

Session II: 11¹⁵-12⁴⁵

Chairpersons: Gerda Rogl and Remon Pop-Iliev

11¹⁵-11³⁰ High pressure torsion - a rapid tool for the production of high ZT skutterudites

Ramakrishnan Anbalagan¹, Ernst Bauer², Jiri Bursik³, Andriy Grytsiv⁴, Gerda Rogl⁴, Peter Rogl⁴, Michael Zehetbauer⁵

¹Institute of Atomic and Molecular Sciences, Taipei City, Taiwan, Province of China;

²Institute of Solid State Physics, TU Wien, Vienna, Austria; ³Academy of Sciences of the Czech Republic, Brno, Czech Republic; ⁴Christian Doppler Laboratory for Thermoelectricity, TU Wien, Vienna, Austria; ⁵Faculty of Physics, University of Vienna, Vienna, Austria

11³⁰-11⁴⁵ Advanced concepts for processing integral-skin multilayered cellular polymeric composites

Remon Pop-Iliev

UOIT- University of Ontario Institute of Technology Faculty of Engineering & Applied Science Canada, Canada

- 11⁴⁵-12⁰⁰ **Interaction between flow and faceted crystal growth**
Mihaela Stefan-Kharicha, Abdellah Kharicha, Andreas Ludwig, Meghuai Wu
Montanuniversitaet Leoben, Department Metallurgy, Simulation and Modelling
Metallurgical Processes, Leoben, Austria
- 12⁰⁰-12¹⁵ **Tool geometry effect on microstructure and properties of friction stir welded 5083 and 7075 aluminium alloys**
Izabela Kalembe-Rec¹, Mateusz Kopycia¹, Damian Miara², Krzysztof Krasnowski²
¹Faculty of Metal Engineering and Industrial Computer Science, AGH University of Science and Technology, Av. Mickiewicza 30, 30-059 Krakow, Poland; ²Instytut Spawalnictwa (Institute of Welding), 16-18 Bł. Czesława Str., 44-100 Gliwice, Poland
- 12¹⁵-12³⁰ **Development of highly piezoelectric coaxial fiber for energy harvest by using thermal drawing and post-process towers**
Thinh Tam Luong, Anh Tuan Luu, Quang Van Duong, Thu Thi Nguyen, Seung Tae Choi
School of Mechanical Engineering, Chung-Ang University, Republic of Korea
- 12³⁰-12⁴⁵ **Fabrication and application of polyvinylidene fluoride (PVDF) fabric sensors for in situ health monitoring of fibrous composite structures**
Seung-Hwan Chang, Kyung-Chae Jung
Chung-Ang University, School of Mechanical Engineering, Seoul, Republic of Korea

SECOND ORAL SESSION

Small Conference Hall

Session I: 09⁰⁰-10³⁰

Chairpersons: Rosalía Cid Barreno and Smilja Markovi

- 09⁰⁰-09¹⁵ **Epitaxial Fe₃O₄/La_{0.7}Ca_{0.3}MnO₃ thin film heterostructures for spintronic devices**
Rosalía Cid Barreno^{1,2}, Juan Rubio Zuazo^{1,2}, Eduardo Salas Colera^{1,2}, Germán R. Castro^{1,2}
¹SpLine CRG BM25 Beamline, European Synchrotron Radiation Facility (ESRF), 38000 Grenoble, France
²Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas (ICMM-CSIC), 28049 Madrid, Spain

- 09¹⁵-09³⁰ **Fe₃O₄-based heterostructures for semiconductor spintronics**
Iciar Arnay, Juan Rubio-Zuazo, German R. Castro
ICMM-CSIC (Instituto de Ciencia de Materiales de Madrid), Ciudad Universitaria de Cantoblanco, 28049 Madrid, Spain; BM25-SpLine, ESRF (European Synchrotron Radiation Facility), 71 Avenue Martyrs, 38000 Grenoble, France
- 09³⁰-09⁴⁵ **Synthesis of TiO₂ -WO₃ composite nanofibers by electrospinning for application in photocatalysis and fuel cells**
Vincent Otieno Odhiambo, Orsolya Kéri, Imre Miklós Szilágyi
Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Hungary
- 09⁴⁵-10⁰⁰ **The new integrated process flow sheet for production of Fe-NiAl composite microgranules for the additive technology.**
Vitalii V. Sanin¹, Mikhail R. Filonov², Evgenii A. Levashov³, Yurii S. Pogozhev³, Vladimir I. Yukhvid⁴, Denis M. Ikornikov⁴
¹NUST «MISIS», Scientific-educational center "Nanomaterials and nanotechnologies", Moscow, Russia; ²NUST «MISIS», Department of Science and innovation, Moscow, Russia; ³NUST «MISIS», Division of Powder Metallurgy and Functional Coatings, Moscow, Russia; ⁴ISMAN Department SHS Melts and Cast Materials, Chernogolovka, Russia
- 10⁰⁰-10¹⁵ **Reducing the deformation temperature of AZ31 magnesium alloy through CCT approach**
Mohammad Mirghasemi, Ali Reza Eivani, Seyyed Hosein Seyedein, Hamid Reza Jafarian
School of Metallurgy and Materials Engineering,, Iran University of Science and Technology, Tehran, Iran
- 10¹⁵-10³⁰ **Eco-technology: the application of calcined waste mine overburden clay materials as cement substitution**
Pozhhan Mokhtari, Sorour Semsari Parapari, Noyan Ozkan, Mehmet Ali Gulgun
Department of Material Sciences and Nano-Engineering, Sabanci University, Tuzla, Istanbul, Turkey

Break: 10³⁰-11⁰⁰

Session II: 11⁰⁰-12¹⁵

Chairpersons: Dragana Jugovi and Pozhhan Mokhtari

- 11⁰⁰-11¹⁵ **Structural and electrochemical study of lithium iron (II) pyrophosphate**
Dragana Jugovi¹, Miloš Milovi¹, Miodrag Mitri², Valentin Ivanovski², Sre o Škapin³, Dragan Uskokovi¹
¹Institute of Technical Sciences of SASA, Belgrade, Serbia; ²Vin a Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia; ³Jožef Štefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia
- 11¹⁵-11³⁰ **Li₄Ti₅O₁₂. Promissing anode material for Li-ion batteries synthesized via mechanochemically assised route**
Martin Fabián¹, Markéta Žukalová², Ladislav Kavan², Vladimír Šepelák¹, Mamoru Senna³
¹Institute of Geotechnics, Slovak Academy of Sciences, 040 01 Košice, Slovak Republic; ²J. Heyrovsky Institute of Physical Chemistry, Acad. Sci. Czech Republic, 182 23 Praha, Czech Republic; ³Faculty of Science and Technology, Keio University, 223-8522, Yokohama, Japan
- 11³⁰-11⁴⁵ **CTAB- and pluronic F-127-assisted microwave processing of ZnO particles with modified morphology and optical properties**
Smilja Markovi¹, Ivana Stojkovi -Simatovi², Sanita Ahmetovi², Ljiljana Veselinovi¹, Stevan Stojadinovi³, Vladislav Rac⁴, Sre o Škapin⁵, Dragan Uskokovi¹
¹Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade, Serbia; ²University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia; ³University of Belgrade, Faculty of Physics, Belgrade, Serbia; ⁴University of Belgrade, Faculty of Agriculture, Belgrade, Serbia; ⁵Jožef Stefan Institute, Ljubljana, Slovenia
- 11⁴⁵-12⁰⁰ **Synthesis of tribological WS₂ powder from oxide precursor**
Nataša Gaji¹, Željko Kamberovi², Zoran An i³, Jarmila Trp evska⁴, Beatrice Plešingerova⁴, Jovana oki³
¹University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy in Belgrade Ltd., Belgrade, Serbia; ²University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia; ³University of Belgrade, Innovation center of Faculty of Chemistry Ltd., Belgrade, Serbia; ⁴Technical University of Košice, Faculty of Materials, Metallurgy and Recycling, Košice, Slovakia
- 12⁰⁰-12¹⁵ **Thermochemistry aspects of mechanochemistry activation of the flotation processes**
Milan M. Petrov, Marina S. Blagojev, Ljubiša D. Andri , Dragan S. Radulovi
Institute for Technology of Nuclear and other Raw Materials, Belgrade, Serbia

THIRD ORAL SESSION

Friday, September 7, 2018

Main Conference Hall

Session I: 9⁰⁰-10⁴⁵

Chairpersons: Nenad L. Ignjatovi and Milena Špírková

09⁰⁰-09¹⁵ **CaP that kills: the intrinsic antimicrobial effect of calcium phosphate nanoparticles**

Victoria Wu

Advanced Materials and Nanobiotechnology Laboratory, Garage & Backyard @ Woodbridge, Irvine, CA 92604, USA

09¹⁵-09³⁰ **Cell-selective toxicity of hydroxyapatite-chitosan oligosaccharide lactate particles loaded with a steroid cancer inhibitor**

Nenad Ignjatovi¹, Marija Saka², Ivana Kuzminac², Vesna Koji³, Smilja Markovi¹, Victoria Wu⁴, Vuk Uskokovi⁵, Dragan Uskokovi¹

¹Institute of Technical Sciences of the Serbian Academy of Science and Arts, Knez Mihailova 35/IV, P.O. Box 377, 11000 Belgrade, Serbia; ²University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovi a 3, 21000 Novi Sad, Serbia; ³University of Novi Sad, Faculty of Medicine, Oncology Institute of Vojvodina, Put Dr Goldmana 4, Sremska Kamenica 21204, Serbia; ⁴Advanced Materials and Nanobiotechnology Laboratory, Irvine, USA; ⁵Department of Bioengineering, College of Medicine and College of Engineering, The University of Illinois at Chicago, Chicago, 851 South Morgan Street, Chicago, IL 60607-7052, USA

09³⁰-09⁴⁵ **Synthesis of antimicrobial cobalt ferrite/gold nanocomposites**

Sonja Jovanovi^{1,2}, Lea Udovc¹, Jelena Rmuš², Matjaž Spreitzer¹, Marija Vukomanovi¹

¹Institute Jožef Stefan, Advanced Materials Department, Ljubljana, Slovenia; ²University of Belgrade, Vinca Institute of Nuclear Sciences, Laboratory of Physics, Belgrade, Serbia

09⁴⁵-10⁰⁰ **New agents for no-chemotherapy of socially significant diseases: structure and properties of nitrosile [1Fe-2S] ferredoxins mimetics – nitric oxide donors**

Nataliya A. Sanina

Russian Academy of Sciences Institute of Problems of Chemical Physics, 1, Acad. Semenov Av., 142432, Chernogolovka, Russia

10⁰⁰-10¹⁵ **Characterization of the TiNi surface after modified by electron beam and its effect on the morphology and cytoskeleton of mesenchymal stem cells**

Ekaterina Yu. Gudimova¹, Ludmila L. Meisner^{1,3}, Evgenii V. Yakovlev², Olga I. Shabalina^{1,3}

¹Institute of Strength Physics and Materials Science SB RAS, Tomsk, Russia; ²Institute of High Current Electronics SB RAS, Tomsk, Russia; ³National Research Tomsk State University, Tomsk, Russia

10¹⁵-10³⁰ **Bias voltage effect in the development of new beta/alpha-Ti-Nb-Zr biocompatible coating with low Young's modulus and high toughness for medical applications**

Emilio Frutos¹, Miroslav Karlík^{2,3}, José Antonio Jiménez⁴, Tomas Polcar^{1,5}

¹Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Technická 2, Prague, Czech Republic; ²Department of Materials, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 120 00 Prague, Czech Republic; ³Charles University, Department of Physics of Materials, Ke Karlovu 5, 121 16 Prague, Czech Republic; ⁴Centro Nacional de Investigaciones Metalúrgicas (CENIM-CSIC), Avd. Gregorio del Amo no 8, 28040 Madrid, Spain; ⁵nCATS, University of Southampton, University Road, Southampton SO17 1BJ, United Kingdom

10³⁰-10⁴⁵ **Waterborne polycarbonate-based polyurethane films**

Milena Špírková, Ji í Hodan, Jana Kredatusová and Lu ka Machová

Institute of Macromolecular Chemistry AS CR, Heyrovského nám. 2, 162 06 Prague 6, Czech Republic

Break: 10⁴⁵-11¹⁵

Session II: 11¹⁵-12¹⁵

Chairpersons: Jan Kusinski and Natalia Kamanina

11¹⁵-11³⁰ **Nanotechnology approach in optical materials modification**

Natalia Vladimirovna Kamanina

Lab for Photophysics of media with nanoobjects Vavilov State Optical Institute, Kadetskaya Liniya V.O., dom.5, korpus 2, St.- Petersburg, 199053, Russia
St.-Petersburg Electrotechnical University ("LETI"), Russia

11³⁰-11⁴⁵ **Synthesis of highly porous monolithic 3D nanomaterials based on aluminum oxides: development of methods for their functionalization using structural and chemical modification**

Anatole N. Khodan¹, Alexander G. Martynov¹, Andrei V. Bykov⁵, Yulia G. Gorbunova¹, Aslan Yu. Tsivadze¹, Mohamed R. Amamra², Andrei V Kanaev², Alexander E. Baranchikov³, Vladimir K. Ivanov³, Sergey P. Kopitsa⁴, Andrei A. Konovko⁵, Khursand E. Yorov⁶

¹A.N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS (IPCE RAS) Moscow, Russia; ²Laboratoire des Sciences des Procédés et des Matériaux CNRS, Université Paris 13, Villetaneuse, France; ³N.S. Kurnakov Institute of General and Inorganic Chemistry RAS (IGIC RAS) Moscow, Russia; ⁴B.P. Konstantinov Petersburg Nuclear Physics Institute, National Research Center "Kurchatov Institute", Gatchina, Russia; ⁵M.V. Lomonosov Moscow State University, Physics Faculty, Chair of General Physics and Wave Processes, Moscow, Russia; ⁶M.V. Lomonosov Moscow State University, Department of Materials Science, Moscow, Russia

11⁴⁵-12⁰⁰ **Amorphous FeSiB ribbons crystallized by using laser interference treatment**

Jan Kusinski¹, Olaf Czyz¹, Agnieszka Radziszewska¹, Roman Ostrowski², Antoni Rycyk², Jarosław Kanak³, Małgorzata Kac⁴

¹AGH – University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, Department of Surface Engineering and Materials Characterisation, 30 Mickiewicza, 30-059 Krakow, Poland; ²Military University of Technology, Institute of Optoelectronics, Warsaw, 2 Gen. S. Kaliskiego, 00-908 Warsaw, Poland; ³AGH – University of Science and Technology, Faculty of Computer Science, Electronics and Telecommunications, Department of Electronics, 30 Mickiewicza, 30-059 Krakow, Poland; ⁴Institute of Nuclear Physics Polish Academy of Sciences, ul. Radzikowskiego 152, 31-342 Krakow, Poland

12⁰⁰-12¹⁵ **Correlation methods of analysis in studies of mechanochemical reactions**

Dmitriy S. Rybin, Grigoriy N. Konygin

The Udmurt Federal Research Center of the Ural Branch of the Russian Academy of Sciences, Physical-Technical Institute, Department of Physics and Chemistry of Nanomaterials, Laboratory of Mechanoactivation of Organic Systems, Izhevsk 426001, Russia

FOURTH ORAL SESSION

Small Conference Hall

Session I: 9⁰⁰-10³⁰

Chairpersons: Aleksandr Kryshstal and Andrey V. Zadesenets

- 9⁰⁰-9¹⁵ **In situ aberration-corrected STEM of metal-induced crystallization: the case of the Ag/Ge couple**
Aleksandr Kryshstal¹, Sergiy Bogatyrenko², Alexey Minenkov², Paulo Ferreira^{3,4,5}
¹AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science & International Centre of Electron Microscopy for Material Science, Krakow, Poland; ²Karazin National University, Department of Physics and Technology, Kharkiv, Ukraine; ³Iberian International Institute of Nanotechnology, Braga, Portugal; ⁴The University of Texas at Austin, Materials Science & Engineering Program, Austin, USA; ⁵University of Lisbon, Instituto Superior Técnico, Mechanical Engineering Department and IDMEC, Lisboa, Portugal
- 9¹⁵-9³⁰ **Microstructure characterization of a nanostructured austenitic steel annealed under high hydrostatic pressure**
Agnieszka T. Krawczynska¹, Stanislaw Gierlotka², Przemyslaw Suchecki¹, Daria Setman³, Boguslawa Adamczyk-Cieslak¹, Michal Gloc¹, Witold Chrominski¹, Malgorzata Lewandowska¹, Michael Zehetbauer³
¹Warsaw University of Technology, Faculty of Materials Science and Engineering, Warsaw, Poland; ²Institute of High Pressure Physics UNIPRESS, Warsaw, Poland
³University of Vienna, Faculty of Physics, Vienna, Austria
- 9³⁰-9⁴⁵ **Double complex salts as precursors of bimetallic nanoalloys**
Evgeny Y. Filatov, Andrey V. Zadesenets, Sergey V. Korenev
Nikolaev Institute of Inorganic Chemistry of Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia; Novosibirsk State University, Novosibirsk, Russia
- 9⁴⁵-10⁰⁰ **Oxalatopalladates of Co, Ni and Zn as precursors of nanoalloys: from thermal properties to supported catalysts**
Andrey V. Zadesenets, Ilia A. Garkul, Sergey V. Korenev
Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russian Federation
Novosibirsk State University, Novosibirsk, Russia
- 10⁰⁰-10¹⁵ **Ni-Pd/Al₂O₃ catalyst in the form of foam for dry methane reforming**
Vesna Nikoli¹, Zoran An i², Dragana Radovanovi¹, Jelena Uljarevi¹, Maja Stevanovi¹
¹University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy in Belgrade Ltd, Belgrade, Serbia; ²University of Belgrade, Innovation Center of the Faculty of Chemistry, Belgrade, Serbia

10¹⁵-10³⁰ **Modeling transport through an environment crowded by obstacles of different shapes and sizes**

Dijana Dujak¹, Aleksandar Kara², Ivana Lončević³, Ljuba Budinski-Petković³, Zorica M. Jakšić⁴, Slobodan B. Vrhovac⁴

¹University of Zenica, Faculty of Metallurgy and Materials, Zenica, Bosnia and Herzegovina, ²University of Zenica, Polytechnic faculty, Zenica, Bosnia and Herzegovina, ³University of Novi Sad, Faculty of Technical Sciences, Novi Sad, Serbia, ⁴University of Belgrade, Institute of Physics Belgrade, Scientific Computing Laboratory, Center for the Study of Complex Systems, Belgrade, Serbia

Break: 10³⁰-11⁰⁰

Session II: 11⁰⁰-12⁰⁰

Chairpersons: Jan Grym and Ekaterina D. Grayfer

11⁰⁰-11¹⁵ **Interfaces and mechanisms: a molecular dynamics approach to fine tuning manipulation of interfaces**

Alberto Fraile¹, Hakan Yavas¹, Emilio Frutos¹, Teodor Huminiuc², Tomas Polcar^{1,2}

¹Department of Control Engineering, Czech Technical University, Czech Republic; ²Engineering Science, Faculty of Engineering and the Environment. University of Southampton, United Kingdom

11¹⁵-11³⁰ **Properties of ZnO nanorods grown in continuous-flow reactors**

Jan Grym, Roman Yatskiv, Hana Faitová, Šárka Kučerová, Nikola Baštinová, Ondřej Ernohorský, Stanislav Tiagulskyi, David Roesel, Jan Vaniš

Institute of Photonics and Electronics of the CAS, Prague, Czech Republic

11³⁰-11⁴⁵ **The use of layered nanomaterials in composites with metals and their compounds**

Ekaterina D. Grayfer, Mariia N. Kozlova, Sofya B. Artemkina, Pavel A. Poltarak, Anastasiia A. Poltarak, Elena E. Plotnikova, Vladimir E. Fedorov

Nikolaev Institute of Inorganic Chemistry (NIIC) of the Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia; Novosibirsk State University, Novosibirsk, Russia

11⁴⁵-12⁰⁰ **Dielectric behaviour of polyimide/silica based nanocomposites at low temperatures**

Marius Andrei Olariu¹, Arcire Alexandru¹, Elena Hamciuc²

¹Gh. Asachi" Technical University, Electrical Engineering Faculty, B-dul D. Mangeron 67, Iasi-700050, Romania; ²Petru Poni" Institute of Macromolecular Chemistry, Aleea Gr. Ghica Voda 41A, 700487 Iasi, Romania

POSTER SESSION I

Tuesday, September 4, 2018, 20⁰⁰-22⁰⁰

SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

- P.S.A.1. **Plasma assisted strategies for advanced synthesis and processing of materials**
Siavash Assadolahi^{1,2}, Daniele Benetti³, Claude Côté¹, Ryan Porter¹, Sean Wolfe¹, Fabian Ambriz Vargas³, Diego Mantovani⁴, Andreas Ruediger³, Luc Stafford², Andranik Sarkissian¹
¹Plasmionique Inc, Varennes, QC, Canada; ²University of Montreal, QC, Canada; ³INRS-EMT, Varennes, QC, Canada, ⁴Biomaterials Engineering Unit, Saint-François d'Assise Hospital, Laval University, QC, Canada
- P.S.A.2. **Polimorphous transformations in mechanoactivated molecular crystals**
Dmitriy S. Rybin¹, Grigoriy N. Konygin¹, Kirill N. Susloparov², Alla A. Zhygalova²
¹The Udmurt Federal Research Center of the Ural Branch of the Russian Academy of Sciences, Physical-Technical Institute, Laboratory of Mechanoactivation of Organic Systems, Izhevsk, RU; ²Mezomax Inc, San Francisco, USA
- P.S.A.3. **Microstructure development of the Cu-Ti-TiB₂ composite obtained by laser sintering**
Jelena Staši, Dušan Boži
Centre of Excellence-CextremeLab, Institute of Nuclear Sciences "Vin a", University of Belgrade, Mike Petrovića Alasa 12-14, PO Box 522, 11001 Belgrade, Serbia
- P.S.A.4. **Anomalous electron pulse annealing in Ti implanted GaP**
Zbigniew Werner¹, Marek Barlak¹, Alexey Markov², Dmitry Proskurovsky², René Heller³
¹National Centre for Nuclear Research, Otwock, Poland; ²High Current Electronics, Institute, Tomsk, Russia; ³Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany
- P.S.A.5. **The effect of nitrogen ion implantation on the properties of WC-Co composites used in wood-based materials machining**
Jacek Wilkowski¹, Marek Barlak², Roman Böttger³, Zbigniew Werner², Joanna Wachowicz¹, Paweł Czarniak¹
¹Warsaw University of Life Sciences - SGGW, Faculty of Wood Technology, Department of Mechanical Processing of Wood, Warsaw, Poland; ²National Centre for Nuclear Research wiersk - NCBJ, Plasma and Ion Technology Division (FM2),

Otwock, Poland, ³Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Ion Beam Center, Dresden, Germany

P.S.A.6. **Shungite - a russian mineral: possible application as a microwave absorber**

Nina Obradovi¹, Mihajlo Gigov², Aleksandar or evi³, Frank Kern⁴, Svetlana Dmitrovi⁵, Branko Matovi⁵, Antonije or evi^{6,7}, Vladimir Pavlovi¹

¹Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade, Serbia; ²Mining Institute Ltd., Batajni ki put 2, 11080 Belgrade, Serbia; ³Faculty of Science, Department of Chemistry, Biochemistry and Environmental Protection, University of Novi Sad, Trg Dositeja Obradovica 3, 21000 Novi Sad, Serbia; ⁴Universität Stuttgart, Institut für Fertigungstechnologie keramischer Bauteile (IFKB), D- 70567 Stuttgart, Germany; ⁵University of Belgrade, Vin a Institute of Nuclear Sciences, Mike Petrovi a Alasa 12-14, 11000 Belgrade, Serbia; ⁶School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11000 Belgrade, Serbia; ⁷Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia

P.S.A.7. **Sintering of alumina doped with different oxides, followed by sensitive dilatometer**

Suzana Filipovi¹, Nina Obradovi¹, Smilja Markovi¹, Antonije or evi^{2,3}, Aleksandra Dap evi⁴, Jelena Rogan⁴, Vladimir Pavlovi⁴

¹Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade Serbia; ²School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11000 Belgrade, Serbia; ³Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia; ⁴Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia

P.S.A.8. **Ni_{1-x}Mo_x dispersed alloys: synthesis and catalytic properties in 1,2-dichloroethane decomposition process**

Yuliya V. Rudneva¹, Yury V. Shubin¹, Pavel E. Plyusnin¹, Yurii I. Bauman², Ilya V. Mishakov²

¹Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia; ²Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

P.S.A.9. **The influence of the method of preparation and temperature of thermal treatment on the phase composition of the NiO-Al₂O₃ catalyst using the X-ray diffraction method**

Matilda M. Lazi .

Technical College of Applied Sciences in Zrenjanin, Zrenjanin, Serbia

- P.S.A.10. **Chalcogenides of niobium and molybdenum with stoichiometry metal: chalcogen = 2:3**
M.N. Kozlova¹, A.N. Enyashin², E.D. Grayfer¹, V.E. Fedorov¹
¹Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia; ²Institute of Solid State Chemistry UB RAS, Ekaterinburg, Russia
- P.S.A.11. **Crystallographic structure of electron pulse annealed GaP implanted with Ti**
Marek Barlak¹, Zbigniew Werner¹, Alexey Markov², Dmitry Proskurovsky², René Heller³
¹National Centre for Nuclear Research, Otwock, Poland; ²High Current Electronics Institute, Tomsk, Russia; ³Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany
- P.S.A.12. **The influence of boron on synthesis and characteristics of PM copper-zirconium alloys**
Dušan Boži, Jelena Staši, Jovana Ruži
Centre of Excellence-CextremeLab, Institute of Nuclear Sciences “Vinča”, University of Belgrade, Mike Petrovića Alasa 12-14, PO Box 522, 11001 Belgrade, Serbia
- P.S.A.13. **Synthesis and structure of zinc(II) complex with 2-acetylpyridine - aminoguanidine**
Mirjana M. Radanovi¹, Ljiljana S. Vojinovi -Ješić¹, Marko V. Rodić¹, Željko K. Jakić², Katalin Mészáros Szécsényi¹
¹University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Novi Sad, Serbia; ²University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro
- P.S.A.14. **Influence of boron on modified characteristics of iron-based alloys with particular reference to boronizing**
Andjelka Milosavljević¹, Radica Prokić-Cvetković¹, Zoran Radaković¹, Aleksandar Jovović¹, Vuk Adžić¹, Zoran Marković²
¹ University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia;
² University of Belgrade, Faculty of Economics, Belgrade, Serbia

SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATIONS

P.S.B.1. Autowaves of localized plastic deformation in a material with an unstable phase structure

Vladimir I. Danilov, Vadim V. Gorbatenko, Dina V. Orlova, Lidia V. Danilova
Institute of Strength Physics and Materials Science of Siberian Branch of Russian Academy of Sciences, Russia

P.S.B.2. High temperature stability of YSZ and mullite-YSZ coatings deposited by atmospheric plasma spraying

David Jech¹, Pavel Komarov², Karel Sláma ka¹, Michaela Remešová¹, Lucie Dyková¹, Ladislav elko¹
¹Brno University of Technology, CEITEC – Central European Institute of Technology, Materials Characterization and Advanced Coatings, Brno, Czech Republic;
²Novosibirsk State Technical University, Faculty of Mechanical Engineering and Technologies, Novosibirsk, Russia

P.S.B.3. Barium-magnesium-aluminium-silicate environmental barrier coatings: powder manufacturing and plasma spraying

Lenka Klakurková, Ladislav elko, David Jech, Michaela Remešová, Martin Juliš, Pavel Gejdoš, Karel Sláma ka
Brno University of Technology, CEITEC, Materials Characterization and Advanced Coatings, Brno, Czech Republic

P.S.B.4. Magnetic and mechanical properties of nickel-based superalloy after laser induced deformation

An elka Milosavljevi¹, Suzana Poli², Mileša Sre kovi³, Sanja Petroni⁴, Darko Vasiljevi⁵, D.Bekri¹, Dušan Nasradin⁵,
¹University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia;
²Central Institute for Conservation, Belgrade, Serbia; ³University of Belgrade, Faculty of Electrical Engineering, Belgrade, Serbia; ⁴University of Belgrade, Institute of Nuclear Science Vinca, Belgrade, Serbia; ⁵Institute of Physics, Belgrade, Serbia

- P.S.B.5. **Influence of diffusion coatings on magnetic properties of 41CrMo₄ steel**
Zina Pavloušková¹, David Jech¹, Ladislav Jelko¹, Rostislav Huzlík², Tomáš Bulín²,
Lenka Klakurková¹, Jiří Švejcar¹, Jozef Kaiser¹
¹Brno University of Technology, CEITEC, Materials Characterization and Advanced
Coatings, Brno, Czech Republic; ²Brno University of Technology, Faculty of
Electrical Engineering and Communication, Dept. of Electrical Engineering, Brno,
Czech Republic
- P.S.B.6. **Electrical and magnetic properties of multiferroic BiFeO₃-based flexible composites**
Nikola I. Ilić¹, Guilhermina F. Teixeira², Jelena D. Bobić¹, Mirjana M. Vijatović
Petrović¹, Adis. S. Džunuzović¹, Maria A. Zaghete², Biljana D. Stojanović¹
¹University of Belgrade, Institute for Multidisciplinary Research, Materials science
department, Belgrade, Serbia; ²State University of Sao Paulo, Chemistry Institute,
Araraquara, Sao Paulo, Brasil
- P.S.B.7. **Characterization of different MMC coatings deposited by PTA and FS processes**
Vesna M. Maksimović¹, Aleksandar M. Maslarević², Gordana M. Bakić³,
Miloš B. Vukić³, Bratislav M. Rajičić³, Vladimir D. Pavkov¹
¹University of Belgrade, Vinča, Institute of Nuclear Sciences, Belgrade, Serbia;
²University of Belgrade, Innovation Center, Faculty of Mechanical Engineering,
Belgrade, Serbia; ³University of Belgrade, Faculty of Mechanical Engineering,
Belgrade, Serbia
- P.S.B.8. **Determination of ceramic proppant impact on efficiency of shale gas production and the environment**
Joanna Szymanska, Paweł Wisniewski, Jarosław Mizera
Warsaw University of Technology, Faculty of Materials Science and Engineering,
Warsaw, Poland
- P.S.B.9. **Temperature dependence of thermal conductivity of graphene monolayer in the framework of Debay and Calaway models**
Stevó J. J. J. imovski¹, Dejan Raković²
¹Academy of Criminalistic and Police Studies, Belgrade, Serbia; ²University of
Belgrade, Faculty of Electrical Engineering, Serbia

POSTER SESSION II

Wednesday, September 5, 2018, 20⁰⁰-22⁰⁰

SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATIONS

P.S.B.10. Cup anemometer tribology and revised IEC standard

Ivan Popovi , Miodrag Zlatanovi

University of Belgrade, School of Electrical Engineering, Serbia

P.S.B.11. Prediction of new B₆O structures and their properties using ab initio data mining approach

Jelena Zagorac^{1,2}, Dejan Zagorac^{1,2}, Dragana Jordanov¹, Milena Rosi¹, Maria ebela¹, Jelena Lukovi^{1,2}, Branko Matovi^{1,2}

¹Institute of Nuclear Sciences Vin a, Materials Science Laboratory, Belgrade University, Belgrade, Serbia; ²Center for synthesis, processing and characterization of materials for application in the extreme conditions-CextremeLab, Belgrade, Serbia

P.S.B.12. Impact of thickness on properties of high-entropy and conventional metallic glasses

Ramir Risti¹, Ahmed Kuršumovi², Ignacio A. Figueroa³, Emil Babi⁴

¹Department of Physics, University of Osijek, Trg Ljudevita Gaja 6, HR-3100 Osijek, Croatia; ²Department of Materials Science, Cambridge University, Pembroke Street, Cambridge CB2 3QZ, UK; ³Institute for materials research-UNAM, Ciudad Universitaria Coyoacan, C.P. 04510 Mexico D.F., Mexico; ⁴Department of Physics, Faculty of Science, Bijeni ka cesta 32, 10002 Zagreb, Croatia

P.S.B.13. Crystal structure and X-Ray spectroscopic properties of R.E.2Ni12P5 compounds

Ivan D. Shcherba¹, Henrik Noga², Viktor N. Antonov³, Olga V. Zhak¹, Dragan Uskokovi⁴, Bohdan M. Jatcyk⁵

¹Ivan Franko National University of Lviv, Ukraine; ²Institute of Technology, the Pedagogical University of Cracow, Podchorazych st. 2 Cracow 30-084 Poland; ³Institute of Physics of Metals, NASU, Kyiv, Ukraine; ⁴Institute of Technical Sciences of SASA Knez Mihailova 35/IV, PO Box 377 11000 Belgrade, Serbia; ⁵Lviv National University of Veterinary Medicine and Biotechnologies, Lviv, Ukraine

- P.S.B.14. **Study of the interaction between graphene oxide and 12-tungstophosphoric acid in their nanocomposite**
Željko Mravik¹, Danica Bajuk-Bogdanovi², Smilja Markovi³, Janez Kova⁴, Ivanka Holclajtner-Antunovi², Zoran Jovanovi¹
¹University of Belgrade, Vinca Institute of Nuclear Sciences, Laboratory of Physics, Belgrade, Serbia; ²University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia; ³Institute of Technical Sciences of SASA, Belgrade, Serbia; ⁴Jožef Stefan Institute, Department of Surface Engineering and Optoelectronics, Ljubljana, Slovenia
- P.S.B.15. **Transport coefficients of Ar⁺ in BF₃ gas**
Željka D. Nikitovi, Vladimir D. Stojanovi, Zoran M. Raspopovi
Institute of Physics, University of Belgrade, Pregrevica 118, Belgrade, Serbia
- P.S.B.16. **The influence of basalt content on the properties of austenitic stainless steel 316L**
Vladimir D. Pavkov¹, Gordana M. Baki², Vesna Maksimovi¹, Branko Matovi¹, Tatjana Volkov-Husovi³
¹University of Belgrade, Vinca Institute of Nuclear Sciences, Belgrade, Serbia; ²University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia; ³University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia
- P.S.B.17. **Comparative study on noble metal based nanocatalysts on different supports for low temperature fuel cells application**
Ljiljana M. Gaji Krstaji¹, Velimir R. Radmilovi^{2,6}, Peter Ercius³, Borka M. Jovi⁴, Vladimir D. Jovi⁴, Piotr Zabinski⁵, Nevenka R. Elezovi⁴
¹Institute of Technical Sciences SASA, Knez Mihajlova 45, 11000 Belgrade, Serbia; ²Faculty of Technology and Metallurgy University of Belgrade, Karnegijeva 4, Belgrade; ³National Center for Electron Microscopy, LBNL University of California, Berkeley, USA; ⁴Institute for Multidisciplinary Research University of Belgrade, P.O. Box 33, 11030 Belgrade, Serbia; ⁵AGH University of Science and Technology, Faculty of Non-Ferrous Metals, Al. Mickiewicza 30, Krakow, Poland; ⁶Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia
- P.S.B.18. **Experimental Study of Drying Process of Porous Materials**
Abdulhamied Twier,²Elhassen Ali A. Omer,³Ramadan A. Almadani,⁴Mustafa Jarnaz,⁵Abdurrahman Houssein
¹Industrial Authority, Tripoli, Libya; ²Mechanical Engineering department, Engineering faculty, Zawia University, Zawia, Libya; ³Libyan Authority for Research of Natural Science and Technology, Tripoli, Libya; ⁴Libyan Academy for Higher Studies, Tripoli, Libya; ⁵Faculty of Engineering, Zintan University, Zintan, Libya

SYMPOSIUM C: NANOSTRUCTURED MATERIALS

- P.S.C.1. **Production of synthesis gas by carbon dioxide over catalytically active molybdenum based carbide and nitride nanowires**
Mrzel Aleš¹, Damjan Vengust¹, Janez Kova¹, Venkata Dasireddy², Blaž Likozar²
¹Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia; ²National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia
- P.S.C.2. **Nanofibrous polyaniline preparation by the oxidative polymerization of aniline with the oxidant in excess: Raman and FTIR spectroscopy study**
Jana Mišurović, Gordana Irić-Marjanovi
University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia
- P.S.C.3. **One-pot synthesis of biocompatible NaYF₄:Yb,Er nanoparticles for cell labeling**
Ivana Dini¹, Marina Vuković¹, Lidija Manić², Aleksandar Krmpotić³, Olivera Milošević²
¹Innovation Center of the Faculty of Chemistry, University of Belgrade, Serbia; ²Institute of Technical Sciences of SASA, Belgrade, Serbia; ³Photonic Center, Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia
- P.S.C.4. **Shape-controlled synthesis of CeO₂ nanoparticles: effects of different precursors on the formation of oxygen vacancies**
Igor Čer¹, Jelena Bijelić¹, Chenwei Li^{2,3}, Bernd Smarsly², Herbert Over²
¹Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8/A, 31000 Osijek, Croatia; ²Physikalisch-Chemisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 17, 35392 Gießen, Germany; ³Key Laboratory for Advanced Materials, Research Institute of Industrial Catalysis, School of Chemistry and Molecular Engineering, East China University of Science and Technology, Shanghai 200237, China
- P.S.C.5. **Characterization of mechanochemically synthesized CuInS₂/ZnS nanocomposite**
Erika Dutková¹, Nina Daneu², Zdenka Bujáková¹, Matej Baláž¹, Jaroslav Kováčik³, Jaroslav Kováčik Jr.³
¹Institute of Geotechnics, Slovak Academy of Sciences, 04001 Košice, Slovakia; ²Jožef Stefan Institute, Department for Nanostructured Materials, Ljubljana, SI-1000, Slovenia; ³Institute of Electronics and Photonics, Slovak University of Technology, 81219 Bratislava, Slovakia

- P.S.C.6. **Preparation and characterization of nanostructured silver supported on carbonaceous material obtained by hydrothermal carbonization process**
Branka V. Kaluđerović¹, Vesna L.J. Mandušić², Djuro M. Čoklečić³, Jelena Hranisavljević², Srđan Milanović¹, Zlatko L.J. Rakoćević⁴
¹University of Belgrade, Serbia, INN Vinca, Center for the synthesis, processing and characterization of materials for use in extreme conditions, Belgrade, Serbia; ²University of Belgrade, Serbia, INN Vinca, Laboratory of Radiobiology and Molecular Genetics; ³University of Belgrade, Serbia, INN Vinca, Laboratory of Chemical Dynamics and Permanent Education; ⁴University of Belgrade, Serbia, INN Vinca, Laboratory of Atomic Physics, Serbia
- P.S.C.7. **Morphological, microstructural and magnetic characteristics of electrodeposited Ni-Fe-W-Cu alloy powders**
Tomislav Trišović, Miroslav Spasojević, Aleksa Marić, Milica Spasojević
Institute of Technical Sciences of Serbian Academy of Science and Arts, Belgrade, Serbia; Joint Laboratory for Advanced Materials of SASA, Section for Amorphous Systems; Faculty of Technical Sciences, Belgrade, University of Kragujevac, Belgrade, Serbia; Faculty of Chemistry, University of Belgrade, Belgrade, Serbia
- P.S.C.8. **Adsorption of arsenic(III) from aqueous solution on carbon cryogel and carbon cryogel/ceria composite**
Tamara Z. Minović Arsić¹, Ana M. Kalijadis¹, Bojan M. Jokić², Milovan M. Stoiljković¹, Biljana M. Babić³
¹University of Belgrade, Vinča Institute of Nuclear Sciences, Belgrade, Serbia; ²University of Belgrade, Faculty of Applied Arts, Belgrade, Serbia; ³University of Belgrade, Institute of Physics Belgrade, Belgrade, Serbia
- P.S.C.9. **Peculiar optical features of molecular crystalline films**
Jovan P. Šetrajčić^{1,2}, Igor J. Šetrajčić¹, Ana J. Šetrajčić –Tomić³
¹University of Novi Sad, Faculty of Sciences, Department of Physics, Novi Sad, Vojvodina, Serbia; ²University "Union – Nikola Tesla", Faculty of Sports, Novi Beograd, Vojvodina, Serbia; ³University of Novi Sad, Faculty of Medicine, Department of Pharmacy, Novi Sad, Vojvodina, Serbia

SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES

- P.S.D.1. **Lipid production with a high palmitoleic acid content by *Debaryomyces globosus* yeast under conditions of continuous cultivation**
Nadezda N. Stepanova¹, Grigorii I. Morgunov², Svetlana V. Kamzolova¹
¹G.K. Skryabin Institute of Biochemistry and Physiology of Microorganisms, Russian Academy of Sciences, Pushchino, Moscow region, 142290, Russia; ²Peoples' Friendship University of Russia (RUDN University), Moscow, 117198, Russia
- P.S.D.2. **New multifunctional materials based on steel slag**
Ivana Milašević¹, Ljubica Ivanović¹, Irena Nikolić^{1,2}, Dijana Petrović², Smilja Marković³, Vuk Radmilović⁴, Velimir R. Radmilović^{5,6}
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- P.S.D.3. **Biological markers of the petroleum alkane fraction as a forensic tool for determining the presence of petroleum pollutants in the environment**
Nada Vidović¹, Ivan Samelak¹, Milica Balaban¹, Mališa Antić², Tatjana Šolević - Knudsen³, Branimir Jovanović⁴
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POSTER SESSION III

Thursday, September 6, 2018, 20⁰⁰-22⁰⁰

SYMPOSIUM E: BIOMATERIALS

- P.S.E.1. **Addition of porogens improved the characteristics of biodegradable implants made of poly(-caprolactone)/calcium phosphate ceramic composites**
Chang-Chin Wu^{1,2}, Kai-Chiang Yang^{3,4}, Feng-Huei Lin⁵
¹Department of Orthopedics, En Chu Kong Hospital, New Taipei City, Taiwan; ²Department of Orthopedics, National Taiwan University Hospital, College of Medicine, National Taiwan University, Taipei, Taiwan; ³Department of Organ Reconstruction, Institute for Frontier Medical Sciences, Kyoto University, Kyoto, Japan; ⁴School of Dental Technology, College of Oral Medicine, Taipei Medical University, Taipei, Taiwan; ⁵Ins. of Biomed. Eng., National Taiwan University, Taiwan
- P.S.E.2. **The application of hydroxyapatite as the Bletilla striata polysaccharide carrier for sarcopenia treatment**
Ya-Jyun Liang¹, Jia-Yu Hong¹, Chun-Han Hou², Feng-Huei Lin¹
¹National Taiwan University, Institute of Biomedical Engineering, Taipei, Taiwan; National ²Taiwan University Hospital, Department of orthopedic surgery, Taipei, Taiwan
- P.S.E.3. **Hydroxyapatite/gelatin particles embedding stromal cell-derived factor-1 for bone tissue engineering**
Chih Hsiang Fang¹, Yi Wen Lin¹, Jui Sheng Sun², Feng Huei Lin^{1,3}
¹Institute of Biomedical Engineering, College of Medicine and College of Engineering, National Taiwan University, Taipei 100, Taiwan; ²Department of Orthopedic Surgery, National Taiwan University Hospital, Taipei, Taiwan; ³Division of Biomedical Engineering and Nanomedicine Research, National Health Research Institutes, Miaoli 350, Taiwan
- P.S.E.4. **A novel multilayer capsule as desensitizing agent for dental hypersensitivity**
Kuo-Hui Chiu¹, Hsiu-Min Chen¹, Yuan-Yu Hsia¹, Ting-Ru Chung², Chih-Yu Shu³, Chia-Yung Lin⁴, Cherng-Jyh Ke^{1,3}
¹China Medical University, College of Biopharmaceutical and Food Sciences, Department of Biological Science and Technology, Taichung, Taiwan; ²China Medical University, College of Medicine, Department of Biomedical Imaging and Radiological Science, Taichung, Taiwan; ³China Medical University Hospital, Biomaterial Translational Research Center, Taichung, Taiwan; ⁴Taichung Hospital, Ministry of Health and Welfare, Department of Dentistry, Taichung, Taiwan

- P.S.E.5. **Electrospun silk fibroin composite scaffold for tendon repair**
Yi-You Huang
Institute of Biomedical Engineering, National Taiwan University, Taipei, Taiwan.
- P.S.E.6. **BMP-2 and insulin delivered from plasma synthesis of carbon-based nanocarriers for bone regeneration**
Yi Wen Lin¹, Chih Hsiang Fang¹, Jui Sheng Sun², Feng Huei Lin^{1,3}
¹Institute of Biomedical Engineering, College of Medicine and College of Engineering, National Taiwan University, Taipei 100, Taiwan; ²Department of Orthopedic Surgery, National Taiwan University Hospital, Taiwan; ³Division of Biomedical Engineering and Nanomedicine Research, National Health Research Institutes, Miaoli 350, Taiwan
- P.S.E.7. **Rare earth dual-doped multifunctional hydroxyapatite particles for potential application in preventive medicine**
Nenad Ignjatovi¹, Lidija Man i¹, Zoran Stojanovi¹, Marko Nikoli², Sre o Škapin³, Ljiljana Veselinovi¹, Dragan Uskokovi¹
¹Institute of Technical Sciences of the Serbian Academy of Science and Arts, Knez Mihailova 35/IV, P.O. Box 377, 11000 Belgrade, Serbia; ²Photonic Center, Institute of Physics Belgrade, University of Belgrade, Zemun, Belgrade, Serbia; ³Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia
- P.S.E.8. **The processing and application of modified dental composites and dental inserts based on Mg-doped HAP**
or e Veljovi¹, Tamara Mati¹, Giuma Ayoub¹, Maja Ležaja Zebi², Vesna Mileti², Rada Petrovi¹, or e Jana kovi¹
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- P.S.E.9. **Hybrid dental composites with improved mechanical properties**
Abdulsalam. A. Elmadani¹, Ivana M. Radovi², Marija N. Radojevi¹, Miloš. Petrovi¹, Dušica. B. Stojanovi¹, Petar S. Uskokovi¹, Vesna J. Radojevi¹
¹University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia; ²University of Belgrade, Vin a Nuclear Institute, Belgrade, Serbia
- P.S.E.10. **Biomimetic evaluation of novel -TCP/alginate macroporous scaffolds in perfusion bioreactors for potential in bone tissue engineering**
Nataša Stanojevi , Milica Andrejevi , Jovana Zvicer, Jasmina Stojkovska, or e Veljovi , Bojana Obradovi
University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia
Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia

- P.S.E.11. **The morphology of the osteoporotic rabbit bone after implantation of strontium doped biphasic ceramic**
Mara Pilmane¹, Iize Salma², Girts Salms², Janis Locs³
¹Institute of Anatomy and Anthropology; ²Institute of Stomatology, Riga Stradins University; ³R.Cimdins Centre for Biomaterial Innovation and Development, Riga, Latvia
- P.S.E.12. **Spider silk coated with maghemite nanoparticles-synthesis and characterization**
Svetlana Dmitrovi¹, Vojislav Spasojevi¹, Goran Brankovi², Georgios Constantinides³, Aleksandra Zarubica⁴, Branko Matovi¹
¹University of Belgrade, "Vin a" Institute of Nuclear Sciences, Belgrade, Serbia; ²University of Belgrade, Institute for Multidisciplinary Research, Belgrade, Serbia; ³Cyprus University of Technology, Lemesos, Cyprus; ⁴University of Niš, Faculty of Science and Mathematics, Department of Chemistry, Niš, Serbia
- P.S.E.13. **Cefazolin-loaded polycaprolactone fibers produced via blend and co-axial electrospinning**
Anela N. Radisavljevi¹, Dušica B. Stojanovi², Srđan D. Periši¹, Vesna J. Radojevi², Mirjana D. Rajili -Stojanovi², Petar S. Uskokovi²
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- P.S.E.14. **In silico simulation of carvedilol absorption from oral films and nanofibers**
Marija N. Radojevi¹, Sandra V. Cviji², Dušica B. Stojanovi¹, Svetlana R. Ibrić², Petar S. Uskokovi¹
¹University of Belgrade - Faculty of Technology and Metallurgy, Department of Materials Science and Engineering, Karnegijeva 4, 11120 Belgrade, Serbia; ²University of Belgrade - Faculty of Pharmacy, Department of Pharmaceutical Technology and Cosmetology, Vojvode Stepe 450, 11221 Belgrade, Serbia
- P.S.E.15. **Stability of the magnetite particles dispersed in different surfactans using wet stirred media milling**
Zdenka Bujáková¹, Erika Dutková¹, Erika Tóthová¹, Jozef Kováčik², Matej Baláž¹
¹Institute of Geotechnics, Slovak Academy of Sciences, Watsonova 45, 04001 Košice, Slovakia; ²Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 04001 Košice, Slovakia

- P.S.E.16. **Electrochemical characterization of Mg-Zn bulk materials prepared by powder metallurgy method**
Pavel Doležal¹, Michaela Krystýnová², Jozef Minda¹, Stanislava Fintová¹, Mat j B ezina¹, Josef Zapletal¹, Jaromír Wasserbauer²
¹Brno University of Technology, Faculty of Chemistry, Materials Research Centre, Purkynova 464/118, 612 00 Brno, Czech Republic; ²Brno University of Technology, Faculty of Mechanical Engineering, Institute of Materials Science and Engineering, Technická 2896/2, 616 69 Brno, Czech Republic
- P.S.E.17. **Improvement of biocompatibility by formation of nanotubular oxide layer on the ultrafine-grained Ti-13Nb-13Zr alloy**
Veljko R. oki¹, Dragana R. Barjaktarevi ¹, or e N. Veljovi ¹, Ivana D. Dimi ¹, Vesna V. Koji ², Marko P. Rakin¹
¹University of Belgrade, Faculty of Technology and Metallurgy, 11120 Belgrade, Serbia; ²University of Novi Sad, Faculty of Medicine, Oncology Institute of Vojvodina, 21204 Sremska Kamenica, Serbia
- P.S.E.18. **The longterm chemical degradation of magnesium alloy AZ31 and AZ61 processed by method squeeze casting in SBF solution**
Helena Doležalová Weissmannová¹, Ivana Ro áková², Pavel Doležal^{2,3}
¹Brno University of Technology, Faculty Chemistry, Institute of Chemistry and Technology of Environmental Protection, Brno, Czech Republic; ²Brno University of Technology, Faculty of Mechanical Engineering, Institute of Materials Science and Engineering, Dept. of Metal Materials, Brno, Czech Republic; ³Brno University of Technology, Faculty Chemistry Materials Research Centre (MRC), Brno, Czech Republic
- P.S.E.19. **Crystal structures of mixed chloride-azide zinc (II) and chloride-isocyanate cadmium (II) complexes with the condensation product of 2-quinolinecarboxaldehyde and girard's reagent**
Tanja Keški¹, Milica Milenkovi ¹, Božidar obelji ¹, Dušanka Radanovi ², Katarina An elkovi ¹
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**TWENTIETH ANNUAL CONFERENCE
YUCOMAT 2018
Herceg Novi, September 3-7, 2018**

Abstracts

Oral Presentation

MRS-Serbia 2018 Award

Organo-metallic lead iodide perovskites: a material science approach

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Laboratory of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne,
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Materials are the linchpin of technological progress. For example, all energy related applications like photovoltaics, fuel cells, thermoelectrics, (harvesting, storing and transmitting) heavily depend on newly developed, more performing materials. This is well illustrated by the organometallic lead iodide perovskite ($\text{CH}_3\text{NH}_3\text{PbI}_3$) which has recently revolutionized the field of Due to the handshaking of physics, chemistry and material science the material's processing and quality has increased, it has turned out that this material has opened the imagination for novel applications.

In this talk I will describe the activity of my laboratory in relation to this material in thermoelectrics, in magnetic data storage, in photodetection and in photovoltaics in nuclear environment.

Acknowledgment

This work was performed in collaboration with Endre Horvath, Marton Kollar, Balint Nafradi, Alla Arakcheeva, Xavier Mettan, Pavao Andricevic, Konstantins Matulnikovs, Laszlo Mihaly, Karoly Holczer, Katalin Kamaras and many others. It is supported by the ERC Advanced Grant "Picoprop", and ERC Proof of Concept Grant "Picoprop4CT".

PL.S.I.1.

Synthesis and properties of two-dimensional carbides and nitrides (MXenes)

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Two-dimensional (2D) materials with a thickness of a few nanometers or less can be used as single sheets, or as building blocks, due to their unique properties and ability to assemble into a variety of structures. Graphene is the best-known example, but several other elemental 2D materials (silicene, borophene, etc.) have been discovered. Numerous compounds, ranging from clays to boron nitride (BN) and transition metal dichalcogenides, have been produced as 2D sheets. By combining various 2D materials, unique combinations of properties can be achieved which are not available in any bulk material. The family of 2D transition metal carbides and nitrides (MXenes) has been expanding rapidly since the discovery of Ti_3C_2 in 2011 [1,2]. Approximately 30 different MXenes have been synthesized, and the structure and properties of numerous other MXenes have been predicted using density functional theory (DFT) calculations [3]. Moreover, the availability of solid solutions on M and X sites, control of surface terminations, and the discovery of ordered double-M MXenes (e.g. Mo_2TiC_2) offer the potential for synthesis of dozens of new distinct structures.

This paper will describe the synthesis of MXenes by selective etching of layered ceramic precursors, including various MAX phases. Delamination into single-layer 2D flakes and assembly into films and 3D structures will be discussed.

The versatile chemistry of the MXene family renders their properties tunable for a large variety of applications. Oxygen or hydroxyl-terminated MXenes, such as $Ti_3C_2O_2$, have been shown to have redox capable transition metal layers on the surface and offer a combination of high electronic conductivity with hydrophilicity, as well as fast ionic transport. This, among many other advantageous properties, makes the material family promising candidates for energy storage and related electrochemical applications, but applications in optoelectronics, plasmonics, electromagnetic interference shielding, electrocatalysis, medicine, sensors, water purification/desalination and other fields are equally exciting [4].

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PL.S.I.2.

AIM-ing for single-atom precision for heterogeneous catalysts

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A grand challenge in the field of heterogeneous catalysis is to identify and fully characterize sites that are competent for catalysis of desired chemical transformations, ideally with high selectivity, high activity, and high stability. We have found that automated AIM (ALD-like chemistry in MOFs, where ALD is atomic layer deposition and MOF is metal-organic framework) can be used for chemically clean vapor-phase installation of uniform arrays of identically structured catalysts on the reactive nodes of suitably chosen MOFs (typically 6- or 8-connected hexa-zirconium (IV) oxo, hydroxo, aqua nodes of high-stability, high-area (>1,000 m²/g) mesoporous MOFs such as MOF-808, PCN-222, or NU-1000). This methodology, along with a solution-phase analogue termed SIM, can yield metal-oxygen, metal-sulfur, or metal(0) clusters of predetermined size, shape, and chemical composition, as well as desired monometallic catalytic complexes. The uniformity of the obtained catalysts reflects the crystallographic uniformity of the nodes to which the catalysts are grafted.

Thus, MOF nodes can be usefully viewed as uniquely well-defined nanoscopic supports for similarly well-defined catalysts. This presentation will outline the approach to synthesis and characterization, including *operando* synchrotron-based characterization, of MOF-supported arrays of well-defined clusters, and then illustrate, via one or two brief, unpublished, case studies, their application as catalysts for desirable, but challenging gas-phase chemical transformations. Together with input from computational modeling, these kinds of experiments can be used to address fundamental questions in contemporary, materials-based, Catalysis Science that require atomically precise knowledge of the siting and composition of pre-catalysts, activated catalysts, co-catalysts, reactants and products, *i.e.* questions of chemical selectivity, chemical confinement, and modulation of activity via control over catalyst metal-atom nuclearity, and general questions regarding emergent complexity in catalytic systems.

PL.S.I.3.

Applying chemistry to make today's best tunable millimeter wave dielectric even better

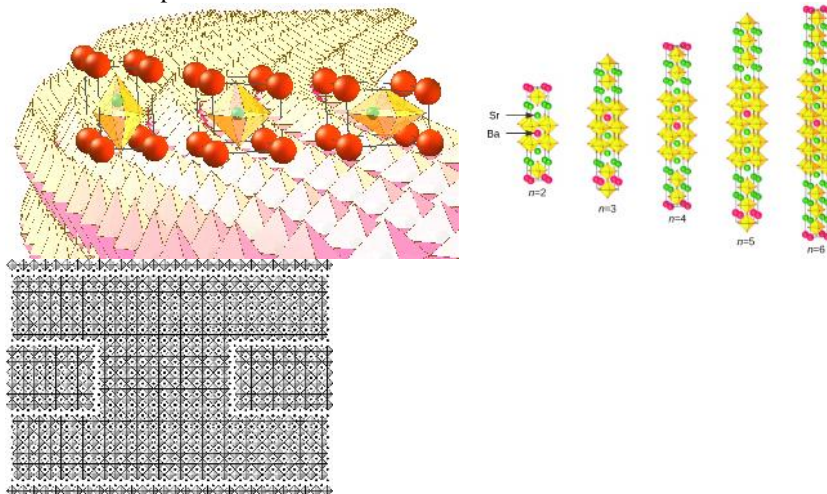
Darrell G. Schlom

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Today's tunable dielectric with the highest figure of merit at room temperature is strained films of $(\text{SrTiO}_3)_6\text{SrO}$. The low loss at frequencies up to 125 GHz comes from the defect mitigating nature of the $(\text{SrTiO}_3)_n\text{SrO}$ Ruddlesden-Popper structure; the tunability arises from imposing strain to induce a ferroelectric instability. Unfortunately the necessity for strain limits the film thickness to around 50 nm, which reduces the device tuning that can be achieved. In this talk I will describe a chemical alternative to strain to induce a ferroelectric instability—the introduction of barium into this Ruddlesden-Popper titanate. No barium-containing Ruddlesden-Popper titanates are known, but this atomically engineered superlattice material can be made thicker and we demonstrate a 300% improvement in the figure of merit of this this new $(\text{SrTiO}_3)_{n-m}(\text{BaTiO}_3)_m\text{SrO}$ tunable dielectric.

This work was performed in collaboration with the coauthors listed in the references below.



Strain engineering, dimensional confinement, epitaxial stabilization, and defect engineering applied to make today's best tunable dielectric even better in new $(\text{SrTiO}_3)_{n-m}(\text{BaTiO}_3)_m\text{SrO}$ tunable dielectrics.

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PL.S.I.4.

Ultra-high resolution study by aberration-corrected TEM of pyrochlore BZN supplying information on displacive atom-site disorder

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Pyrochlores, chemical formula $A_2B_2O_7$, form an extended class of materials with interesting properties. The compound $Bi_{1.5}ZnNb_{1.5}O_7$ (BZN) is prototypical. Its excellent dielectric properties make it attractive, e.g. for capacitors, tunable microwave devices and electric-energy storage equipment. Investigating BZN we report on the first study on a pyrochlore by atomic-resolution transmission electron microscopy. In this study – at the forefront of what modern electron microscopy can do – we are able to realize picometer-precision in our images of the close atom pairs with a separation of only 20 pm. We find that the position of the atomic intensity maxima do not coincide with the projected Wyckoff positions of the basic pyrochlore lattice. This supplies atomic-scale evidence for displacive disorder on split (cage-like) A-type sites. From our studies on atom mobility during microscopic observation we can conclude that it is the Zn-atom jumps and not those of Bi or Nb that are responsible for dielectric relaxation.

PL.S.I.5.

Electric field control of magnetism

Ramamoorthy Ramesh

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Complex perovskite oxides exhibit a rich spectrum of functional responses, including magnetism, ferroelectricity, highly correlated electron behavior, superconductivity, etc. The basic materials physics of such materials provide the ideal playground for interdisciplinary scientific exploration with an eye towards real applications. Over the past decade the oxide community has been exploring the science of such materials as crystals and in thin film form by creating epitaxial heterostructures and nanostructures. Among the large number of materials systems, there exists a small set of materials which exhibit multiple order parameters; these are known as multiferroics, particularly, the coexistence of ferroelectricity and some form of ordered magnetism (typically antiferromagnetism). The scientific community has been able to demonstrate electric field control of both antiferromagnetism and ferromagnetism at room temperature. Current work is focused on ultralow energy (1 attoJoule/operation) electric field manipulation of magnetism as the backbone for the next generation of ultralow power electronics. In this lecture, I will describe our progress to date on this exciting possibility. The lecture will conclude with a summary of where the future research is going.

PL.S.II.1.

Correction of aberrations – past – present – and future perspectives

Harald Rose
Ulm University, Ulm, Germany

Aberration correction can be considered as a quantum step in the development of the electron microscope. The correction of spherical aberration, the improved electrical and mechanical stability of the basic instrument, the development of monochromators, detectors, and corrected energy filters have transformed the electron microscope from a crude imaging instrument into a high-performance analytical instrument providing sub-eV spectroscopic information and sub-Angstrom spatial resolution at voltages above about 80kV. The additional correction of the chromatic aberration and the off-axial coma has further improved the performance of the microscope, giving atomic resolution down to 20kV. The requirements necessary for achieving successful aberration correction are illustrated by outlining the evolution of correctors starting from simple systems and ending with the most advanced corrector employed in the SALVE microscope. This microscope has reached a resolution limit of 15 Å which is about seven times smaller than the resolution limit of a non-corrected TEM. The improvement of resolution and contrast in the SALVE microscope by means of the Cc/Cs corrector will be documented by experimental results. The correction of chromatic aberration enables the use of elastically and inelastically scattered electrons for image formation without loss of intensity and degradation of resolution. This possibility is especially important for imaging dose-limited objects. Moreover, the action of other correctors will be shown for different microscopes operating in the range between 10V and 300kV. Perspectives will be suggested to further increase the information on the atomic structure of radiation-sensitive objects and to enable optical sectioning with atomic resolution.

PL.S.II.2.

Prospects and challenges for high-resolution transmission electron microscopy

Rafal E. Dunin-Borkowski, Lei Jin, András Kovács, Andreas Thust
Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg
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When combined with careful sample preparation, modern spherical aberration corrected transmission electron microscopes can be used to provide direct images of the internal structures of materials with a spatial resolution that can approach 50 pm. The positions of individual atomic column positions in such images can be measured with pm precision to provide indirect information about local functional properties, such as ferroelectric polarization, on a unit cell scale. When combined with a precise knowledge of aberration coefficients and other parameters that describe the electron optics and stability of the microscope, quantitative comparisons between individual experimental images and quantum mechanical image simulations on an absolute scale can now be used to obtain information about the local sample thickness and atomic arrangement on the sample surface. With the recent introduction of chromatic aberration correction, a spatial resolution of better than 0.1 nm can be achieved at microscope accelerating voltages of below 50 kV, providing new opportunities for high-resolution imaging of electron-beam-sensitive materials, while the combination of high-resolution transmission electron microscopy with off-axis electron holography and electron magnetic circular dichroism offers exciting prospects for the direct imaging of local magnetic properties in materials and devices on the atomic scale. In this talk, a selection of challenges and opportunities for the further development of high-resolution transmission electron microscopy will be presented and discussed. In particular, improvements in spatial resolution towards the diffraction limit are likely to require radical changes to the design of electron microscopes, while more precise measurements of local material properties will require the automation of longer experiments, a better knowledge of microscope and specimen parameters, the use of ultra-high-vacuum technologies and improved specimen stages to provide a clean and stable sample environment, quantitative comparisons of experimental measurements with both complementary techniques and advanced simulations, and new approaches for data handling and storage.

PL.S.II.3.

High precision STEM studies of spatial strain distribution in nanostructures with correlation to properties

Eva Olsson

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Strain engineering can be used to tune the properties of advanced materials. Catalytic activity of metal nanoparticles and electrical properties of semiconducting nanowires are examples of structures where the strain induced effects have a strong influence on the performance in applications. We are using high resolution annular dark field (ADF) scanning transmission electron microscopy (STEM) imaging to obtain high resolution (better than 1 Å) and high precision (better than 1 pm) information about the local atomic structure [1]. We use in situ microscopy to perform electrical conductivity and nanoscale mechanical strain measurements using an electromechanical setup. We use also STEM combined with nanobeam electron diffraction to quantitatively evaluate the nanoscale strain distribution [2]. In addition, we have studied electric field induced changes on the atomic scale using in situ microscopy [3]. New aspects of material properties and mechanisms, not obvious from measurements on the macro scale are revealed using in-situ electron microscopy where interfaces and defects affect the material properties on the macro, micro, nano and atomic scale. The knowledge is crucial for not only the understanding of the mechanisms that are involved but also for the design of materials and devices with tailored properties.

[1] T. Nilsson Pingel, M. Jørgensen, A.B. Yankovich, H. Grönbeck and E. Olsson, "Influence of atomic site-specific strain on catalytic activity of supported nanoparticles", Nature Communications 2018, DOI: 10.1038/s41467-018-05055-1.

[2] L. J. Zeng, C. Gammer, B. Ozdol, T. Nordqvist, J. Nygård, P. Krogstrup, A.M. Minor, W. Jäger and E. Olsson, "Correlation between electrical transport and nanoscale strain in InAs/In_{0.6}Ga_{0.4}As core-shell nanowires, Nano Letters 2018, DOI:10.1021/acs.nanolett.8b01782.

[3] L. de Knoop, M. J. Kuisma, J. Löfgren, K. Lodewijks, M. Thuvander, P. Erhart, A. Dmitriev and E. Olsson, "Electric-field-controlled reversible order-disorder switching of metal tip surface", accepted for publication in Physical Review Materials July 2018.

PL.S.II.4.

Unconventional imaging by scanning transmission electron microscopy

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Different approaches of using STEM to study the evolution and physical properties of nanomaterials are presented. When exploring the dynamics and stability of tiniest clusters of Pt atoms at elevated temperatures, we benefit from the high spatial resolution of aberration-corrected STEM and overcome the limited temporal resolution by applying an unusual fast scanning mode. This results in large sets of noisy data that require advanced data processing including machine learning and molecular dynamics simulations. In contrast, it is the limited depth of field of an aberration-corrected STEM probe which improves the resolution in liquid cell STEM while controlling nucleation and growth mode of metallic nanoparticles by the electron beam. Using differential phase contrast STEM, electrostatic fields, potentials and charges of individual atoms can be mapped. This is applied to study the periodic modulation of the ferroelectric polarization of a doped multiferroic material at atomic resolution.

PL.S.II.5.

Growth of wide bandgap semiconducting layers: a transmission electron microscopy study

Bela Pecz

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The talk gives an overview of development of wide bandgap semiconductors via the growth of heteroepitaxial layers and their investigation by transmission electron microscopy. The feedback of microscopy helped crystal growers to decrease the dislocation density in nitride layers. Example of epitaxial lateral overgrowth is discussed. Optoelectronic devices request homogeneous layers and sharp interfaces. Beside the optoelectronic devices high power GaN based transistors were also prepared and their self-heating became a major issue. This paper reviews couple of possible solution of that problem with the combination of materials with high thermal conductivity like diamond, or graphene. Finally, some examples of 2D nitride semiconductors will be shown.

PL.S.II.6.

The role of interface complexions on processing ceramic matrix nanocomposites

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The role of dopants in processing materials is an important issue, especially given the contradicting reports of retarded or accelerated grain growth by dopants and impurities. We have developed a technique to measure dopant solubility limits at the sintering temperature, such that actual dopant levels can be associated with equilibrium grain boundary (GB) segregation (below the solubility limit) or with enrichment (above the solubility limit). New analysis of the GB mobility of alumina as a function of dopant concentration has shown that some segregating dopants increase the GB mobility, i.e. the opposite of solute-drag. The segregating dopants are associated with 2-D structural and compositional (“complexion”) transitions at the GBs, and possible changes in the mechanism of GB migration. This presentation will review recent GB mobility measurements and demonstrate how complexion transitions can be used to control particle location and thus the mechanical properties of particle reinforced ceramic matrix nanocomposites.

PL.S.II.7.

Sub 30 meV in a monochromated Themis Z

Anil Yalcin

Thermo Fisher Scientific, Eindhoven, Netherlands

Since the introduction of monochromators on TEMs, they have been mainly used for low kV imaging as well as for EELS applications down to 0.15-0.2 eV resolution. For studies requiring EELS resolution of 30-50 meV (i.e. phonons), Thermo Fisher introduces UltiMono, delivering sub 30 meV EELS resolution on Themis Z. In this presentation, several UltiMono results will be presented on HR-EELS applications as well as challenges of HR-EELS studies and our solutions to overcome these challenges.

PL.S.II.8.

High-resolution 3D crack visualization in multi-component materials and structures during mechanical loading – A novel application of X-ray microscopy

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The study of the fracture behaviour of multi-component materials is of high interest in materials science and engineering, and the nondestructive 3D imaging of crack propagation in mechanically stressed samples, both bulk samples (e.g. composites) and thin film stacks (e.g. 3D patterned microelectronic structures), with high spatial resolution is essential for the validation of models based on materials physics and chemistry as well as fracture mechanics, and eventually for the design of advanced materials with tailored mechanical properties. In addition, it is needed for gauging the in-service mechanical performance and reliability of advanced products and systems. Laboratory transmission X-ray microscopy (TXM) and nano X-ray computed tomography (nano-XCT) offer intrinsic advantages for 3D in-situ imaging of cracks in multi-component materials and structures, since it is nondestructive, i.e. the local strain state is not modified by sample preparation. In this talk, we present a novel micro-double cantilever beam (micro-DCB) test in an X-ray microscope for a nondestructive 3D visualization of crack propagation with high spatial resolution during mechanical loading. This approach allows to identify the weakest (cohesive or adhesive) bindings in the material or of an interface and it provides several benefits over existing methods. It is applicable across a range of disciplines, from materials science and microelectronics to life sciences.

The potential of the novel approach is demonstrated for two examples: 1) Nafion®, a synthetic polymer, filled with platinum particles: The mechanical stability of Nafion®, which is caused by the polymer backbones, is of particular importance for the use as solid polymer electrolyte (proton conductor) in proton exchange membrane (PEM) fuel cells, e.g. for automotive applications. 2) an on-chip interconnect stack of an integrated circuit: The robustness of the backend-of-line (BEoL) stack against chip-package interaction (CPI) is evaluated, and the weakest layers and interfaces are identified, which is valuable information for reliability engineering and design-for-reliability (DFR) in semiconductor industry.

PL.S.III.1.

An update on advanced electron microscopy for cancer nanotechnology research

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We have been engaged in an interdisciplinary research effort on nanotechnology for early cancer detection for thirteen years now. Our role has been to apply advanced nano characterization technologies to reveal details of the structures and methodologies of highest significance. Recent results include:

- Application of electron tomography to identify the location of gold nanorods inside or on extracellular vesicles
- Structure and chemical identity of theranostic gold-ion oxide nanoparticles (GIONs)
- Synthesis and characterization of graphite-encapsulated ferromagnetic iron nanoparticles from ball-milling assisted low-pressure chemical vapor deposition
- In situ environmental TEM studies of the degradation of field-emitting carbon nanotubes in an oxidizing environment
- Raman and electron energy loss spectroscopy of model lithographic gold nanostructures for surface enhanced Raman spectroscopy (SERS) applications

An overview of these studies will be described.

We gratefully acknowledge support of this work from the Center for Cancer Nanotechnology Excellence for Translational Diagnostics (CCNE-TD) at Stanford University through an award (grant No. U54 CA199075) from the National Cancer Institute (NCI) of the National Institutes of Health (NIH).

PL.S.III.2.

Recent developments in combination nanopreparations against cancer

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Nanopreparations of various anti-cancer drugs are causing great interest from pharmaceutical scientists. Both, non-targeted and targeted nanopreparations are under development, including combination nanopreparations containing more than one active ingredient or, more than one specific ligand. Some of those will be discussed here.

Resveratrol (RES), a natural polyphenol with pleiotropic health benefits, has proven chemopreventive effects in all the stages of cancer including initiation, promotion and progression. However, the poor physico-chemical properties of RES severely limit its use as a free drug. To counter its drawbacks as a free drug, for glioblastoma (GBM) treatment, RES was loaded into PEGylated liposomes (RES-L). Since transferrin receptors (TfRs) are up-regulated in GBM, the liposome surface was modified with transferrin moieties (Tf-RES-L) to make them cancer cell-specific. The RES-L were stable, had a good drug-loading capacity, prolonged drug-release in vitro and were easily scalable. As shown by flow cytometry and confocal microscopy with U-87 MG cells, the Tf-RES-Ls were significantly more cytotoxic and induced higher levels of apoptosis accompanied by activation of caspases 3/7 in GBM cells compared to free RES or RES-L. In a subcutaneous xenograft mouse model of GBM, a tumor growth inhibition study and a modified survival study showed that Tf-RES-Ls were more effective than other treatments in their ability to inhibit tumor growth and improve survival in mice.

Among many approaches for active tumor-targeting, arginine-rich cell penetrating peptides (such as octaarginine, R8) and ligands specific to target over-expressed receptors on cancer-cell surfaces, are popular. We have prepared doxorubicin(DOX)-loaded liposomes, surface-modified with, R8 and transferrin (Tf) (Dual DOX-L), to improve targeting of A2780 ovarian carcinoma cells via the over-expressed transferrin receptors (TfRs) with the subsequent R8-mediated intracellular DOX delivery. Flow cytometry analysis with fluorescently-labelled DualL showed 2-fold higher cancer-cell association than other treatments after 4 h treatment. Blocking entry pathways of R8 (macropinocytosis) and Tf (receptor-mediated endocytosis, RME) resulted in a decreased cancer-cell association of DualL. Confocal microscopy confirmed involvement of both entry pathways and cytoplasmic liposome accumulation with nuclear DOX delivery for Dual DOX-L. Dual DOX-L exhibited enhanced cytotoxicity in vitro and was most effective in controlling tumor growth in vivo in an A2780 ovarian xenograft model compared to other treatments.

Other combination preparation include those combining pro-apoptotic drugs and drugs targeting cancer cell energy metabolism as well as nanopreparation with theranostic properties, i.e. combining therapeutic and diagnostic agents in a single nanoparticle.

PL.S.III.3.

The future of medicine: implantable nanosensors

Thomas J. Webster

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There is an acute shortage of organs due to disease, trauma, congenital defect, and most importantly, age related maladies. Synthetic materials used in medical device and tissue engineering applications today are typically composed of micron sized particles/grains and associate surface roughness. Although human cells are on the micron scale, their individual components, e.g. proteins, are composed of nanometer features. By modifying only the nanofeatures on synthetic material surfaces without changing surface chemistry, it is possible to increase tissue growth of any human tissue by increasing the endogenous adsorption of adhesive proteins (and their bioactivity) onto the material surface. In addition, our group has shown that these same nanofeatures and nano-modifications can reduce bacterial growth without using antibiotics, which may further accelerate the growth of antibiotic resistant microbes. Finally, material nanofeatures have been shown to stimulate the growth and differentiation of stem cells, which may someday be used to treat incurable disorders, such as neural damage. This talk will summarize techniques and efforts to create nanofeatures for a wide range of medical device and tissue engineering applications, particularly those that have received FDA approval and are currently being implanted in humans.

PL.S.III.4.

Ceramic nanoparticles for advanced biomedical applications: from bone to brain

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Structural complexities of ceramics are the key to explaining their display of a broad range of interesting properties, yet the control of these complexities has not been harnessed to the fullest extent and translated to the medical domain. In the first part of the lecture I will talk about the studies on calcium phosphate nanoparticles and the control of their physical and chemical properties with the goal to yield new properties relevant for various biomedical applications, ranging from tunable drug delivery kinetics to gene delivery to cancer cell targeting to intrinsic antibacterial activity. This will be placed in the context of an ongoing effort to expand the application repertoire of calcium phosphate nanoparticles beyond their traditional use as components that impart osteoconductivity and high compressive strength to tissue engineering constructs. In the second part of the lecture I will talk about the ongoing work on the use of composite nanoparticles modeled after the stratified structure of the planet Earth for permeation of the blood-brain barrier and brain tumor targeting.

PL.S.III.5.

Solid-state oxygen abstraction from stable oxides for energy storage materials

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Oxygen deficient oxide materials, including less stable oxides of lower oxidation number, are of great technological significance. They are conventionally prepared from stable oxides by heating under reducing atmosphere. Opposite processes, i.e. from metals by sparingly oxidizing under controlled oxygen partial pressure are less popular but some attempts were also made. Abstraction of lattice oxygen from stable oxides, mostly with highest oxidation number, is not just a simple reduction. Mechanisms of such phenomena are well documented in the interests of semiconductor technology and catalytic activity. However, such accumulated knowledges are not always taken over for the preparative methods of modern functional materials. When electrophilic species are coexisting and participate in such a preparative process, abstraction of lattice oxygen creates oxygen vacancies, leading to subsequent reduction of the oxides. The same principle is directly extended to the anion exchange, e.g. toward oxyhalides when an electrophilic materials we use contain halogens. The presentation is based on the related recent studies carried out by the author and his colleagues on V_2O_5 , TiO_2 , SiO_2 and SnO_2 . Some new insights why and how are those less stable oxides exhibit their functionalities are discussed in view of their application to energy storage devices, among others thermal energy storage via latent heat during phase change, and Li-ion battery anode is briefly referred.

PL.S.III.6.

High energy density electrodeposited Li and Na-ion battery electrodes

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Lithium-ion battery electrodes are nearly universally formed via tape casting of a slurry containing a mixture of active material, binder, and conductive carbon. However, the electrochemical and mechanical properties of slurry cast electrodes are often limited by weak interconnections between particles and between the particles and the substrate. We suggest conformal electrodeposition of high-quality electrode materials would provide opportunities to enhance battery performance (energy density, power density, and flexibility) and broaden the scope of available electrode form factors (size, shape, porosity, and 3D integration). We have now made considerable advances in the direct electrodeposition at modest temperatures of high performance tin-based Li-ion anodes and LiCoO₂, NaCoO₂, LiMn₂O₄, and Al-doped LiCoO₂-based Li-ion cathodes. The electrolytically active materials were formed either as solid films, or where significant volume changes upon cycling are present, via a templating process, as a 3D mesostructured film. The capacities are near-theoretical, and in the case of the electroplated oxides, the crystallinities and electrochemical capacities of the oxides are comparable to powders synthesized at much higher temperatures (700 ~ 1000 °C). The electrodeposition method significantly broadens the scope of battery form factors and functionalities, enabling a variety of highly desirable battery properties including microbatteries, and high energy, high power, and flexible designs.

PL.S.III.7.

(Early actinoid metal)-boron-carbon systems: phase equilibria, crystal structures and physical properties

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As generation IV nuclear fuels include actinoid carbides in combination with B₄C control rods, interest has been revived in the corresponding phase relations for the An-B-C systems. Preliminary studies of phase relations in the ternary systems {Th,U,Np,Pu}-B-C prompted the formation of two main isotypic series of ternary compounds {Th,U,Np,Pu}BC (UBC-type, space group Cmcn or ThBC-type, space group P4122) and {Th,U,Np,Pu}B₂C (ThB₂C-type, space group R-3m). Since then isothermal sections have been established for all four systems revealing further compounds, the crystal structures of which have recently been defined from single crystal and powder X-ray intensity data.

Phase equilibria in the system Th-B-C, established at 1400 °C, reveal four ternary thorium boron carbides: ThBC, ThB₂C, Th₃B₂C₃, "ThBC₂". Whereas the structures of the former are already established earlier, the crystal structure of the latter (hitherto described as "ThBC₂"), has now been defined from single crystal data as a new and unique orthorhombic structure type with the proper formula Th₂B₂C₃ (space group Pnnm, #58; a=1.30655(9) nm, b=0.39757(3) nm, c=0.36507(3) nm). The crystal structure of Th₂B₂C₃ is characterized by C-branched infinite chains ...B-C1-B-B-C1-B... whereby each boron atom is additionally linked to a C2-atom. Boron atoms are in a typical triangular prismatic metal coordination, C₁-atoms center a bi-pyramid, Th₄B₂, and C₂-atoms are surrounded by 5 pyramidal Th-atoms and one B-atom. Bonding from carbon atoms to thorium appears to correspond to the sum of radii for C₂, whereas distances dTh-B slightly exceed the sum of the radii. According to the formula Th₂B₂C₃ (formerly "ThBC₂"), the phase relations for the Th-B-C system have been revised.

Density functional theory calculations were made for all thorium boron carbides as well as for the homologous uranium boron carbides (including also isotypic CeB₂C) within the pseudopotential approach of VASP utilizing the general gradient approximation for the exchange correlation functional. Structural parameters optimized were in good agreement with the experimental values. Relativistic calculations by including spin-orbit coupling were performed for the electronic structure. Atomic volumes and charges were computed by the concept of Bader yielding the ionic charges and the charge transfer among the atoms. Particularly the analysis of the electronic structure for Th₂B₂C₃ shows features of chains and corresponding structural subunits with π -like bonding. The DFT heat of formations were studied along the sections which involve all the ternary {Th,U} boron carbides: ThB₄ - ThC₂ and B - ThC as well as for the corresponding U-sections.

Physical properties have been elucidated for two series of compounds [Th,U,Np,Pu]BC and [Th,U,Np,Pu]B₂C revealing interesting magnetic and electrical behavior dependent on the amount of spdf hybridization.

PL.S.III.8.

Solid-state synthesis of lead-free (K/Na)_{0.5}Bi_{0.5}TiO₃ piezoceramics: peculiarities and their influence on the electrical properties

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Investigating the literature on the lead-free (K_{1-x}Na_x)_{0.5}Bi_{0.5}TiO₃ based piezoelectric materials, a strong inconsistency of the reported data and properties can be observed. To clarify the inconsistencies, we investigated the formation mechanism of Na_{0.5}Bi_{0.5}TiO₃ (NBT) and K_{0.5}Bi_{0.5}TiO₃ (KBT). Synthesis of NBT commences with the formation of a sodium deficient end member, which then reacts further towards a nominal composition. During the reaction, the symmetry changes from cubic to rhombohedral. The change in the symmetry and microstructure result in the differences in the electrical properties. The most striking difference is the change of piezoelectric constant d₃₃, which increases from 82 pC/N to 97 pC/N with increasing sodium deficiency. The A-site deficiency was shown to be responsible for high leakage current, which can be used for high-temperature ionic conduction¹. A-site deficiency exists also in KBT compound, where the formation of a stoichiometric compound is not possible due to thermal instability of the matrix phase. During the solid-state synthesis of KBT, several secondary phases are formed. Among them, the hygroscopic K₂O-rich liquid phase is the most important as it deteriorates the electrical properties of the ceramics. This phase is formed by transformation of potassium tetra-titanate to potassium hexa-titanate. Inevitably, polytitanates form at low temperatures and they are stable. The K₂O-rich phase was identified by careful investigation of the phase relations around KBT and microstructural changes of thermally and chemically etched samples. By eliminating the hygroscopic liquid phase, the electrical properties are greatly improved: a two-fold increase in the dielectric constant, an increase in the remanent polarization to 29 mC/cm² and a 3-fold increase in the piezoelectric d₃₃ coefficient were observed. In this work, we will show the evidences leading to the conclusion that the main reasons for the inconsistencies are an inappropriate selection of the synthesis conditions and insufficient characterization of the synthesized ceramics before measuring their electrical properties. Selected synthesis peculiarities and their impact on the dielectric and ferroelectric properties will be presented. In addition, the methods for identification and analyses of the minor factors influencing the properties of the ceramics will be discussed.

1 Li et al, Nature Materials, vol.13, 31–35, 2014

PL.S.IV.1.

A unified computational approach for dislocation-based plasticity

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Discrete dislocation dynamics (DD) simulations have been widely used to gain a better understanding of the mechanisms involved in the deformation of metals. While there are a number of variants of DD simulations, they all involve the calculation of the stress at each dislocation, the resolving of that stress as a force, and solving the equations of motion. Sub-scale models are used to describe such processes as junction formation, cross-slip, and climb. In traditional DD approaches, the stresses are found by summing analytical expressions (usually based on isotropic elasticity). Recently we have shown that the stress calculation can be done using a fast Fourier transform (FFT) method based on an eigenstrain representation of the plasticity. The FFT-DD approach is faster than conventional methods and enables use of anisotropic elasticity with little change in computational time. In addition, it is straightforward to include any type of additional eigenstrain, allowing us link the FFT-DD method directly within the FFT-polycrystal framework developed by Lebensohn, which enables direct simulations of dislocation-based plasticity in fully polycrystalline systems. In this talk, we will show recent applications of the FFT-DD-polycrystal method. We will also show how this same framework enables straightforward modeling of such phenomena as precipitate/inclusion/solute hardening, creep, etc., providing a unified approach for dealing with complex deformation phenomena.

PL.S.IV.2.

Materials characterization and integrated computational materials engineering: providing solutions for near-net shape manufacturing

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There have been, over the past four decades, various processing schemes introduced that are focused on near net-shape manufacturing of components. These are often based on powder metallurgy approaches, and include hot isostatic pressing (HIP) and additive manufacturing (AM), but more recently include processes such as solid state joining. The full exploitation of these processing schemes has been frustrated by a number of limiting factors including anisotropic and coarse microstructures, issues with prior-particle boundaries, porosity, residual stress, and deficits in certain mechanical properties. This presentation describes an effort aimed at overcoming some of these problems through application of a combination of sophisticated materials characterization and integrated computational materials engineering. The focus has been on the production of equiaxed microstructures and improved fatigue properties of Ti alloys, and the reduction of the influence of ppb's in Ni-base superalloys. The results of these experiments will be discussed in terms of the increased use of these processing approaches for the manufacture of turbo-machinery.

PL.S.IV.3.

On the nucleation of planar faults in single crystal Ni-base superalloys

Gunther Eggeler

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Under conditions of low temperature ($< 800^{\circ}\text{C}$) and high stress ($> 600\text{ MPa}$) creep, $a\langle 112 \rangle$ fault ribbons form in the microstructures of single crystal Ni-base superalloys. New experimental shear creep results are presented which show that a macroscopic $\langle 112 \rangle \{111\}$ shear test deforms much faster than a $\langle 110 \rangle \{111\}$ shear test. The reason is, that the two dislocation families with different Burgers vectors, which are needed in order to start the nucleation of a $a\langle 112 \rangle$ fault experience the same high resolved shear stress during $\langle 112 \rangle \{111\}$ shear testing.

Diffraction contrast microscopy is performed to provide microstructural evidence for the presence/absence of planar faults.

Moreover, creep activation parameters n (stress exponent) and Q (apparent activation energy) are measured for the two macroscopic shear systems and are discussed in the light of previous results published in the literature.

PL.S.IV.4.

Quo vadis quantum matter?!

Davor Pavuna

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Successes of the twentieth century physics made a remarkable impact on the society in areas ranging from basic science and space technology to improved medical tools or computing and financial modeling ... In remarkable advancements in materials, the confirmation of electron or simple Drude model (both around 1900) led eventually to discovery of superconductivity and several striking metal-insulator related subjects, like semiconductor technology, quantum Hall effects, photonics, high- T_c superconductivity, topological insulators, gorilla glasses and artificially engineered multi-ferroics.

However, we still do not fully understand the physics of metal-insulator transition or complex cooperative phenomena, especially in chemically or artificially constructed low-dimensional heterostructures in the nanoscale limit. Quantum Matter is an active field and I will present several examples from our research. It is evident that we have to fully master the sub-nano-scale and emergence of novel cooperative - competitive phenomena, also in biosystems: in short, many challenges for the new generation!

PL.S.IV.5.

Ultimate atom resolution

Richard W. Siegel

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The materials research community has been seeking ever higher experimental resolution of atoms with increasing success in a variety of environments over many years. In parallel with these efforts, theoretical modeling of atoms and their material environments has achieved a high level of atom resolution that has enhanced our understanding of these environments. These developments have enabled greater and more precise visualization of atom interactions and organization. They have also been important in stimulating and capturing young people's interest in the world around them and how that world is made up of atoms, molecules, and materials. This interest and initial learning can begin even at a very early age, long before any formal schooling begins. In order to encourage young people of all ages to become interested in materials and to gain a greater understanding of them, we created the Molecularium® Project (www.molecularium.com) at Rensselaer almost 20 years ago. This award-winning effort utilizing state-of-the-art atom simulations has produced several media, including *Molecularium – Riding Snowflakes* (2005), *Molecules to the MAX!* (2009), *NanoSpace*® (2012), and *My Molecularium* (2017), which now capture young people's interest through entertainment with significant scientific content – *stealth education*. This talk will highlight these media that are now being used by children, parents and teachers to increasingly develop science literacy and to entice eager young minds into the exciting world of materials.

PL.S.IV.6.

Probing mechanical behaviour at small length scales: from spatially resolved toughness in Pt-Ni-Al bond coats on superalloys to small scale cantilever creep for residual life assessment

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Small scale test methods are now available to probe mechanical behaviour in uniaxial loading, bending and fracture for the determination of location-specific mechanical properties. This talk focuses on materials and length scales that are relevant to industrial applications in coatings, weldments and residual life assessment of samples extracted from high temperature components. The first example is one of bond coats on superalloys where we demonstrate the use of micro scale tests to study the ductile-brittle transition as a function of platinum content and the variation in fracture toughness across a 0.1 mm graded Pt-Ni-Al diffusion aluminide. A new method is presented using a clamped beam under central loading that leads to stable crack propagation under load control and allows the determination of R-curves and fatigue crack growth with sub-micrometre spatial resolution. The second example describes our efforts to adapt the age-old technique of bending creep to small size cantilever testing for creep evaluation of steam turbine components from which extracted specimens need to be as small as possible. It transpires that the assumption of steady state creep characterized by a single stress exponent allows a good match to be established between bending and uniaxial creep parameters, while length scale effects start to appear below a critical size of ~ 1 mm in coarse grained aluminium. Challenges in using such creep data under non-steady state conditions for predictions based on uniaxial parameters will be discussed.

PL.S.IV.7.

NV centers in diamond: potentials and limitations for quantum metrology

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Among the various isolated impurity sites in diamond, Nitrogen – Vacancy (NV) centers have been extensively studied over the past 25 years or so. The exceptionally intense, non-bleaching fluorescence, which is sensitive to the spin state of the ground state allows for both “ensemble average” and single center ODMR (Optically Detected Magnetic Resonance) spectroscopy. Embedded in a large band gap material, the ground state magnetic sublevels of isolated NV center display remarkably long coherence times at room temperature, enabling precise single center spectroscopy, i.e. sensitive detection of local electromagnetic fields influencing the sublevel structure. An individual, negatively charged NV site is able to measure changes in its local environment, for example to detect a nanometer scale displacement of an elementary charge or a paramagnetic center induced by conformation changes of nearby biological molecules. These exceptional properties make NV centers in diamond the most exciting atomic scale quantum metrology tool available at present.

Almost all practical use of the demonstrated potentials rely on the use of a large number of NV centers at the same time. Interrogation of a large number of NV centers at the same time requires all of the NV centers to experience nearly identical local environment. Controlled positioning of the NV centers relative the objects being measured, typically situated on the surface of the diamond, is a challenge on two fronts. Positioning and orienting the NV centers identically relative to the surface remains an unsolved problem in spite of the tremendous recent developments made ion-implantation and refined MW-CVD diamond growth. Equally difficult is controlling the surface chemistry of the diamond and the target molecules to ensure, that the changes to be monitored dominate other unwanted fluctuations in the environment of the NV centers. Potentials for developments and compromises are discussed.

PL.S.IV.8.

Metastable-watching for the structure and property of low-temperature plasmas

Toshiaki Makabe
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Low-temperature plasmas in argon are widely employed for the basic research and application fields owing to the feature of the non-chemical reactivity, the atomic data accumulation, and the cost performance of the feed gas.

In the present review, we will arrange and correlate the number density between the neutral metastable and the electron in the plasma based on the accumulated experimental and modeling studies. We will also discuss the physical property and the function of the metastable in a plasma, interface, and on a material (electrode) surface in various kinds of plasma sources under non-equilibrium conditions, including our results.

The present talk will work as a bridge between past and future of the study and development of the low-temperature plasma and of the material processing.

PL.S.IV.9.

On the origin of high glass forming ability in metallic systems

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Rapidly cooled atomic and molecular liquids can bypass crystallization and vitrify. While network bonding in silica and chain entanglement in polymers seem plausible mechanisms for inhibiting their crystallization, the corresponding mechanism for metallic systems is less clear. When molten alloy is cooled, the formation of metallic glass (MG) usually competes with that of intermetallic compounds (IC): thus similar free energies (G) of MG and competing IC(s) facilitate vitrification. At low temperatures G is dominated with internal energy which in metallic systems strongly depends on electronic structure (ES). Thus small differences in ES between MG and competing IC(s) promote vitrification, as observed in several binary and ternary transition metal (TM) alloy systems.

This correlation seems applicable to all TM alloys irrespective on their number of alloying components (thus also to high-entropy alloys) and provides a simple way to select compositions with high glass forming ability.

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PL.S.IV.10.

Fundamental aspects of the use of metal hydrides in hydrogen energy and chemical current sources

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The significant aggravation of energy and especially environmental problems, which is observed both in Ukraine and throughout the world, the exhaustion of traditional fossil hydrocarbon fuels put forward the problem of a wider use of alternative energy carriers and, first of all, hydrogen. Hydrogen is a unique energy carrier that has three times the energy intensity compared to traditional fuels, it is easy to store and transport, it can be very effectively converted into electricity, for example, in fuel cells, with the only waste being water.

Clean energy technologies that use hydrogen as energy carrier can be harmoniously combined with systems based on renewable energy sources, primarily solar, wind, geothermal, etc. One of the shortcomings of these sources is the periodicity of their action. Therefore, the issue of accumulation of residual energy and its further utilization becomes topical. The use of hydrogen as a battery of energy in this case is considered the most promising. Hydrogen is conveniently stored in the solid compounds - metal hydrides. In recent years, the focus is on hydrogen storage devices based on magnesium.

The presented report contains an overview of the results of studies carried out in recent years at the IPMS NAS of Ukraine. The aim of the research was to decrease the temperature and improve the kinetics of the decomposition of the stoichiometric hydride MgH_2 using the mechanical dispersion and doping of Ti, Fe, Ni, and Al in the course of its synthesis. The role of separately each of these alloying elements as well as the role of double doping of Al + Ti, Al + Fe, Al + Ni, Ti + Fe in reducing the temperature and improving the kinetics of the decomposition of the hydride phase of MgH_2 mechanical alloys obtained by the method of reactive mechanical alloying. .

O.S.F.1.

The preparation of injectable angiogenic bone cement for femoral head avascular necrosis

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Human tissue depends on blood circulation to transport oxygen, nutrition, carbon dioxide, waste and so forth. If there are problems in transportation of these substances, one's organ and tissue will be necrotic. When this happened in brain, it may lead to stroke or transient ischemia; in heart, it will probably bring myocardial infarction and stenocardia; in bone, it will cause osteonecrosis. Avascular necrosis of the femoral head is also known as aseptic necrosis of the femoral head or osteonecrosis of the femoral head. According to the literature, 300,000 to 600,000 people have avascular necrosis of the femoral head in the United States. It is a disease of weak osseous blood flow of femoral head. This disease commonly occurs in the people who are thirty to fifty years old. The ultimate purpose of every clinical treatment is to save patient's femoral head but it's not an easy work. Making a decision about therapy is related to the patient's other illness, previous life, living environment and so on.

Poly(propylene fumarate) (PPF) is an unsaturated linear polyester that can be cross-linked through the double bonds along its backbone to form a solid polymer. Cross-linking can be carried out through the addition of N-vinyl pyrrolidinone (NVP, a cross-linker), benzoyl peroxide (BP, an initiator) and N,N-dimethyl-p-toluidine (DMT, an accelerator). An orthopedic composite formulation can be formed through the addition of tetracalcium phosphate (TTCP) / dicalcium phosphate (DCPA) as an osteoconductive agent and ginsenoside (Rg1) as an angiogenic agent. Moreover, TTCP/DCPA can improve the mechanical strength of PPF. This composite forms an injectable paste that can be used to fill skeletal defect, acting both as a biodegradable scaffold with angiogenic agent for cell growth and as a mechanical support at the defect site.

The purpose of study is to fabricate an injectable bone cement with biodegradable and angiogenic functions. We anticipate this bone cement can benefit to supporting mechanical strength immediately after injection. As time goes by, it will be degraded within the body gradually followed by releasing angiogenic agent which can stimulate vascularization of surrounding tissue. With the nutritional supply of new microvessel, bone tissue will regenerate onto this cement. Finally, the cement will be replaced by newly formed bone.

O.S.F.2.

Gelatin nanoparticles with anti-inflammatory/anti-angiogenesis agent loading for ocular disease treatment

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With more and more aging population, or accidents, many eye disease become problems to obstruct vision, such as dry eye syndrome (DES) and cornea neovascularization (NV). DES is a common disease causing by instable tear film induce ocular surface inflammation. And cornea NV leads the transparent cornea become opacity due to blood vessels ingrowth. Therefore, the polyphenol extracted from green tea, epigallocatechin gallate (EGCG), with anti-inflammatory and anti-angiogenetic effect was chose as the model drug for treating these two common extraocular diseases. In ophthalmological treatment, topical delivery of ocular therapeutics such as eye-drop is usually used, but ocular barrier of eyes can impede the release of pharmaceutical drugs; particularly solution type is quickly removed to nasolacrimal duct, local bioavailability of the drug decreases. Nanocarriers offer a promising alternative for the treatment of ocular diseases with high availability of therapeutic agent on the ocular surface. The main objective of the study is to develop a new nanomedicine for DES and cornea NV treatment. Gelatin was adapted as the drug(EGCG) carrier with surface coating of hyaluronic acid (HA) to increase drug retention on the cornea for treating DES. With RGD peptide modified on nanoparticle's surface, it can lead to recognized the vascular endothelia cells for angiogenesis inhibition. For DES treatment, a rabbit dry eye model was established to evaluate the therapeutic effect of this EGCG loaded gelatin nanoparticles. This nanoparticle was used as eye drops via twice dosing per day. Clinical signs, corneal fluorescein staining, tear production and inflammation cytokines in cornea were evaluated. Cornea specimens were processed for histological section with H& E stain for histological examination. For cornea NV treatment, an alkali-burned mice model was used. Mice with eye drops dosing once per day were lasted for one week treatment, and then sacrificed. Visual grading of mice eyes was examined. Corneas were then paraffin embedded and stained for histological examination. Furthermore, cornea lysates were examined by enzyme-linked immunosorbent assay (ELISA) was used to evaluate the vascular endothelial growth factor (VEGF) and MMP-9 content in mice cornea. Overall, we've confirmed that gelatin -EGCG self-assembling nanoparticles with HA coating on its surface can effectively treating DES rabbits with inflammation relief and tear selection increased. With RGD modified on particles surface, it can be used as eye drop for treating cornea NV effectively via inhibition VEGF, MMP9 expression in cornea to prevent vessel formation in the damaged cornea.

O.S.F.3.

High throughput generation of alginate-gelatin capsules for human osteoblast-like cells (MG63) long-term cultivation

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Osteoarthritis is the predominant form of arthritis and it remains the leading cause of disability among aged population. Alternative orthopedic repair approaches focus on tissue-engineered bone grafts that have been investigated for the treatment of full-thickness bone defects with promising results. A significant challenge remains in how to engineer a consistent and stable osteochondral interface for achieving integrative osteoarthritis repair. Cell microcapsules have presented a wide range of potential applications. The cellular microenvironments strongly influence cell motility, phagocytosis, growth, and differentiation. The focus of this study, guided by these design criteria, is to evaluate the potential of alginate-gelatin capsules to promote the bone like tissue formation of a calcified bone-like matrix in vitro. Moreover, try to optimal configuration of the hydrogel to construct a microenvironment for cell manipulation and cell engineering. By this way, we can construct an ideal cell microcapsules for orthopedic tissue engineering especially in degenerative arthritis.

O.S.F.4.

Using continuous bioreactor system to cultivate human bone-like tissues for bone tissue engineering

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Age-related orthopedic disorders and bone defects have become a critical public health issue, and cell-based therapy is potentially a novel solution for issues surrounding bone tissue engineering and regenerative medicine. Long-term cultures of primary bone cells exhibit phenotypic and functional degeneration; therefore, culturing cells or tissues suitable for clinical use remain a challenge. A platform consisting of human osteoblasts (hOBs), calcium-alginate (Ca-Alginate) scaffolds, and a self-made bioreactor system was established for autologous transplantation of human osteoblast cell clusters. The described strategy could be used in therapeutic application and opens new avenues for surgical interventions to correct skeletal defects. In order to overcome such limitation and problems, establishing an appropriate scaffold system combining bioreactor system to mimic the microenvironment for cell proliferation and differentiation is the major issue of bone tissue engineering. In this study, a proper platform was established for human osteoblast cell clusters production for autologous transplantation and was consist of human osteoblasts (hOBs), Ca-Alginate scaffolds, and the self-designed bioreactor system. In brief, we harvest osteoblasts from spongy bones which were collected at surgery. Next, we could employ Ca-Alginate scaffolds as cell culture matrices and incubate these cells at our self-made bioreactor system with dynamic fluid. Ca-Alginate scaffolds not only contain highly porous structure but also provide a “soft” growth environment. At the end of incubation, we extract bone-like tissues without any enzymatic treatment. Under osteogenic condition in this self-made bioreactor system, human osteoblasts could differentiate into bone-like tissues with biomineralization. This strategy could create enough bone-like tissues for cell therapy and avoid contaminations. Above all, the results demonstrate that the functionally-closed process bioreactor system provides an economic and safety tool on bone regenerative medicine. In the future, we hope the strategy could be applied on clinical use.

O.S.F.5.

Fabrication of multilayered gold/silica/gadolinium compound core-shell particles and their properties of X-ray imaging and MRI

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The present work describes preparation of a colloid solution of multilayered gold nanoparticle/silica/gadolinium compound core-shell (Au/SiO₂/GdC) nanoparticles and investigation of its properties of X-ray imaging and MRI. The Au nanoparticles with a size of 15.5 nm were produced by reducing hydrogen tetrachloroaurate (III) trihydrate with trisodium citrate dihydrate. Silica-coated Au (Au/SiO₂) particles with a size of 38.0 nm were fabricated by a sol-gel reaction in the presence of the Au nanoparticles. Multilayered Au/SiO₂/GdC nanoparticles with sizes of 43.8±1.9 nm were fabricated by a homogeneous precipitation reaction in the presence of Au/SiO₂ nanoparticles and concentrated with centrifugation. The computed tomography (CT) value of the Au/SiO₂/GdC colloid solution containing 4.3 × 10⁻² M Au was 606 HU: Its converted CT value (CT value divided by Au concentration) was 1.4×10⁴ HU/M. The longitudinal relaxation rate (r₁) of the Au/SiO₂/GdC colloid solution was 2.3 mM⁻¹μs⁻¹.

O.S.F.6.

The self-assembled, microtube array membranes (MTAM) and their applications for cancer translation

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MTAM, a novel class of hollow fibers were fabricated with the internally developed patented electrospinning process. These MTAMs possess many unique microstructures which are applicable in a wide range of applications. One key application is the use of these MTAMs as a 3D culture substrate in the cancer biology and anti-cancer drug development arena where better cell survivability/viability and excellent drug sensitivity have been successfully demonstrated through the MTAM-Hollow Fiber Assay (MTAM-HFA) process. The MTAM-HFA process, brings unprecedented reliability and significantly shorten the time frame for each test cycle at a fraction of the cost of conventional anti-cancer drug screenings. Through the utilization of the MTAM-HFA process, we have successfully tested it for a wide range of cell sources (cell lines and patient derived tumor cells); cancer types (solid and non-solid tumors) and a wide range of anti-cancer drugs (small molecule drug, protein drug and immunotherapy drug such as PD-1). The combination of these elements allowed us to further develop this technique into a personalized medicine platform for anti-cancer treatment (MTAM/Select); and as a system to identify target patient segment for clinical trial phase (MTAM/Trial) for drug developers. Currently, with promising preliminary data, we strive to integrate EpCAM molecules into the MTAMs as a circulating tumor cell (CTC) capture system; and the use of the MTAMs in the encapsulation of hybridoma as a potential long-lasting anti-cancer treatment

O.S.F.7.

Cornea epithelium reconstruction by a new way to engineer cell sheet

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Carbon dioxide plasma treatment following adding Cystine, EDC, and HA generate well-formed two-stage surface-modified PET membranes. The PET membranes seem to be a novel and potential material in engineering cell sheet and could be useful in harvesting cell sheets. The PET membranes surface were successfully modified and by adding a reducing agent, the disulfide bonds can be easily cleaved were confirmed by methylene blue, water contact angle measurement, and ESCA. further, we utilize our cell sheet engineering system successfully cultivated and fabricated rabbit corneal epithelial cell sheet and oral mucosal epithelial cell sheet for autologous cornea epithelium reconstruction. It's were easily detached and be smoothly transferred onto an electrospun PLLA membrane made the carrier, and animal-tested then. The animal test results for autologous corneal epithelium reconstruction also shows the feasibility of our system. We also look forward to the system could be applied to clinical practice in the near future.

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O.S.F.8.

Addition of porogens improved the characteristics of biodegradable implants made of poly(-caprolactone)/calcium phosphate ceramic composites

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Metal implants are routinely used in fixations of bony fragments. However, the excessive mechanical strength causes bony atrophy and/or disuse osteoporosis because of the implants stress-shielding effects and strain-induced bone resorption. The mechanical strength of pure biodegradable polymer fixators is insufficient, and most of these materials are non-radiopaque which are difficult to evaluate the placement postoperatively and difficult to investigate the degradation of the bioabsorbable fixation devices. Therefore, we designed a new composite made of calcium phosphate ceramic (CPC, including tricalcium phosphate [TCP] and tetracalcium phosphate/dicalcium phosphate [TTCP/DCP]) and poly (-caprolactone) (PCL) to fabricate biodegradable orthopedic fixators. After implantations, for these composites dissolved slowly, some porogens had been applied to improve the characteristics of these composites. In this study, calcium sulfate (CS) and strontium (Sr) were added into poly (-caprolactone)/calcium phosphate ceramic (PCL/CPC) composite for fabricating biodegradable orthopedic fixators. The dissolution of CS and Sr can create porous structures in implants. In the meantime, CS can provide calcium ions for hydroxyapatite formations. Moreover, CS can upregulate osteoblasts and inhibit osteoclasts. The strontium has been dispensed clinically as an anti-osteoporosis regimen which improves osteoblast's functions and depresses those of osteoclast. Different weight ratios of CS or Sr are added into the PCL/CPC. We examined the mechanical properties, microstructure, degradation time, and the material mediated cytotoxicity of PCL/CPC/CS and PCL/CPC/Sr composites. The degradation pattern will be established. After the in-vitro study, the formula of PCL/CPC/CS and PCL/CPC/Sr will be selected to prepare the bone screws, which are implanted into rabbit femurs. Computed tomography and histologic examination will be applied to evaluate the in-vivo performance and osseointegration of these new implants.

The results revealed that the addition of CS accelerates the biodegradation and enhanced apatite formation of the PCL/ CPC composite screw. In PCL/CPC/Sr group, the Sr-impregnated bone fixator improves osseointegration in osteoporotic animals.

O.S.F.9.

The application of hydroxyapatite as the *Bletilla striata* polysaccharide carrier for sarcopenia treatment

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Sarcopenia is a disease of muscle mass loss and muscle function decline caused by aging. There are no effective drug without side effects to treat sarcopenia. *Bletilla striata* is a chinese herb. The polysaccharide isolated from *Bletilla striata* (BSP) have wound healing and anti-inflammatory property. But BSP is easily broken down in the body, so we need drug carrier to prolong drug effect. Hydroxyapatite (HAp) is one of the components of bones and teeth in the human body, has well biocompatibility and biodegradability. This study will develop hydroxyapatite particles as drug carriers carrying BSP (HAp-BSP, BHAp); it also may provide patients with calcium ions which lack in the body and reduce the drug injection frequency. In this study, we will perform the material test, in vitro cell biocompatibility test and in vivo test. In this study, we successfully to induce muscle injury that similar to sarcopenia, and HAp-BSP could decrease the symptoms caused by induced. It was confirmed that HAp-BSP had its anti-oxidation and promoting tissue capacity.

O.S.F.10.

Hydroxyapatite/gelatin particles embedding stromal cell-derived factor-1 for bone tissue engineering

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A bone fracture is a damage in the continuity of the bone, which may be the result of high force impact or stress, osteoporosis, osteopenia, bone cancer, or osteogenesis imperfecta. Bone grafts or bone tissue engineering are the use of a combination of cells, engineering and materials methods to improve or replace biological tissues. For the bone grafts, there are three critical properties in bone tissue engineering, osteoinduction, osteoconduction, and osteogenesis. However, most of bone tissue engineering lacks osteoinduction. Stromal cell-derived factor-1 (SDF-1) is a well-characterized chemokine for attracting stem cells and thus a strong candidate for promoting regeneration. Therefore, the purpose of this study is to develop an osteoinductive bone graft, hydroxyapatite/ gelatin particles loaded with stromal cell-derived factor-1 for bone tissue engineering. In primary results, the particles synthesized by spattering in three hundred micro-meter to five hundred micro-meter, and the component was similar to the natural bone. In vitro study, there was no cytotoxicity in the particles, and stem cells differentiated or develop into preosteoblasts co-culture with particles. All the results indicated hydroxyapatite/ gelatin particles, which is osteoinductive bone grafts could use to bone tissue engineering for bone regeneration.

O.S.F.11.

A novel multilayer capsule as desensitizing agent for dental hypersensitivity

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Dental Hypersensitivity (DH) is a very common oral disease in Taiwan. According to the statistics, over 30% Taiwanese suffer the dental hypersensitivity and most of them have no cognition with the disease. However, the therapeutic of DH currently is filling the Dentin Pore with Calcium Phosphate Minerals (CPM), which is a mechanical filling and is not able to completely fit the dentin pore. In this case, we developed a new multilayer capsule for dentinal tubules filling. The material characteristics could not only evaluate the adhesion between capsules and dentin pore but enhanced the regeneration ability of dentin. The capsules filled in dentin pore could provide a microenvironment for dentin regeneration and avoid the stimulate. As the materials used in capsules fabricating are biodegradable, the capsules in dentin pore would degrade after dentin regenerate. We expect the capsules might be a long-term treatment for dental hypersensitivity.

O.S.F.12.

Electrospun silk fibroin composite scaffold for tendon repair

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Applying electrospun nanofibers to the regenerative medicine is an emerging field. Electrospinning is a remarkably simple, robust, and versatile technique capable of generating fibers with diameters down to the nanoscale. A number of approaches to fabricate scaffolds from electrospun nanofibers have been developed. We developed a new strategy for tendon repair by using electrospun silk fibroin (SF) composite scaffolds. The silk fibroin composite has 3D aligned silk fibers and high porosity. It also incorporated bioactive molecules to mimic the native tendon architecture and provide biomimic microenvironment. Experimental results demonstrated that primary tenocytes exhibited better native spindle-shaped morphology, cell infiltration and cell proliferation on the silk fibroin composite (tendon-ECM supplemented scaffold) compared with SF scaffold. In addition, SF/tendon-ECM scaffold in promoting injured tendon repair was more efficiency than SF scaffold in rat tendon injured model. All the results suggest silk fibroin composites can improve tendon tissue engineering to facilitate tendon repairing.

O.S.F.13.

BMP-2 and insulin delivered from plasma synthesis of carbon-based nanocarriers for bone regeneration

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Insulin and bone morphogenetic protein-2 (BMP-2) have been widely used in the fields of tissue engineering stimulate bone formation. The aim of this study was to determine whether Insulin and BMP-2 are involved in the homing of human mesenchymal stem cells (hMSCs) for bone regeneration and to innovate strategy of developing the carbon-based nanocarriers as drug delivery systems. We evaluate the properties of carbon-activated plasma-polymerized nanoparticles (nanoP3) can be synthesized in dusty plasmas with tailored properties; this includes an examination of how the different features of carbon nanocarriers affect tissue growth, how these properties to them might be leveraged in regenerative tissue therapies and how substances jeopardize their toxicity and biological interaction. In vitro, both Insulin and BMP-2 also have been confirmed to induce the homing of hMSCs. Observations based on ALP activity, type I collagen, OC gene expression, and mineralized formation were increased in the BMP-2 and insulin-treated group compared with control group. These findings support our hypothesis that the localized release of Insulin and BMP-2 promote bone regeneration.

O.S.G.1.

Vertical alignment of BaTiO₃ nanoparticles for enhanced piezoelectric performance

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In general, particle-polymer composite nanogenerators, in which the particles are dispersed in the polymer matrix, are less power generation than the oriented particle composite because of the particle randomness and a thick insulating polymer layer. If the nanoparticles are unidirectionally oriented in a polymer matrix to form a bundle of chains, the stress-induced energy can be more concentrated and easier transferred to the electrodes. Here, we present a facile electrical orientation method to obtain vertically aligned BaTiO₃ nanoparticle arrays in a polymer matrix for the improved piezoelectric power generation. Compared to the randomly dispersed nanoparticle composite, the vertically aligned BaTiO₃ array film has an excellent electrical output performance (ca. 3 V and 650 nA) and more than twice the transparency because of reducing light scattering by gathering BaTiO₃ nanoparticles. In addition to the improved piezoelectric performance and transparency due to the alignment of the nanoparticles, we found that the (200) diffraction plane of BaTiO₃ is transformed by an electric field. Furthermore, it is demonstrated that electric power generated by a mechanical micorloading of 4 μm denting depth using a nanoindenter equipment can pass through the polymer insulating layer in the well-aligned composite system but no the dispersed system.

O.S.G.2.

High performance photodetector using graphene barristor

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Graphene has attracted an enormous attention for various applications including transparent conducting electrode, photonic and electronic device applications. The enthusiasm for the electronic device applications has been substantially diminished as the research on the bandgap generation was not so fruitful and many of drawbacks such as self-heating and poor stability etc. were disclosed [1]. In case of photonic applications, small photoactive volume and high defect density of graphene limited the sensitivity of graphene based photonic devices. As the quality of CVD graphene and the device stability have been substantially improved by a vacuum transfer process and the integration processes adapted to the graphene [2, 3], a new approach combining the graphene with photoactive semiconductor is getting attention as a way to increase the photoresponsivity [4]. Furthermore, the extra band bending on graphene-semiconductor Schottky diode based photodetector resulted in very high photoresponsivity with a very low dark current. In this talk, the performance and operation mechanism of graphene-semiconductor Schottky diode based photodetector will be discussed.

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O.S.G.3.

High performance Al alloys development by simultaneous increasing strength and its trade-off properties

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The structural metallic alloys have been developing to get high strength and ductility, since structural metals require high strength for safety and high ductility for easy fabrication or high reliability. However, nearly all of fabrication ways for increasing strength must sacrifice ductility. For practical application of metal and alloys, many metal alloys should be under went the plastic deformation including cold and hot working to make appropriate shape, the increasing total sum of trade off relation, here, strength and ductility after plastic deformation is also very important. During plastic deformation, for example, hot working over the recrystallization temperature could not show effective strengthening, while, the cold working under the recrystallization temperature must show the drastic decrease of ductility.

While conducting the studies on aging and deformation behavior of Al alloys, we found that cold worked specimens at room temperature had higher strength and ductility than as-aged counterpart. This is extremely unique phenomenon since ductility drop is inevitably accompanied with cold working. For this, we deliberately utilized the non-conventional microstructure of discontinuous precipitate, which later turned into nano-lamellar precipitate, by over-aging.

O.S.G.4.

Improving the mechanical properties and wettability of metals by control interfacial characteristics: Study based on first-principles

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To get high strength and ductility in second-phase strengthening alloys, we introduce the novel methodology that combines the morphology control by conventional metallic alloy developing method including alloy design and thermo-mechanical process and the control of interface energy based on density functional theory (DFT) calculations. To adjust the interface energy between the precipitate and matrix through the additional element in Al-Zn alloys, we investigate the interface energy between Al matrix and Zn particles with and without Cu atoms using DFT simulations. The results show that Cu atoms prefer to reside near the Al/Zn interface and reduce the interface energy. Besides, the lattice misfit between the Zn precipitate and the Al matrix decreased drastically by additional Cu. Thus, we expect that Cu ions play a role of reducing the strain and interface energy between Al and Zn phases, leading to a small size and uniform distribution of Zn particles in Al matrix. As a result, we achieved simultaneous increase in strength and ductility in cast Al-Zn-Cu alloy.

Meanwhile, metal ultra-thin films have attracted much attention as a favorable candidate for flexible transparent conducting electrodes (FTCE) due to high electrical conductivity and good ductility of metals. However, the growth of metal nanoclusters induces high sheet resistance and low transmittance in FTCE. Much effort has been made to obtain the continuous metal ultra-thin films such as forming an alloy or introducing a surfactant layer. Here, we suggest that impurities at the initial state of metal deposition can modulate the interface between metal and substrate and suppress the growth of metal islands based on the first-principle calculations. Our simulations show that impurities such as oxygen (O) and nitrogen (N) prefer to reside at the interface between metal and insulator and on the surface of metal films. Analysis of the electronic structure of Cu films reveals that these impurities stabilize the Cu ions by lowering of non-bonding states of Cu at the interface and surface. Thus, O and N impurities can reduce the interface and surface energies, leading to the enhancement of the wettability of metal films. Finally, we confirm experimentally that these metal ultra-thin films with impurities show good conductivity and transmittance.

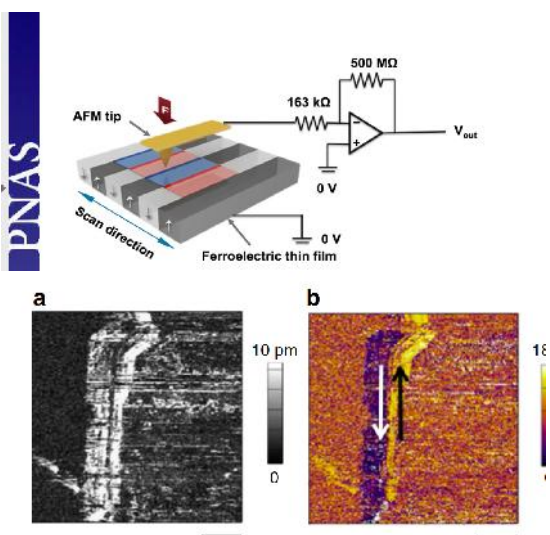
O.S.G.5.

Hybrid materials imaging initiative: past, present and future

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Renaissance established the scientific method, a system by which both observation and reason are employed in order to test the proposed mechanisms for planetary motion. Descartes promoted science by first questioning everything and then building up a theory based on sound observational evidence. Materials science is no exception in the sense that visualization of order parameters or materials properties provides the solid ground on which materials theory and design can flourish. Here I will present our current research thrusts to visualize polarization, electrical charges and ionic transport to understand the emerging phenomena on materials surfaces as well as interfaces and how they help design future memory and energy storage devices [1,2]. Last but not least, I will discuss the vision of materials imaging initiative.



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O.S.G.6.

Circular double-patterning lithography using a block-copolymer template and atomic layer deposition

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One-dimensional (1-D) nanostructures have attracted much attention for nanoscale electronics, photonics including electron transport channel, electrode in sensors, photocatalyst. Owing to the high surface-to-volume ratios and structural uniqueness, the 1-D nanostructures can present excellent electron transport efficiency and the significantly reduced electron-hole recombination. Herein, we present a novel and feasible methodology is developed to fabricate well-ordered, freestanding 1D n-ZnO/p-Si nanotube (NT) and nanorod (NR) arrays via double patterning technology with block copolymer (BCP) self-assembly, atomic layer deposition (ALD), and inductively coupled plasma (ICP) dry etching. In order to obtain the highly ordered nanotube pattern, we employed a self-assembled Si-containing poly(styrene-4-(tert-butyl)dimethylsilyl)oxystyrene (PS-b-PSSi) BCP on SU-8/p-Si wafer as a template. After n-ZnO formation on the self-assembled BCP template by ALD, ICP etch-back process was performed to produce well-defined n-ZnO/p-Si nanotube arrays with diameters of 52 nm (outer) and 25 nm (inner) using the huge difference of etching rates between ZnO and Si. We also successfully obtained an n-ZnO/p-Si nanorod pattern by precisely controlling the ALD cycles and ICP etching time. The electrical property was measured by conductive atomic force microscopy (C-AFM), showing a typical rectifying behavior of diode. This simple and useful approach provides a very convenient route to fabricate high-density nanodiode patterns without using high-cost photolithography.

O.S.G.7.

Various nanoarchitectural hybrid materials for high-performance supercapacitors

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Supercapacitor known as electrochemical capacitor has attracted considerable interest over the past few decades, due to their valuable properties of the rapid charging/discharging, long cycle life, good cycle stability, high power density and the ability to deliver up to ten times more power than conventional batteries. Here, we present high-performance supercapacitor with various capacitive materials, the nanoarchitectures, and the energy storage mechanism. The performance of supercapacitor electrode depends on the interactive site with an electrolyte, the nanostructural morphologies, and the high conductivity rather than the intrinsic nature of the nanomaterials. We introduce the electrochemical performances and the various morphologies of nanomaterials fabricated according to the processing methods and materials. Those fabricated nanoarchitectures are of nanocubes, nanorods, nanoplates, nanowires, nanospheres, etc. We also cover future research plans and challenges for the next generation of high-performance supercapacitors.

O.S.G.8.

High-performance hybrid energy storages enabling ultrafast charging and high energy density along with robust cycle life

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Energy storage devices for future hybrid plug-in electric vehicles (EVs) and pure EVs must satisfy more challenging standards in energy and power densities over long repeated charge/discharge cycles. Currently, the dominating electrochemical energy storage remains on a lithium ion battery (LIB) with high energy density although an electrochemical capacitor (EC) with high power density along with robust cycle life has great potential for many energy storage devices. Meanwhile, it was found that the sole usage of a LIB or an EC could not give simultaneously high energy and power densities because of its complementary ion storage mechanism. Therefore, hybrid electrochemical energy storages are of great interest as they have the potential to achieve both high energy and power densities. Herein, we propose high-performance hybrid full-cell capacitors on a new class of paradigm structures for anode and cathode electrodes. These results support that assembling the cathode with many metal encapsulated anode structures could pave a new route to realize the hybrid full-cell energy storage devices requiring both high energy and power densities over long repeated charge/discharge cycles along with excellent rate capability, in addition to design a new class of high-performance energy storage structures.

O.S.G.9.

Thermal management by electrochemical process: thermoelectric and radiative cooling materials

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Since the birth of electronic technology, the heat flux generation from electronic devices has increased and this trend is expected to continue. There are two solutions; active and passive cooling techniques, to maintain the device temperature without performance degradation. Active cooling technology integrated with electronic devices is very efficient in electronic heat management applications. Due to the size restriction, the thermoelectric cooler (TEC) is a candidate. For passive cooling techniques, radiation should be controlled rather than conduction and convection. For thermoelectric materials, we tailored nanocomposite embedded structure in Bi-Te and Sb-Te films, resulting in allowed the realization of intriguing TE performance based on interfacial energy-barrier scattering. The TE performance of nanocrystalline films is optimized by tailoring the energy band offset employed in the energy-filtering mechanisms. In addition, for radiative cooling, we fabricated Porous metal sheet by electrochemical process in order to control heat transfer or/and radiation heat transfer of metal material. The pores of porous structure can inhibit the transfer of heat, resulting the reduced thermal conductivity. And porous metal structure were synthesized by stacking polystyrene (PS) beads on Au/Ti/Si substrate by using spin coating, followed by the electrodeposition of Ni. Porous Ni films were obtained by the resolving PS beads in water. The thermal property of porous Ni films was $47 \text{ W}\cdot\text{m}/\text{K}$, which is more than 2 times smaller than the bulk counterpart ($102 \text{ W}\cdot\text{m}/\text{K}$). The more details will be presented.

O.S.G.10.

Solution plasma synthesized carbon-supported hybrid catalysts for energy converting systems

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Carbon-based materials have been widely utilized as the electrode materials in energy conversion and storage technologies, such as fuel cells and metal–air batteries. In these systems, the oxygen reduction reaction is an important step to determine the overall performance. A novel synthesis route, named solution plasma process, has been recently utilized to synthesis various types of metal-based and hetero-atom doped carbon catalysts. Mostly importantly, this innovative method can fabricate N-doped carbon matrix, as well as control the C-N bonding states by choosing the structure of the original precursor without annealing post-treatment. This review summarized cutting-edge technologies involving synthesis and modeling of carbon-supported catalysts synthesized via solution plasma process, followed by current progresses on the electrocatalytic performance of these catalysts. Herein, provides the fundamental and state-of-art performance of solution plasma synthesized electrode materials, as well as the remaining scientific and technological challenges for this process.

O.S.G.11.

3-dimensional hybrid nanostructures: novel fabrication strategies and applications

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Despite their high demand and various promising applications, the fabrication of 3D nanostructures is not straightforward. We suggest that nanotransfer printing (nTP) may be a more practical solution controllably build 3D nanostructures. An nTP technique is usually composed of several steps - preparation of nanostructured elastomeric replica, deposition of functional materials, and transfer of functional nanostructures. The nanostructures can be transferred onto other substrates by contacting the mold on the surface of the receiver substrate. To overcome the issues of resolution limit (typically several tens of nm) and low transfer yield of conventional nTP, we developed and demonstrated that solvent-assisted nanotransfer printing (S-nTP) can controllably generate extremely fine (down to sub-10 nm) functional nanostructures with excellent transfer yield (~100%). The excellent uniformity of the printed nanostructures is another advantage of nTP, as it makes it possible to obtain highly uniform and reproducible 3D nanostructures composed of different materials. In this talk, I will introduce several applications of 3D hybrid nanostructures such as 3D Pt, Au, and Ir nanocatalysts with outstanding catalytic activity and durability and plasmonic nanostructures for highly efficient surface-enhanced Raman spectroscopy (SERS).

O.S.G.12.

Virus: The Next Generation Material

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Evolution by natural selection from the ancient past creates numerous nanomaterials, of which only the best is selected and propagated in generations of proteins and genes. Proteins and genes coordinate the spatial and temporal control of the synthesis of organic and inorganic nanomaterials, and generally form a hierarchical structure with specific functions. Moreover, further modification of the structure to manipulation capability was a key component of evolutionary pressure by natural selection. However, most of the nanostructures in nature are stereostuctured and poorly formed, sometimes arranged at low levels, making it difficult to imitate very accurately. Our M13 bacteriophage-based self-assembly approach can be good candidate to overcome those obstacles. M13 bacteriophages are very beneficial for self-assembly. M13 bacteriophage can be mass-replicated with a specific *E. coli* as a host, so that an almost perfectly uniform monomer can be mass-produced easily and inexpensively. In addition, it is possible to express various chemical functional groups on the surface protein of M13 bacteriophage through genetic engineering technology. Due to above-mentioned advantages of the M13 bacteriophage, we are conducting research on application to various sensors, full color pixels and piezoelectric nanogenerators.^{1,2,3}

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O.S.I.1.

Anion-mediated photophysical behaviour in a C₆₀ fullerene [3] rotaxane shuttle

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The realisation of functional molecular machines is heralding an era of nanotechnology where researchers can wield unprecedented control over molecular components for application in fields as diverse as artificial photosynthetic devices and nanomedicine. The unique structure and properties of fullerenes also offer bountiful opportunities for application in these fields amongst others. To this end, we have used anion templation to construct a multi-station [3]rotaxane molecular shuttle containing a central fullerene moiety. Mediated by the nature of the counter anion, the rotaxane's macrocycles reversibly shuttle between stations along their half of the axle track. Crucially, the macrocycles are functionalised with electron-donating ferrocenyl, whilst electron-accepting moieties are incorporated into the axle component. Thus, we carried out a suite of photophysical and electrochemical studies to probe the system's photophysical behaviour. A striking visible fluorescent response is seen in the presence of chloride ions suggesting its utility as a novel sensor.

O.S.I.2.

Synthesis and densification of monolithic nanocrystalline SiC ceramics

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Cubic SiC nanopowder synthesis by sol-gel process with the average grains size of 15 nm was densified by using high-pressure “anvil-type with hollows” apparatus. Mechanical properties of the samples (hardness, toughness) were determined and a correlation between the final microstructures and the mechanical behavior was established. Increasing applied pressure reduces the pore density and replaces free surface by grain boundaries. The best result was obtained at pressure of 4 GPa. Relative high densification was obtained for temperatures at 1500 °C. Fully densified sample (> 99%) was obtained at a sintering temperature of 1900 °C for only 60 s. This sample exhibits micro-hardness and Young’s model of elasticity of 330 GPa and 450 GPa, respectively.

O.S.I.3.

First principles investigations of structural, electronic, elastic and mechanical properties of barium sulfide from standard to extreme high pressures

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Barium sulfide (BaS) is an important precursor to other barium compounds with applications from ceramics and flame retardants to luminous paints and additives, and recent research shows potential technological applications in advanced electrical and optical devices. Pressure induced phase transitions of barium sulfide has been investigated. Novel BaS modifications have been calculated on ab initio level using Hartree-Fock, DFT and the hybrid B3LYP functional. We predict metastable BaS polymorphs which have not-yet been observed in the experiment or previous calculations. We investigate the electronic, mechanical, elastic, vibrational and thermodynamical properties of BaS and our calculations were in very good agreement with previous experimental and theoretical observations. Furthermore, we investigate the electronic properties of experimentally known structures, as well as novel predicted modifications of BaS at extreme pressure conditions. In this way, we address new possibilities of synthesizing BaS and possible band gap tuning which can have great applications in opto-electrical technologies.

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O.S.I.4.

Tuning of the stoichiometry of PLD grown SrO thin films via fluency optimization

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In recent years the integration of functional oxides with silicon has attracted significant attention. However, achieving epitaxial integration is a challenging task due to silicon reactivity and dissimilar properties with respect to oxides. Nowadays, state-of-the-art approaches rely on simultaneous deoxidation and passivation of a silicon surface where SrO- and Sr-based buffers have proved highest chemical and structural compatibility. An important characteristic of buffer layers both from the perspective of their quality and subsequent growth of functional oxides is stoichiometry. In the present work we have used fluency control as an optimization route for PLD growth of stoichiometric SrO thin films in 0.012 mbar O₂. X-ray reflectivity (XRR), X-ray diffraction (XRD), reflection high energy electron diffraction (RHEED) and Rutherford backscattering spectrometry (RBS) have been used for assessment of the atomic composition and crystallographic properties. It was found that fluency increase leads to gradual increase of SrO layer thickness. The density of the SrO layers, obtained by XRR, was used for calculation of areal density which enabled determination of atomic composition of the layers. The results show that the best crystallinity was obtained for the most stoichiometric film and that the strontium amount varies from 0.62 to 0.41 at. % for fluency between 1 and 3 J/cm².

O.S.I.5.

Conduction in calcium containing LaAlO₃ solid solutions prepared via ball milling

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In this study, the effects of Ca ions substitution on the densification, microstructure, and physical properties of La_xCa_{1-x}AlO₃ ceramics were investigated. The results indicate that doping with Ca ions not only enhances the densification but also promotes the grain refinement of La_xCa_{1-x}AlO₃ ceramics. On top of that the XPS spectroscopy revealed the real positions of Ca ions in the structure of synthesized perovskites. The conduction of La_xCa_{1-x}AlO₃ ceramics was significantly raised by Ca substitution. In this paper the electrical properties of synthesized samples are discussed in connection to their structural properties.

O.S.I.6.

Novel reactive infiltration process for production of fine grained Fe-Al intermetallics

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FeAl intermetallics are potential candidates to substitute Cr/Ni based (stainless) steel parts used in high volume end consumer products such as in the lock industry, electronics, process industry and automotive industry, in order to reduce consumption of the critical raw materials. Their impact would therefore be much higher if a cost effective industrial process would be available, that allows manufacturing complex 3-D geometries of almost unlimited shapes from small grain size (0.1-5 μm) high ductility material. In this work a novel processing method has been investigated. It involves reactive infiltration of liquid Al and its alloys into the porous Fe preforms with the aim to obtain fine grained Fe-Al. Initially, preliminary DTA experiments were conducted to analyse the effect of the melt temperature and composition on the thermodynamic effects of reaction between the preform and the melt. It was found that the pure Al melt interacts with Fe porous preform intensively with high exothermic effect, thus causing a great risk of melting of the preform or can lead to formation of rather porous material. In the next step, a pressure - assisted technique i.e. suction casting was applied. A series of experiments of molten Al and FeAl₂ melt were infiltrated into a porous Fe-based preforms produced by three different methods (selective laser melting (SLM) and Kochanek-process (KE) and Metal Injection Melting (MIM)). The design of the device for a full preform infiltration and further process parameters tuning (e.g. suction pressure) were the main challenging issues. As a result, the successfully infiltrated preforms were obtained and a feasibility of the process was proven. To determine intermetallic phases, X-ray diffraction (XRD), scanning electron microscopy and (SEM) and electron backscattered diffraction (EBSD) were applied. The extend of preform infiltration and intermetallic formation process was found to be dependent on the processing parameters such as the suction pressure as well as on the perform and melt temperatures. Follow the infiltration, a post treatment process was performed to impose a phase transformation into the ultra-fine desired FeAl phases.

O.S.I.7.

Properties of composite parts manufactured with help of LATP technology

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The current growth of composite parts application in various industries, creates the need for developing manufacturing solutions that would increase productivity at a lower cost, but at the same time yield products with superior properties. The process of setting laser automatic tape placement (LATP) shows great potential for efficient production of large composite structures. However, there are uncertainties about the mechanical performance of the final product that are associated with the defects caused by the process. During manufacturing process, laminate is subjected to several heating and cooling cycles which will result in residual stresses inside the final laminate. Heating and cooling are affected by many parameters such as layup speed, temperature of laser power, layup sequences, ambient temperature etc.

In this paper, some of the defects that may arise in the process will be detected. Experiments are conducted on thermoplastic composites with different thermoplastic matrices. The results show that the LATP process is very effective in heating and consolidating the surface of the layers. The results have shown that the mechanical properties depend on parameters for LATP technology. The experimental research was performed at Mikrosam AD from Prilep on their LATP machine, whereas three-point bending test and short-beam strength test select the best variable combination. Tests have revealed minimal percent of voids in the manufactured laminate and good interfacial properties of the laminate.

O.S.I.8.

High pressure torsion - a rapid tool for the production of high ZT skutterudites

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It is well known that severe plastic deformation (SPD) introduces defects, enhances the dislocation density and refines the grains to nano size. This way the figure of merit, ZT, of ball-milled and hot pressed skutterudites could be enhanced. In this paper a new method to produce skutterudites is designed. SPD via high-pressure torsion (HPT) at elevated temperatures and in argon atmosphere was used to directly consolidate skutterudite powders into a solid disc. ZTs, of these samples are in the range of those produced via high-energy ball milling and hot pressing; thus time and energy consuming ball milling and hot pressing can be avoided. Synchrotron measurements from room temperature to 550°C provide insight in the changes of grain size and dislocation density; SEM and TEM investigations reveal the modifications of this HPT produced material.

Hardness and elastic moduli, due to grain refinement, are higher than for the reference sample, compacted via hot pressing.

With already existing large HPT facilities as well as industrially produced skutterudite powders, a new fast and cheap mass production of skutterudite legs is envisaged.

O.S.I.9.

Advanced concepts for processing integral-skin multilayered cellular polymeric composites

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Rotational molding, despite its very lengthy processing cycles and intensive energy consumption, proved to be the best suited method for the manufacture of very large and complex-shaped single-piece hollow articles. A patented (US 8,628,704 B2) melt extrusion-assisted rotational foam molding process, referred to as Rapid Rotational Foam Molding, advantageously decouples the step of in-mold melting and shaping of the plastic from its foaming step. By exploiting and building on this unique synergy between traditional rotational molding and the extrusion foaming process it becomes possible to explore a pioneering attempt for implementing both chemical and physical blowing agents in rotational foam molding, individually or in combination. This concept provides unprecedented possibilities for seamlessly producing integral-skin rotationally molded cellular composites that not only can include foamed layers or core morphological structures of two different kinds that have been generated by two different polymeric resin grades using two different kinds of blowing agents by design, but also can be fully encapsulated by a solid skin layer made of a resin of a third kind. Thereby, a novel class of ultra low-density eco-friendly cellular polymeric composites with dramatically reduced foam cell sizes that will possess currently non-achievable properties can be manufactured.

O.S.I.10.

Interaction between flow and faceted crystal growth

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The growth of faceted crystals occurs often in nature and industry, involving always the presence of flow. Insulin, silicon, pyrite, quartz, gallium are only few examples of faceted crystals. The present paper presents a numerical model for the simulation of faceted crystal growth, taken into account the incidence of flow. The growth in faceted crystals is the results of interface kinetics and flow hydrodynamics. This model was applied to the Fe_2Al_5 faceted crystal, presenting a hexagonal crystal shape. These faceted crystals (Fe_2Al_5), so called top dross particles are forming during the production of Zn coated steel sheets (Galvanizing industry). In the galvanizing industry their occurrence is a problem and therefore it should be limited. Comparison was made between simulation and experimental observation of crystal shape. The growth was found to be the result of the coupling between the interfacial kinetic and the hydrodynamic induced kinetics.

O.S.I.11.

Tool geometry effect on microstructure and properties of friction stir welded 5083 and 7075 aluminium alloys

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Friction stir welding is a solid-state joining process, which actually is developed to joining dissimilar materials. One of scopes of future research on dissimilar friction stir welding is selection of design of tool for the joining. The tool forms a principal element in the process. The tool functions are heating of workpieces, moving the material to produce the joint and also hampering outflow of the plasticized material. Thus the tool plays a major role in heat generation, material flow and formation of weld. This research addresses the microstructural and mechanical characterization of 5083-H111 and 7075-T651 friction stir welds depending to tool geometry. All used tools consisted of a spiral shoulder, but a different pin design: Triflute, Whorl or threaded taper. This investigation shows that the tool geometry has a clear influence on the degree of intermixing of alloys joined and the extent of the weld area.

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O.S.I.12.

Development of highly piezoelectric coaxial fiber for energy harvest by using thermal drawing and post-process towers

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In this study, highly piezoelectric coaxial fibers with PVDF-based polymer was fabricated by using thermal drawing and post-process towers. Polycarbonate (PC) mixed with carbon black (CB) nanoparticles was used as the flexible core electrode composite. A cylindrical preform made of PC/CB composite core and PVDF-based polymer sheath is thermally drawn to reduce the diameter of the macroscopic preform into the order of several hundreds of microns. The drawn fiber is annealed at 140 °C for 24 hours to increase their crystallinity. Then, the annealed coaxial fiber is angularly polarized by in-situ corona discharge poling process with the post-process tower, and AgNW was coated on the poled coaxial fiber as the outer electrode. The developed highly piezoelectric coaxial fiber can be used in wide range of flexible electronics applications, especially in wearable energy harvest fabrics if we weave or knit textiles with the developed highly piezoelectric coaxial fibers.

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O.S.I.13.

Fabrication and application of polyvinylidene fluoride (PVDF) fabric sensors for in situ health monitoring of fibrous composite structures

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There are many widely used conventional strain or impact sensors like fiber Bragg grating sensors (FBG sensors) and strain gauges but they have some critical drawbacks such as limited sensing area, intrinsic brittleness and so on. They are easy to break when they are applied to some harsh conditions and curved surfaces. On the other hand, electroactive polymer (EAP) films are soft and flexible, therefore they can be easily applied to many structures for measuring impact and vibration. Even the film sensors they are hardly to be applied to excessively curved surfaces. In this paper, fabric type sensor composed of a polyvinylidene fluoride (PVDF) was designed and fabricated for checking feasibility of real-time in situ health monitoring of composite structures such as wind blades. Electro-mechanical characteristics was investigated and its sensing performance was evaluated by experimental protocol.

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O.S.II.1.

Epitaxial $\text{Fe}_3\text{O}_4/\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ thin film heterostructures for spintronic devices

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Highly spin-polarized oxides as Fe_3O_4 (magnetite) and $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ (LCMO, a mixed-valence manganite) are of special interest for the design of new spintronic devices.

Bulk Fe_3O_4 experiences a metal-to-insulator transition at $T_v=120$ K, while LCMO shows an insulator-to-metal transition close to room temperature (T_c). Three different coupling states are foreseen in a $\text{Fe}_3\text{O}_4/\text{LCMO}$ heterostructure (metal/insulator above T_c , metal/metal between T_c and T_v and insulator/metal below T_v). The ability to tune the conductivity coupling of the bilayer gives the unique possibility to design transport based devices working simultaneously in perpendicular and parallel configurations.

We report the epitaxial growth of thin $\text{Fe}_3\text{O}_4/\text{LCMO}$ bilayers by PLD on SrTiO_3 (001) and (111) substrates. LCMO was crystallized at 800C under 1 bar of flowing oxygen, while Fe_3O_4 was deposited at different temperatures to artificially tune its morphology from homogeneous to nanostructured.

The experimental conductivity of the heterostructures reveals the overimposed transitions occurring in magnetite and manganite individual layers, identifying the three coupling states. A correlation between the lattice (structure and morphology), transport and magnetic coupling between layers will be presented.

O.S.II.2.

Fe₃O₄-based heterostructures for semiconductor spintronics

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Magnetite is predicted to be half metallic, which is translated in a 100% spin polarization at the Fermi level. The integration of Fe₃O₄ films on silicon is of huge interest for semiconductor spintronics. However, the functionality of the system is strongly influenced by the structural and morphological properties of the system, especially regarding the interface quality. Because of this it is fundamental to understand the interaction between the silicon surface and the deposited films and to develop new strategies for the preparation of high quality heterostructures without formation of mixed layers at the interfaces that can hinder the spin injection in Silicon. We report on different Fe₃O₄-based heterostructures prepared through different buffer layers, concretely Fe₃O₄/SiO₂/Si and Fe₃O₄/SrTiO₃/Si. The synthesis parameters were optimized in order to obtain single phase magnetite films. Strong efforts were made to characterize the buried interfaces and understand the interaction between magnetite, silicon and the buffer layer.

O.S.II.3.

Synthesis of TiO₂ -WO₃ composite nanofibers by electrospinning for application in photocatalysis and fuel cells

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Titanium dioxide and tungsten oxide nanocomposites were prepared using electrospinning and annealing, and their features and applications were studied in detail. The aim of the study was to fine tune the properties of nanocomposites by using different proportions of titanium dioxide and tungsten oxide precursors. For the nanofiber synthesis, polyvinylpyrrolidone, titanium(IV)- bis-lactato-bisammonium dihydroxide and ammonium metatungstate were dissolved in a mixture of water, acetic acid and ethyl alcohol. The nanofibers formed after electrospinning were calcined by heating at a rate of 5°/min until 600°C to remove the polymer component. The titanium dioxide and tungsten oxide nanocomposites were characterized using TG/DTA-MS, XRD, SEM-EDX, TEM, FTIR, and Raman. The as-synthesized nanomaterials were studied for their application in photocatalysis and fuel cell electrodes.

O.S.II.4.

The new integrated process flow sheet for production of Fe-NiAl composite microgranules for the additive technology.

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The fabrication of complicated items by conventional methods including casting, machining, spark erosion, thermo-mechanical treatment act. is labor and material consuming process. The challenge here can be solve by the additive technology (AT). The most promising kind of AT is SLS and SLM (selective laser sintering/melting) that requires starting materials in the form of spherical granules (micro granules) with strictly defined size and morphology (spherical shape). In this communication, we will present some recent results for obtaining the Fe-NiAl composite micro granules for AT by integrated technique including:

- synthesis of Fe-NiAl cast layer consumable electrodes (CLCE) by combined use SHS metallurgy and subsequent electrovacuum remelting and casting into steel pipes,
- production of Fe-NiAl composite microgranules of CLCE by centrifugal plasma sputtering (CPS).

Process-dependent parameters have been worked out and optimized. The structural and phase composition of electrodes and micro granules have been investigated.

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O.S.II.5.

Reducing the deformation temperature of AZ31 magnesium alloy through CCT approach

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Severe plastic deformation (SPD) is a term used for a group of different deformation techniques to apply a significantly high amount of deformation on the material and thereby, reducing the grain size towards submicron and nanoscale. In order to achieve ultrafine grain structure, the deformation must be conducted below the recrystallization temperature and repeated for few times. However, due to the lack of slip systems, room temperature deformation of Mg alloys is not possible and leads to cracking and failure of the samples which prohibits repeating the process. SPD processing of these alloys above recrystallization temperature results in minimum expected achievement in terms of grain refinement. In this study, copper casing tube (CCT) approach has been used to increase the workability and thereby, reducing the working temperature of AZ31 magnesium alloy. Various casing thicknesses have been utilized to find the optimum thickness. It is found that the sample of AZ31 alloy can be deformed at 175 °C with no surface cracking. This reduction in deformation temperature results in reducing the recrystallized fraction of the samples and the average achieved grain size. In addition, an enhancement in strength and ductility of the sample is observed.

O.S.II.6.

Eco-technology: the application of calcined waste mine overburden clay materials as cement substitution

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Cement manufacturing is a major source of greenhouse gases and it causes more than 5 percent of CO₂ production. Few studies tried to solve the emission production by the cement industry concentrating on intervention of the other affordable and attainable materials such as clay. In fact, an ordinary way to reduce the CO₂ emission attributed to cement production is to substitute a large portion of Portland clinker in cement to create blended cements, or replace an OPC in concrete mixture with proper supplementary cementing materials (SCM). Recently, the usage of the industrial by-products such as fly-ash and blast-furnace slag as substitution was widespread, but the amount of these materials is significantly less than the cement production and industrial demands. So, alternative sources like calcined clay were considered by the manufactures. In this research, 2 types of clayey mine overburden materials (M&T) are used as partial cement substitute. "M" contains proper amount of clay while "T" contains carbonates. Each of these clays have been used as cement substitution and their compressive strength were found acceptable. By mixing these two clay and calcination of them, we have tried to intensify the compressive strength of calcined clay cement. To evaluate the raw materials, several types of analyses have been performed. First, the potential reactivity of normal clays is analysed by the thermo-gravimetry method to identify the optimum dihydroxylation temperature. Then, the phase analysis has done by means of X-ray diffractometer (XRD) while the scanning electron microscopy (SEM) photos elaborate phases present in the raw material. The calcined clay cement paste samples have been prepared for compressive strength measurement and the results shows the quiet acceptable compressive performance of the provided mixture. The results which is obtained from the compressive strength tests, shows higher strength performance of the samples. It means that the mine overburden clay type powders could be a proper substitution for the cement in term of cement paste or concrete. Also, it is found that it is possible to intensify the compressive strength of the sample by mixing two types of them to compensate the lack of effective phases which could affect on reactivity.

O.S.II.7.

Structural and electrochemical study of lithium iron (II) pyrophosphate

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Lithium iron(II) pyrophosphate, $\text{Li}_2\text{FeP}_2\text{O}_7$, attracts attention of researchers for application as a cathode material in rechargeable lithium batteries. $\text{Li}_2\text{FeP}_2\text{O}_7$ has somewhat higher voltage than commercial LiFePO_4 (3.5 and 3.4 V, respectively), thus enables higher energy density, and also provides the possibility of two-electron reaction during intercalation. Within this study, pristine $\text{Li}_2\text{FeP}_2\text{O}_7$ and its composite with carbon $\text{Li}_2\text{FeP}_2\text{O}_7/\text{C}$ were synthesized, with the carbon being formed by the pyrolysis of organic precursor *in situ* during formation of $\text{Li}_2\text{FeP}_2\text{O}_7$ at high temperature. The polymer of methylcellulose was used as carbon source because of its ability to reversibly, depending on temperature, dissolve or gel in water. The structural, electrical and electrochemical characteristics of prepared powders were investigated by means of X-ray diffraction analysis, Mössbauer spectroscopy, impedance spectroscopy and galvanostatic charge/discharge testing. The results imply that *in situ* formation of carbon alters lattice parameters, decreases crystallite size, and facilitates lithium ion intercalation/deintercalation processes.

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O.S.II.8.

Li₄Ti₅O₁₂. Promising anode material for Li-ion batteries synthesized via mechanochemically assisted route

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Nanocrystalline spinel phase Li₄Ti₅O₁₂ (LTO) was synthesised via a solid state route by calcining a precursor mixture at 600 °C. The precursor was prepared from a stoichiometric mixture of TiO₂ nanoparticles and an ethanolic solution of Li acetate and activated by ball-milling. The structure of synthesized sample was investigated by X-ray diffraction, Raman and ⁶Li MAS NMR spectroscopy. The capacity of our optimised material (142 mAh/g) is superior to that of commercially available spinel, despite the considerably smaller BET-specific surface area of the former (S_a = 1.4 m²/g). The superior properties of our material were also demonstrated by galvanostatic charging/discharging. Moreover, it is shown that enhanced surface area clearly influences electrochemical properties of LTO. From these observations, we conclude that the presented low-temperature solid state synthesis route provides LTO with improved electrochemical performance.

O.S.II.9.

CTAB- and pluronic F-127-assisted microwave processing of ZnO particles with modified morphology and optical properties

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Zinc oxide-based materials have a great potential to be applied as photocatalysts in the processes of removal of organic and biological pollutants from drinking and wastewaters. A major drawback of ZnO as visible-light absorber is a band energy gap of 3.37 eV, which restricts the material to absorb UV light only. This drawback can be overcome by modifying the optical absorption properties of zinc oxide particles. Different approaches have been applied to modify the visible light photocatalytic activity of ZnO materials: (1) metal and nonmetal ion doping, (2) hydrogenation, (3) the incorporation of crystalline defects in the form of vacancies and interstitials, (4) the modification of particles morphology and surface topology, etc.

In this study we investigated the influence of different surfactants on the morphology, optical properties and functionality of ZnO particles. Two different surfactants were employed during microwave processing of ZnO particles, cetyltrimethylammonium bromide (CTAB) as cationic and Pluronic F-127 as non-ionic one. The crystal structure and phase purity of the ZnO particles were determined by X-ray diffraction and Raman spectroscopy. Effects of the surfactants on particles morphology and texture properties were observed with field emission scanning electron microscopy (FE-SEM) and nitrogen adsorption-desorption isotherm, respectively. The optical properties were studied using UV-Vis diffuse reflectance and photoluminescence (PL) spectroscopy. Functionality of ZnO particles was studied due to their photocatalytic and electrochemical activities. Photocatalytic activity was examined *via* decolorization of methylene blue under direct sunlight irradiation. Electrochemical behavior of the ZnO samples as anode material was evaluated by linear sweep voltammetry in Na₂SO₄ electrolyte; the oxygen evolution kinetics were determined and compared.

O.S.II.10.

Synthesis of tribological WS₂ powder from oxide precursor

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This paper describes two stages process for synthesis of WS₂ powder on selected temperatures by using WO₃ as a precursor. WO₃ submicron particles were prepared by ultrasonic spray pyrolysis of ammonium meta-tungstate (AMT) at 650°C in the air. WS₂ particles were obtained by sulfurization of the WO₃ particles in presence of additive K₂CO₃ in a nitrogen atmosphere, first at lower temperature (200°C) and followed by reduction at higher temperature (900°C). HSC Chemistry software package 9.0 is used for the analysis of chemistry and thermodynamic parameters of the processes for synthesis of WS₂ powder. The samples of WO₃ and WS₂ powders were characterized by X-ray diffraction (XRD) measurements. The morphology and composition of these samples were examined by scanning electron microscopy (SEM) combined with energy dispersive X-ray analysis (EDX).

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O.S.II.11.

Thermochemistry aspects of mechanochemistry activation of the flotation processes

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The energy that holds together atoms in molecules is a significant value that is measured in tens and hundreds of thousands of joules per mole substance. These molecules, which built most of the world available to us, held together other, much weaker forces. Their energy is measured only in tens of joules per mole, values that we are sometimes prone to neglect by comparing them with the aforementioned. Cohesive pressure is the phenomena in condensed phases and is associated with intermolecular forces. Driving forces in the process of mass transfer of substance in multiphase disperse systems, driven by molecular forces, which resultant is formation of concentration and temperature gradient. Flotation process is carried out in the pulp, apropos, dispersed system which is in dynamic equilibrium with the energy of mixing. Selective forming of surface alloys on minerals in the pulp has a diffusion character is service of mass transfer. Separation processes, liquid-liquid, are actually processes of treating the mineral raw material by flotation contributing to a greater or lesser extent, distribution of useful minerals. The paper presents the process ore flotation Veliki Krivelj and statistically analyzed the mechanism of action the collectors xanthate and aeropromoter.

O.S.III.1.

CaP that kills: the intrinsic antimicrobial effect of calcium phosphate nanoparticles

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One of the main goals of materials science in the 21st Century is the development of materials that can substitute for traditional pharmacotherapies, especially for antibiotics, whose overuse has led to the promotion of microbial resistance. Here we will report on the intrinsic antibacterial effect of amorphous calcium phosphate (ACP) and hydroxyapatite (HAp) against both Gram-positive and Gram-negative bacteria as well as on the synergistic effect that these two calcium phosphate (CaP) phases have when delivered in combination with antibiotics. To determine the antimicrobial mechanism of action of CaP nanoparticles we examined both biological and physicochemical parameters such as intracellular free calcium levels due to nanoparticle solubility; diffusivity and electrostatic attraction to the bacterial cell surface; particle size; genotoxicity; cell membrane damage; and efflux pump inhibition. We show that the antimicrobial effects exist not only for laboratory strains of bacteria, but for clinical, multidrug resistant isolates as well. The results of this work illustrate the potential of CaP nanoparticles as a stand-alone antimicrobial therapy in the face of increasing bacterial multidrug resistance.

O.S.III.2.

Cell-selective toxicity of hydroxyapatite-chitosan oligosaccharide lactate particles loaded with a steroid cancer inhibitor

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The applicative potential of synthetic calcium phosphates, especially hydroxyapatite (HAp), has become intensely broadened in the past 10 years, from bone tissue engineering to multiple other fields of biomedicine. Hybrid systems based on nano hydroxyapatites (HAp) are the subject of numerous studies in preventive and regenerative medicine. HAp nanoparticles coated with bioresorbable polymers have been successfully used as fillers, carriers of antibiotics, vitamins and stem cells in bone tissue engineering, etc. In this study we utilize an emulsification process and freeze drying to load the hybrid system made of nano HAp particles coated with chitosan oligosaccharide lactate (ChOSL) with two different but similar steroid derivatives: 3 -hydroxy-16-hydroxymino-androst-5-ene-17-one (A), C₁₉H₂₇NO₃ and 3 , 17 -dihydroxy-16-hydroxymino-androst-5-ene (B), C₁₉H₂₉NO₃. The cell-selective toxicity of HAp particles coated with of A- or B-loaded ChOSL was examined simultaneously on the following cell lines: human breast carcinoma (MCF-7, MDA-MB-231), human lung carcinoma (A549) and human lung fibroblasts (MRC-5), using dye exclusion (DET) and MTT assays.

¹H NMR, ¹³C NMR and high-resolution time-of-flight mass spectrometry (MS) techniques confirmed the intact structure of the derivatives A or B. FT-IR, XRD, DTA, TGA and DSC techniques confirmed the drug loading process of sterioide (A or B) in core-shell particles based on nano hydroxyapatite. Atomic force microscopy and particle size analyses were used to confirm that the particles were spherical with sizes between 80 and 240 nm. The measured values of electrokinetic parameters (zeta potential, electrophoretic mobility and conductivity) were significantly different for the steroid free carrier (HAp/ChOLS) and A- or B-loaded ChOSL. The value of the topological molecular polar surface area (TPSA, the sum of the surfaces of polar atoms and groups in the molecule), were also different for drug free carrier and A- or B-HAp/ChOLS. Highly selective anticancer activity was noted towards breast cancer cells (MDA-MB-231) by B-loaded HAp/ChOLS. DET testing after 48 hours (after incubation and recovery) of the treatment with A-HAp/ChOSL and B-HAp/ChOSL particles showed a high viability of healthy cells (over 80%). The lowest viability was found in MDA-MB-231 cancer cells treated with B-HAp/ChOSL (28%). The obtained results of the DET and MTT tests showed that the particles of A-HAp/ChOLS exhibited nearly four-fold greater cytotoxicity towards breast cancer

cells (MDA-MB-231) than towards healthy cells (MRC-5). B-HAp/ChOSL particles exhibited nearly six times greater cytotoxicity to all breast cancer cells than to healthy ones.

O.S.III.3.

Synthesis of antimicrobial cobalt ferrite/gold nanocomposites

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Combining antimicrobial and magnetic properties is foreseen as a good option in designing novel generations of antimicrobials. It is expected that this type of materials will be capable of targeted and localized activity that can be removed upon demand.

In the present work, we present our work on designing antimicrobial nanocomposites based on amino acid-functionalized gold nanoparticles (AuNPs) and cobalt ferrite nanoparticles (CFO NPs). Initially, the hydrophobic CFO NPs were synthesized via solvothermal method with oleic acid as a surface capping agent. In order to use CFO NPs for bio-application the ligand exchange was performed. As-prepared hydrophilic CFO NPs were sonochemically combined with functionalized gold and further characterized by X-ray powder diffraction (XRD), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR) and superconducting quantum interference device (SQUID).

Synthesized materials were identified as nanocomposites with CFO and gold phases. Morphologically they contained larger AuNPs (approx. 20 nm in diameter) surrounded with smaller 5-nm sized CFOs. The surface of NPs was decorated with specific ligands, which provided them special functionality. The magnetic measurements confirmed their paramagnetic nature while antimicrobial tests proved their bacteriostatic activity against *E. coli*, *S. epidermidis* and *P. aeruginosa*. We will discuss about optimization of surface properties to provide the most optimal combination of magnetic and antimicrobial activity of the composite.

O.S.III.4.

New agents for no-chemotherapy of socially significant diseases: structure and properties of nitrosile [1Fe -2S] ferredoxins mimetics – nitric oxide donors

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Nitric oxide (NO), known for more than 20 years, is involved in various physiological and pathophysiological processes in mammalian organisms [1]. A significant experimental material has been accumulated and demonstrated that NO participates both in the development of pathological processes and in their correction by chemotherapeutic methods [2]. The obtained data on the multifaceted biological activity of this radical-mediator and its reactions with biological substrates in cells are successfully used in the development of effective drugs - NO (NO-therapy) or inhibitors of NOS activity (anti-NO-therapy).

There has been an exponential growth of interest in the study of nitrosyl complexes of transition metals, in particular, iron complexes in recent years [3, 4].

Representatives of a new family of low-toxic water-soluble exogenous NO donors, namely, dinitrosyl iron complexes with sulfur-containing aliphatic ligands derived from thiourea were first isolated in the crystalline state at IPCP RAS on the basis of a detailed study of the chemical nature of the Fe-S and Fe- N active nitrosyl ferredoxin sites [5].

Results of a fundamental study of the structure and properties of these compounds in solid phase and in solutions, as well as the potential practical application of these compounds for NO-therapy of antitumor and cardiovascular diseases, will be presented in the presentation.

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O.S.III.5.

Characterization of the TiNi surface after modified by electron beam and its effect on the morphology and cytoskeleton of mesenchymal stem cells

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The correlations between features of cells morphology and their cytoskeleton and the surface characteristics of the samples TiNi alloy before and after electron-ion-plasma treatments – roughness, chemical conditions and phase compositions of the thin oxide films on these surfaces are discussed. In the paper were studied TiNi samples: (i) the initial state, (ii) after microsecond low-energy high-current electron beam (LEHCPEB) pretreatment aimed, (iii) of Ti-Ta-Ni surface alloys formed in result of a 20-multiple magnetron deposition of Ti70Ta30 thin films and their liquid-phase mixing with the TiNi substrate by a LEHCPEB. The experiment “in vitro” was performed on culture of mesenchymal stem cells (MSCs) of rat marrow. Separate attention is paid to electron-microscopic studies of the interaction of MSC with sample surfaces before and after their modification and on the interface of the cell-surface of the alloy. The work was carried out at the financial support of RSF according (Project No.18-19-00198, 26.04.2018).

O.S.III.6.

Bias voltage effect in the development of new beta/alpha-Ti-Nb-Zr biocompatible coating with low Young's modulus and high toughness for medical applications

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The ideal surface modification, in form of coating, on biomaterial for orthopedic implant applications is one that exhibits excellent biocompatibility with no adverse cytotoxicity, excellent corrosion resistance, and a good combination of mechanical properties such as high strength and low elastic modulus. Sputtering techniques are extremely versatile to produce nanostructured, homogeneous, dense, compacts and crack-free coatings. This technique offers multiple possibilities to design in-situ complex (near) pure beta-Ti textured coatings as function of the bias voltage used, thanks to the introduction of a non-reversible martensitic transformation from body centered cubic crystal structure, beta, to orthorhombic crystal structure, alpha". The focus of this work is to design Ti-XNb-YZr (X=13, 26, 22, 34 w.% and Y=10, 25, 20, 24 w.%) coatings, manipulating their microstructure, texture, grain size and residual stress magnitude in order to get non-linear elastic behavior as well as low Young's modulus and high yield strength.

O.S.III.7.

Waterborne polycarbonate-based polyurethane films

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Functional properties of films made from novel waterborne polyurethane dispersions (PUDs) were studied. Simplified acetone method omitting the chain-extension step was used for PUD synthesis. Some PUDs contain D,L-lactide-based oligomer in the PU backbone. The set of methods enabling the material analysis from segmental up to macroscopic levels (e.g. FTIR, tensile characteristics, AFM, SEM, DSC and TGA) was used. Tensile properties of flat and regular films made from PU dispersions depend significantly on the sample composition and vary from 2.7 to 33.8 MPa (Young's modulus), 0.2 to 28.0 MPa (tensile strength), 112 to 1193 % (elongation-at-break) and 0.5 to 93.2 mJ/mm³ (toughness). PUDs can be in practice used either alone or together with water-dispersible additives as the matrix for diverse 2D nanocomposite biomaterials.

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O.S.III.8.

Nanotechnology approach in optical materials modification

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It should be remarked that at present time the nanotechnology methods are widely used in order to modify the basic properties of the optical materials. In the current paper the nano-structuration of the optical materials will be presented using the two approaches. The first approach [1,2] is connected with the surface modification of the optical materials by carbon nanotubes (CNTs) in order to reveal the change of the spectral, mechanical, laser and wetting phenomena. In this case the CO₂-laser is used to deposit the CNTs in vertical position at the surfaces of the optical materials. Currently the emphasis is given on the surfaces modifications of such materials: LiF, KBr, Sc, ZnS, PVA, etc. Mechanisms responsible for the material spectral and mechanical parameters change will be discussed and supported by the analytical and quantum-chemical simulation.

The second approach [3,4] is coincided with the structuration of the body of the optical materials. Some polymers and monomers, as well as the liquid crystals have been sensitized by the fullerenes, quantum dots (QDs), shungites, graphene oxides, etc. and studied by the pulsed nanosecond Nd-laser. The refractive properties change via estimation of the laser-induced refractive index have been shown and explained by the increased local volume polarizability. In the current paper the influence of the optical materials body sensitization on the surface wetting angle will be shown with good advantage.

The results obtained have been received via supporting by Russian Foundation for Basic Research, grant No.13-03-00044 (2013-2015), by FP7 Marie Curie International researchers exchange proposal "BIOMOLEC" (2012-2015), by the Russian Project "Nanocoating-GOP" (2012-2015), as well as by Russia-Israel project "Adaptaciya" (2017).

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O.S.III.9.

**Synthesis of highly porous monolithic 3D nanomaterials based on aluminum oxides:
development of methods for their functionalization using structural and chemical
modification**

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Synthesis and processing of 3D nanomaterials consisting of nanofibrils of $\text{Al}_2\text{O}_3 \cdot n\text{H}_2\text{O}$ were studied in the temperature range of 20 – 1700 °C. We have shown that structure of these materials can be presented as a 3D network consisting of nanofibrils of aluminum oxyhydride/oxide (NOA). A remarkable property of the NOA material is the preservation of the monolithic state during annealing although the density of NOA monolith increases from ~ 0.02 up to ~ 3 g/cm³, the total porosity decreasing from 99.3% to 25% and remains open up to 4 hour annealing at 1300 °C. Two mechanisms of the morphological and structural transformations in NOA are evidenced and quantitative physical model was proposed allowing the estimations of all this changes as the morphological evolution of the averaged NOA fibril. Applying the 3D model allows to explain the phenomenon of the preservation of the integrity of NOA monoliths during annealing by an important role of surface diffusion which provides an isotropic decrease in the parameters of the 3D structure without a significant increase in internal stresses, and samples integrity are preserved.

With the purpose of functionalization of NOA materials properties, various methods of the structural and chemical modification have been developed: by applying metallorganic compounds (siloxanes, phthalocyanines, oxyquinolines) and by impregnation with nanoparticles <10 nm (TiO_2 , NiO_2 , CeO_x , etc.)

The simplest effective media models using Maxwell-Garnett, Bruggeman and Landau-Lifshitz-Looyenga equations was applied to describe the optical properties of the NOA materials in the THz range, and good agreement with the experimental results was achieved.

This work was supported by the French-Russian collaboration project DRI CNRS No.EDC26176, and by the Russian Foundation for Basic Research Project 17-53-150007 CNRS_a.

O.S.III.10.

Amorphous FeSiB ribbons crystallized by using laser interference treatment

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Iron based $\text{Fe}_{80}\text{Si}_{11}\text{B}_9$ amorphous ribbons after interference laser heating, using variable pulse energy and number of consecutive pulses, as well as as-cast and after conventional annealing at 600°C ribbons were investigated. Performed laser treatment succeeded in periodically distributed, crystallized micro-areas (dots), ~10 μm in diameter, in the remaining amorphous matrix. SEM, TEM and HRTEM observations indicate that pulsed laser interference heating involves structural transformations in the subsurface layer up to ~300 μm . The rapid heating and cooling rates involved in pulsed interference laser heating, permitted to saturate the amorphous FeSiB alloy with the randomly oriented, ultra fine grains of $\alpha\text{-Fe}(\text{Si})$ dispersed in the remaining amorphous matrix. The main structural differences between laser heating and conventional annealing are that laser heating led to create nanograin structure while. Conventional annealing led to create dendrite structure. Magnetization measurements show that the as-cast ribbon and laser light irradiated samples are magnetically soft materials. The results obtained lead to the conclusion, that the dots corresponding to the laser modified regions exhibit a perpendicular magnetic anisotropy. Magnetic force microscopy showed that the laser heating led to change magnetic structure only in laser heated micro-areas (dots), in annealing material magnetic structure are strongly developed.

O.S.III.11.

Correlation methods of analysis in studies of mechanochemical reactions

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The possibility of using the method of two-dimensional correlation spectroscopy for a step-by-step study of deformation-induced conversions and transformations of bioinorganic compounds is shown in this work.

As result of comprehensive research involving direct structural and structure-sensitive spectroscopic techniques, as well as quantum chemical simulations, the conditions necessary to obtain the polymorphic molecular compounds by mechanical activation were formulated, and the interrelation of the kinetics of their production with the amorphization and the formation of nano-dispersed states of molecular crystals (i.e., plane 2-D structures, nanotubes) was established.

The reported study was funded by RFBR according to the research project 16-03-01131- and partially the FASO project AAAA- 17-117022250038-7.

O.S.IV.1.

In situ aberration-corrected STEM of metal-induced crystallization: the case of the Ag/Ge couple

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The effect of low-temperature crystallization of amorphous Ge and Si films in contact with a metal, such that a eutectic couple is formed, was discovered almost 50 years ago. Nevertheless, the mechanism of this reaction is still under debate in the literature. In this work, we have investigated the initial stages of the aforementioned reaction by means of aberration-corrected (S)TEM. A few nm size Ag particles deposited by PVD on thin amorphous Ge film were used as a model for the metal-semiconductor couple. Nucleation and growth of crystalline Ge phase was observed at atomic scale in real time by heating the system in a double corrected FEI Titan Themis operated at 200 keV. A new insight into the mechanism of metal-induced crystallization will be presented and discussed.

Financial support from the National Science Centre, Poland under grant No. 2016/23/B/ST8/00537 is gratefully acknowledged.

O.S.IV.2.

Microstructure characterization of a nanostructured austenitic steel annealed under high hydrostatic pressure

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In this study the impact of high hydrostatic pressure annealing on the grain boundary character, precipitation rate and susceptibility to intergranular corrosion of a nanostructured austenitic stainless steel is investigated. Samples are deformed by high pressure torsion and subsequently annealed at 900°C for 10 min under a pressure of 0.1 MPa, 2 and 6 GPa. The resulting microstructures are examined using electron beam scattering diffraction, transmission and scanning electron microscopy. Annealing austenitic stainless steel under high hydrostatic pressure leads to a higher percentage of high-angle grain boundaries than annealing under atmospheric pressure, promotes the coexistence of two orientations $\langle 111 \rangle$ and $\langle 100 \rangle$, whereas atmospheric pressure supports mainly $\langle 111 \rangle$ and promotes the nucleation of precipitates and hinders their growth, thereby resulting in a higher number of Cr₂₃C₆ carbides during annealing under 6 GPa, making this sample susceptible to inter-granular corrosion.

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O.S.IV.3.

Double complex salts as precursors of bimetallic nanoalloys

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We present the results of bimetallic nanoparticles synthesis by thermolysis of single-source precursors – double complex salts (DCS). Variation of thermolysis conditions (temperature, heating rate, aging time, etc.) makes it possible to produce a variety of products: thermodynamically stable and metastable solid phases, mono- and polyphase alloys. Changing the atmosphere of thermal destruction allows obtaining both metal solid solutions and mixed oxide phases. On example of three bimetallic systems with different miscibility the features of nanoalloys creation are revealed. Based on CoPt system (unlimited miscibility) formation of the nanoalloys with superstructure ordering depending on the thermolysis atmosphere and catalytic properties are shown. On an example of RhRe system (limited miscibility) possibility of using nanoalloys for phase diagram's reconstruction is presented. Examples of synthesis of nanoalloys in immiscible metals' system (RuCu) by using this approach and their catalytic activity are given. This work was supported by Russian Foundation for Basic Research (17-03-00950-).

O.S.IV.4.

Oxalatopalladates of Co, Ni and Zn as precursors of nanoalloys: from thermal properties to supported catalysts

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Thermal decomposition of complex salts comprising both cationic and anionic coordination entities is a handy way for preparation of bimetallic nanoalloys. Hexaaquocobalt, -nickel and -zinc oxalatopalladates were chosen as precursors of high dispersed equiatomic bimetallic phases. The main advantages of this composition is rather high solubility relatively to other double complex salts and a presence of ligands with remarkably reductive properties. Structurally the salts differ from each other inessentially and thus open up possibility to form solid solutions with partially substituted non-noble metals

Thermal behavior of complex salts strongly depends on atmosphere of decomposition experiment. The heating in both reductive (hydrogen) and inert (helium) atmosphere leads to full reduction of metals. Supported on TiO₂, bimetallic nanoalloys show high photocatalytic activity.

O.S.IV.5.

Ni-Pd/Al₂O₃ catalyst in the form of foam for dry methane reforming

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In this research, catalytic properties of Ni-Pd/Al₂O₃ catalyst synthesized by aerosol impregnation method were examined in the dry methane reforming process. First, reticulated ceramic foams were impregnated by ultrasonically nebulized solution of corresponding chlorides and dried. The catalyst was activated by direct hydrogen reduction, without calcination, at only 533 K. The reforming test was carried out at temperatures of 873, 973 and 1023 K. Since CO and H₂ are the main products of the dry methane reforming, yields of those gasses were measured and obtained results were a base for conclusions about selectivity, activity and stability of the catalyst.

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O.S.IV.6.

Modeling transport through an environment crowded by obstacles of different shapes and Sizes

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Many biological environments, are crowded by macromolecules, organelles and cells of varying size and shape. Experimental and computational evidence suggests that crowding effects may hinder the transport of macromolecules and cells in such environments. We examine the transport of individual agents through crowded environments using a lattice-based nearest neighbor random walk model. We simulate crowding effects by randomly populating the lattice with immobile obstacles of different shapes and sizes up to a chosen density. For given spatial distributions of obstacles (crowders) we demonstrate how anomalous diffusion with strongly non-Gaussian features arises in this model system. We have simulated trajectories of tracer particles over a wide range of obstacle densities, above and below the percolation threshold. In both cases, ballistic motion at short times is followed by a regime of anomalous transport. At large time scales and below the localization transition, generic diffusive behavior is recovered. Above the critical density, the particles are trapped and mean-square displacement (MSD) is bounded by the mean-square cluster size. At the critical density, the dynamics becomes neither diffusive nor trapped, and transport remains anomalous for all times. Diffusion coefficients are extracted from the MSD. With increasing density, diffusion coefficient is more and more suppressed until it vanishes at percolation threshold as a power law. This provides clear evidence for the intimate connection between percolation and our model of a crowded environment; i.e., diffusion is not blocked as long as there is an infinite path through the medium (a purely geometric reason.)

O.S.IV.7.

Interfaces and mechanisms: a molecular dynamics approach to fine tuning manipulation of interfaces

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The design of high-performance materials is driven by controlling and optimizing different mechanical and thermal properties such as strength, ductility, plasticity, and toughness. Nanoscale metallic multilayers (NMMs) are relatively new class of materials with promising potential for changing their conventional counterparts used in the high-end applications, as nuclear, space and aerospace technologies. The superior properties of NMMs are mostly correlated with the advanced design and fabrication of the interfaces at a very confined spaces (~nm). In this presentation, we will present a comprehensive study by means of atomistic simulations, of the dislocation activity and phase transitions that determine the mechanical properties at the nanoscale in Zr-Nb NMMs. The governing mechanisms, in special, the effect of the interfaces, for improved strength, fracture and fatigue will be discussed. Additionally, we will present the experimental characterization of ZrNb NMMs and nano-indentation results showing, for selected geometries, unprecedented hardness close to the theoretical limits.

O.S.IV.8.

Properties of ZnO nanorods grown in continuous-flow reactors

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Investigation of one-dimensional semiconductor nanostructures is at the forefront of research. Despite a large number of applications, the growth of ZnO nanorods from solutions is not well understood and the growth technology mostly relies on empirical results. We report on the growth of ZnO vertical nanorod arrays on electron and ion beam patterned substrates in continuous-flow reactors. Unlike conventional batch reactors, in continuous-flow reactors the solution supersaturation can be accurately set, which enables to control the growth rates, the aspect ratio, the incorporation of dopants and impurities, and the density of defects. To study the electric charge transport in the nanorods, electrical contacts were formed by (i) the deposition of colloidal graphite, (ii) by the nanoprobe in SEM, and (iii) by conductive AFM. The transport properties are correlated with the structural and optical properties investigated by x-ray diffraction and photoluminescence spectroscopy.

O.S.IV.9.

The use of layered nanomaterials in composites with metals and their compounds

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Nanocomposites are actively researched nowadays, because of their improved performance or enhanced properties in many applications, ranging from energy storage to nanomedicine.

We report nanocomposites where we combine various kinds of layered materials with metals, metal oxides or chalcogenides. The first step in the preparation of the nanocomposites is liquid-phase exfoliation of a layered material, such as graphene, *h*-BN, MoS₂, VS₄, TiS₃, NbS₃, etc. We analyze how the nature of the support influences the characteristics of the deposited nanoparticles. For example, in case of chalcogenides, depending on the support, we obtained either Ag or Ag₂S deposited nanoparticles. To illustrate potential applications of the nanocomposite samples, we show their catalytic and photocatalytic activities, as well as performance as electrodes of high-capacity lithium-ion batteries.

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O.S.IV.10.

Dielectric behaviour of polyimide/silica based nanocomposites at low temperatures

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Within the last decades polyimide have been extensively used in various application as of its outstanding electrical properties, meaning low dielectric constant as well as low dielectric losses. However, the increase of demand for wearable flexible electronics is requesting for improvement of thermal behaviour of materials employed for development of polymeric substrate which should ensure long time operability at both normal and extreme working temperatures. We are herein presenting an in-depth study of dielectric properties of polyimide/silica based nanocomposite at temperatures below zero Celsius degrees down to -160°C realized with the help of broadband dielectric spectroscopy. The effect of low temperatures on dielectric polarizations is described in terms of real permittivity and dielectric losses in a frequency domain from 0.1Hz up to 3GHz. Practical aspects of dielectric properties behaviour are considered and discussed in respect to utilization of polyimide/silica based nanocomposite in flexible electronics manufacturing.

Poster Presentation

P.S.A.1.

Plasma Assisted Strategies for Advanced Synthesis and Processing of Materials

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Nanostructured materials have drawn considerable attention from various industrial fields. However, various applications require structures with different building blocks, which makes it necessary to develop specific strategies for selective etching, functionalization, growth or synthesis, with excellent control over their structure as well as their mechanical, chemical, biological, electrical, or optical characteristics, in order to fully exploit their potentials. Moreover, some applications could require doping of the surface structures in order to obtain desirable surface characteristics.

There are variety of techniques used for fabrication of various nanostructured materials, structuring surfaces and improving interfaces. Plasma and vacuum assisted techniques have been used as a strategy to assist the surface engineering and synthesis of some complex nanomaterial structures.

In this presentation we will highlight various plasma assisted strategies, using low or atmospheric pressure plasma, with various examples that we have applied for synthesis of carbon nanostructures [1], surface engineering of biomaterials, fabrication of nanoscale CMOS compatible FTJ devices [2] and efficient synthesis of epitaxial multiferroic films, such as BFCO [3].

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P.S.A.2.

Polimorphous transformations in mechanoactivated molecular crystals

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The physical mechanisms of the hierarchy of the deformation induced structural transformations in molecular crystals, including morphological changes, amorphization and molecular polymorphous conversions in nano-dispersed organic, bioinorganic and organometallic compounds are discussed in this work. Integrated study using direct structural and spectroscopic methods as well as quantum-chemical calculations allowed obtaining the data on polymorphous transformations, taking place during mechanical activation.

One of the possible reasons for lattice polymorphous transformations and amorphization observed during mechanical activation of molecular crystals, might be the spatial molecular isomerization. In this case, the disappearance of the translational invariance of the lattice is conditioned by the simultaneous coexistence of the reactants and reaction products, which have different stereo-organization of the molecular structure. The relationship between kinetics of such transformations and formation of nano-dispersed state in molecular crystals is also discussed. The reported study was funded by RFBR according to the research project 16-03-01131- .

P.S.A.3.

Microstructure development of the Cu-Ti-TiB₂ composite obtained by laser sintering

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Mechanically alloyed Cu-4Ti (wt%) and Cu-1.5B (wt%) powders, after milling of 22 h, were homogenized for 30 min and sintered by pulsed millisecond Nd:YAG laser. Layer-by-layer production of 3D cubes was done using the following parameters: laser frequency 50 Hz, laser pulse duration 1 ms and pulse energy 1.6 J. The morphology and microstructure of laser sintered Cu-Ti and Cu-B single layers, as well as Cu-Ti-B cubes, were characterized by optical and scanning electron microscope with an energy dispersive x-ray spectrometer. Density of the cubes was determined by Archimedes method in water. Vickers microhardness of the samples was determined under the load of 10 g. Depending on the parameters of laser sintering, in the microstructure of single layers and cubes could be identified solid solutions Cu-Ti and Cu-B, particles of free titanium and boron, as well as *in situ* formed TiB₂ particles.

P.S.A.4.

Anomalous electron pulse annealing in Ti implanted GaP

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Ti implanted GaP is considered as a prospective material for high efficiency impurity band solar cells. To achieve the required Ti concentration above a solubility limit, pulse annealing of Ti implanted material is used. We studied details of pulse annealing, using high energy density electron pulses of an energy density in the range 0.3-1.5 J/cm² and pulse duration of 1-2 μs. We observed that GaP samples implanted with moderate Ti dose of 1e15 cm⁻² and treated with electron beam pulses of an energy below the melting threshold (1.1 J/cm²) and studied by cRBS method reveal an anomalous crystallographic structure. Instead of epi-crystallized surface layer, instantaneously molten by the electron pulse, they show a polycrystalline structure in the region of Ti content. This process is analyzed in terms of GaP dissociation inside the material bulk.

P.S.A.5.

The effect of nitrogen ion implantation on the properties of WC-Co composites used in wood-based materials machining

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Cemented tungsten carbides, like WC-Co, are e.g. the liquid-phase sintered composites of hard brittle carbides and a relatively soft, ductile metallic binder. WC-Co is a widely used material in the industry, because it is harder than steel and much cheaper than diamond. Unfortunately, the durability of present WC-Co tools is not satisfactory. Ion implantation is one of a several methods to improve the lifetime of WC-Co tools. Basically an increase of microhardness due to formation of hard nitrides is observed for nitrogen implantation and a friction reduction due to carbon precipitation occurs for carbon implantation. In this paper presents the effect of nitrogen ion energy and applied dose on the surface layer properties of WC-Co tools in contact with wood-based materials.

P.S.A.6.

Shungite - a russian mineral: possible application as a microwave absorber

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The paper presents results of investigation of the influence of mechanical activation of shungite, a Russian natural mineral rich in silica and carbon, on its sintering behavior. The mechanical activation of the starting powder was performed in a high-energy ball mill in time intervals from 0 to 480 minutes. The phase composition of the starting mixtures and sintered samples was analyzed by the X-ray diffraction method. The scanning electron microscopy was performed in order to determine changes in the microstructure. Sintering was performed at various temperatures for 2 h, in an Ar and vacuum atmosphere. Dielectric properties of the sintered samples were measured in the frequency range from 1 to 500 MHz. The obtained results indicate that sintered shungite powder is a good candidate for applications as an absorber of electromagnetic waves in microwave engineering.

P.S.A.7.

Sintering of alumina doped with different oxides, followed by sensitive dilatometer

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Sintered alumina powder represents suitable material for usage in various industry fields (e.g., as chip carriers in electronics, microwaves, jewelry production), due to convenient physical properties, such as sinterability, electrical and mechanical features. Those properties can be modified by addition of different oxides and/or mechanical treatment. Therefore, in this investigation the alumina was doped with 1 wt. % of Cr₂O₃, Mn₂O₃ and NiO, respectively, followed by 1 hour of mechanical activation at 400 rpm in planetary ball mill. Sintering of powder mixtures was tracked by sensitive dilatometer up to 1400 °C. The final density values varied from cca. 2–3.2 g/cm³. Changes in microstructure were observed by means of SEM. The influence of additives along with mechanical activation is monitored through changes in electrical permittivity and loss tangent. Compared to pure alumina, the additives lower the relative permittivity and increase dielectric losses. For a given mixture, the sintering increases the relative permittivity and decreases losses.

P.S.A.8.

Ni_{1-x}Mo_x dispersed alloys: synthesis and catalytic properties in 1,2-dichloroethane decomposition process

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Catalytic decomposition of chlorinated hydrocarbons on Ni-based alloys is the most promising approach in the recycling of Cl-containing organic wastes, which are generated as a result of chemical productions. In this work we show that Ni_{1-x}Mo_x alloys are the most active catalysts in the number of tested bimetallic systems (Ni-Co, Ni-Cr, Ni-Cu, Ni-Fe, Ni-Pt) in the process of decomposition of 1,2-dichloroethane. The process results in formation of carbon nanofiber with high specific surface area (300–400 m²/g). Ni and Mo are thermodynamically immiscible in the region of 10 at.% Mo at T<1000 °C. We successfully prepared Ni_{1-x}Mo_x dispersed alloys with Mo content of 1-13 at.% by the thermolysis of specifically synthesized single-source precursors, containing both metals in desired ratio. The structure and composition of prepared dispersed alloys were confirmed by XRD, TEM, ICP AES and EDX analysis.

The work has been supported by grant of Russian Science Foundation (project 16-13-10192).

P.S.A.9.

The influence of the method of preparation and temperature of thermal treatment on the phase composition of the NiO-Al₂O₃ catalyst using the X-ray diffraction method

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The influence of the method of preparation of the NiO-Al₂O₃ catalyst and subsequent thermal treatment on the phase composition of the catalyst was studied. Catalysts are prepared by co-precipitation, wet impregnation and mechanical mixing of oxide powders and calcined at 400, 700, 1100 °C, respectively. The prepared catalysts were tested by X-ray diffraction. The choice of the catalyst preparation method and calcination temperature significantly influences the phase composition. The phenomena are the result of the formation of different types and degree of interaction of system components, which depend on the contact conditions of the components of the catalyst. The results indicate the possibility of producing nickel spinels in all catalysts. Nickel spinels are undesirable structures in the NiO-Al₂O₃ catalyst because they are difficult to reduce under high temperature conditions in the processes of wet and dry reforming of methane and make it difficult to regenerate deactivated catalysts.

P.S.A.10.

Chalcogenides of niobium and molybdenum with stoichiometry metal: chalcogen = 2:3

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The work reports both experimental and theoretical investigation of transition metal sesquichalcogenides M₂Q₃ (M=Mo, Nb, Ta; Q=S, Se). Mo₂S₃, Nb₂Se₃ and Ta₂Se₃ are known to be synthesized by direct high-temperature reaction between elements; however, Mo₂Se₃, Nb₂S₃ and Ta₂S₃ are not obtained. We synthesized and characterized Mo₂S₃ and Nb₂Se₃ phases and attempted to find out the reasons of instability of compounds, which could not be synthesized by direct reactions. The results of comparative study of phases in Nb-S and Nb-Se systems by DFT calculations are given. For example, when stoichiometry in Nb-Se system is 2:3, there are two competing phases, namely Nb₂Se₃ and intercalated phase Nb_{1.33}Se₂, that crystallizes in the structure of 2H-NbSe₂. The formation of Nb₂Se₃ becomes possible at temperatures higher than 1100°C. The experimental data are in good agreement with the results of calculations.

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P.S.A.11.

Crystallographic structure of electron pulse annealed GaP implanted with Ti

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Ti implanted and electron pulse annealed GaP - a prospective material for high efficiency impurity band solar cells, is studied by RBS technique and reveals an anomalous crystallographic structure, when annealed with high energy density electron pulses of an energy density below 1.1 J/cm² and pulse duration of 1-2 μs. Instead of epitaxially recrystallized layer, molten by the electron pulse, as observed for higher energy density pulses, it reveals a polycrystalline layer in the region of Ti implantation, when the Ti dose is in the range of 1e15 cm⁻² for 120 keV implantation. To study details of this process, we performed TEM and SEM studies of the surface layer. The TEM images are presented and discussed in terms of other results on pulse-induced defects in GaP.

P.S.A.12.

The influence of boron on synthesis and characteristics of PM copper-zirconium alloys

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High conductivity Cu-1Zr (wt%) and Cu-1.1Zr-0.3B (wt%) alloys were prepared by mechanical alloying and subsequent hot pressing. Microstructural changes during mechanical alloying and hot pressing were studied using scanning electron microscopy and X-ray diffraction. In particular, changes in the Cu particle size, structural parameters of the powder mixtures and formation of CuZr phase in binary alloy, i.e. CuZr phase and ZrB₂ particles in ternary alloy during the processes of hot pressing were investigated. The mechanism of *in situ* formation of ZrB₂ particles in ternary copper alloy was also studied. Compared with Cu-Zr alloy obtained using the same procedure, the hardening effect in Cu-Zr-B alloy is greater. In regards to binary Cu-Zr alloys with low content of Zr, hardness decrease in ternary alloy after annealing at 700 °C is considerably milder as a result of the presence of ZrB₂ reinforcing particles in the structure.

P.S.A.13.

Synthesis and structure of zinc(II) complex with 2-acetylpyridine - aminoguanidine

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Due to usually high photoluminescence, group 12 metal complexes are promising candidates for the application in domain of optoelectronic devices, thus their syntheses and characterization are of a particular interest. Single crystals of the titled complex were obtained in the reaction of warm aqueous solutions of 2-acetylpyridine-aminoguanidine hydrogen chloride and zinc(II)-acetate in the presence of sodium-cyanate. The complex has been characterized by elemental analysis, IR spectra, conductometric measurements and X-ray crystallography. The latter has revealed the usual tridentate coordination of the chelating ligand via pyridine, azomethine and nitrogen atom of the imino-group of the aminoguanidine moiety. The zinc(II) is situated in distorted square-pyramidal surroundings of the tridentate Schiff base and two monodentate cyanate ions coordinated through nitrogen atoms.

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P.S.A.14.

Influence of boron on modified characteristics of iron-based alloys with particular reference to boronizing

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The paper deals with the research of the chemical element Boron and its effects on the environment. The obtained experimental results from the performed tests are based on the influence that Boron (B), as an alloying component has on the modified characteristics of multicomponent alloys. In addition, part of the results is related to the chemical heat treatment – boronizing, that has been applied for the surface hardening of iron-based alloys.

P.S.B.1.

Autowaves of localized plastic deformation in a material with an unstable phase structure

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In terms of autowave theory of localized plastic flow macroscopic plastic instabilities, namely Lüders bands and Portevin - Le Chatelier bands, can be considered as a propagation of switching and excitation autowaves correspondently. Until this time, the study of given waves were proceeding using different materials, because they usually can not be observed simultaneously in a same sample. In this respect steels with transformation-induced plasticity (TRIP), with the yield point and stress plateau followed by serrated yielding, allows to study the change of autowaves type from switching to excitation. This paper presents an investigation of that process.

It is found that on the stress plateau several regions of localized deformation is formed by nucleus of a Lüders bands. Next, during the work hardening stage and serrated yielding, the motion of the localized deformation fronts remains limited by that regions and each sharp serrated yield point corresponds to the run of a single front. With the growth of general deformation, the velocity of fronts decreases but they amplitude of deformation increases which finally led to sample destruction.

The work was carried out within the framework of the Program of Fundamental Scientific Research Russian State academies of sciences for 2013-2020.

P.S.B.2.

High temperature stability of YSZ and mullite-YSZ coatings deposited by atmospheric plasma spraying

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Durability of conventional yttria stabilized zirconia (YSZ) coatings with high porosity content was compared with multilayer Mullite-YSZ/YSZ (M-YSZ) coatings by means of isothermal oxidation, cyclic oxidation and burner-rig testing. Both ceramic coatings were deposited by atmospheric plasma spraying from commercial powders. The initial M-YSZ powder mixture consisted of 29 vol. % of Mullite and 81 vol. % of YSZ. The conventional TBC system consisted of ~ 150 µm thick bond coat and ~ 300 µm thick YSZ top coat. The experimental M-YSZ TBC system consisted of ~ 150 µm thick bond coat, ~ 100 µm thick YSZ interlayer and ~ 200 µm thick M-YSZ top coat. Substrate discs were prepared from Inconel 713LC and HA230 superalloys. Lifetime, phase stability, thickness of the thermally grown oxide layer, porosity, and changes in microstructure after testing were evaluated using scanning electron microscope equipped with EDAX analyzer and by XRD technique.

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P.S.B.3.

Barium-magnesium-aluminium-silicate environmental barrier coatings: powder manufacturing and plasma spraying

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As a potential candidate for the top coating in novel Environmental Barrier Coating systems, one representative of a Barium-Magnesium-Aluminium-Silicate (BMAS) family was produced in the form of the powder. Initial compounds were heat-treated to synthesize and the product was crushed in the ball mill device down to the fraction of 20 micrometers. In the next step, the atmospheric plasma spray (APS) technique was used to form a coating on a steel sheet substrate. The aim of this study was to obtain the most favorable technological parameters for the thermal spraying process and therefore two plasma spraying parameters for pure alumina or yttria stabilized zirconia, and other three experimentally designed ones were tested. Despite the same stand-off distance used for coatings manufacturing, thickness and porosity differed in order of tens of micrometers and several percent, respectively. Resulting coatings consisted of a mixture of amorphous and crystalline Al_2O_3 , SiO_2 and MgO phases.

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P.S.B.4.

Magnetic and mechanical properties of nickel-based superalloy after laser induced deformation

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Nickel-based superalloys are used in load-bearing structures at elevated temperature and pressure and in harsh environment. Nickel based superalloys have good mechanical properties, good oxidation and corrosion resistance. Among the most demanding applications for a structural material are those in the turbine engines, in first place for turbine blades. Nickel based superalloys consist of nickel solid solution, strengthening γ' phase (Ni_3Al) and carbides. At room temperature turbine blades are paramagnetic. The earlier studies reported increase in magnetic properties of Ni_3Al after induced deformation. In this paper, the magnetic properties of nickel-based superalloy after deformation induced by laser waves are investigated and discussed. Mechanical characteristics are analyzed with regards to changes of magnetics properties.

P.S.B.5.

Influence of diffusion coatings on magnetic properties of 41CrMo₄ steel

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The knowledge of magnetic and transport properties of construction steels for magnetic circuits plays an important role. Three different techniques: (i) flame spray, (ii) twin wire arc spray and (iii) powder mixture with halide activator were used to produce Si, CuSn6 and Si coatings, respectively, on the 41CrMo₄ steel ring substrates. After the thermal spraying or inserting the steels into the powder mixture was used isothermal heat treatment at the temperatures of 800 °C / 6 hrs, 1000 °C / 4 hrs and 1250 °C / 2 hrs to produce the diffusion coatings. Several coating systems consisting of different phases and thicknesses were manufactured. Opto-digital microscope, scanning electron microscope and digital image analysis, second equipped with energy dispersive microanalyzer, were utilized to characterize the microstructure, chemical composition and thicknesses of the coatings. The influence of coatings on magnetic properties in the frequency range of 50 – 2000 Hz was also measured.

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P.S.B.6.

Electrical and magnetic properties of multiferroic BiFeO₃-based flexible composites

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Flexible composite samples were prepared by hot pressing of BiFeO₃ powders prepared by chemical methods with polyvinylidene fluoride (PVDF). Role of PVDF is not only to make the samples flexible, but also to improve the properties of BiFeO₃, primarily to prevent the problems with high density of leakage currents. Microstructure of composites showed good homogeneity and uniform thickness of around 50 μm. Dielectric, impedance, ferroelectric and ferromagnetic properties of composite samples were studied and compared with those of BiFeO₃ powders or ceramic samples. Flexible samples exhibited improved electrical resistivity, which enables them to withstand significantly higher electric fields and to be weakly polarized. By eliminating the sintering step, it is possible to retain weak ferromagnetism originating from Fe₃O₄ nanoparticles formed during the synthesis in compact samples.

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P.S.B.7.

Characterization of different MMC coatings deposited by PTA and FS processes

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The paper presents the results of characterization metal matrix composite (MMC) of coatings deposited on a steel substrate by plasma transferred arc welding (PTA) and thermal flame spraying (FS) processes. Three erosion protection coatings were deposited: coatings with tungsten carbides (WC) in NiBSi matrix (WC/NiBSi), WC in NiCrBSi matrix (WC/CrNiBSi), and a coating with chrome carbides (CrC) in FeNiSi matrix (FeCrC). Filler materials in the form of powder, substrate and coatings were characterized using LM, SEM, EDS and XRD techniques. The macro/microhardness tests of the coatings, the substrate-coating zones and carbides were carried out by the Vickers method. Also, particle erosion tests for the purpose of determining and comparing mass loss of the coatings were carried out using the high-velocity/high energy erodent particles impact for different erodent particle and impact angles.

P.S.B.8.

Determination of ceramic proppant impact on efficiency of shale gas production and the environment

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Recently, shale gas has become significant source for energy production. However, difficult mining conditions (low-permeability, high reservoir pressure) force into implementation of advanced extraction methods. The most practiced, hydraulic fracturing, must deal with rapid closure of created fracture and its limited conductivity. Ceramic proppant injected into wellbore remains the fracture open due to high mechanical strength and stability in acids, thus intensifies gas-flow by 60%.

The study concerns functionality of proppants granulated and sintered from aluminosilicates with nanotubular/platy morphology, high specific surface area and cation-exchange capacity, improving crush and chemical resistance of proppants and heavy metals capture from environment.

The minerals and proppants were evaluated by PSD, TGA, SEM, BET, EDS, XRF, XRD, μ CT and simulation of proppant embedment. Roundness/sphericity, bulk density, decay in water and acids were also determined. The results confirmed influence of the mineral composition on proppants quality and proved their prospectiveness for sustainable, economic gas production.

P.S.B.9.

Temperature dependence of thermal conductivity of graphene monolayer in the framework of Debay and Calawey models

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The temperature dependence of thermal conductivity of graphene monolayer is analyzed, based on semiclassical Boltzmann transport equation in the approximation of relaxation time in the framework of Debay and Calawey models. In both cases the phonon relaxation mechanisms on impurities, monolayer boundaries, and phonon-phonon interactions are considered. Electron-phonon and electron-electron interactions are neglected as they provide small contributions to thermal conductivity. The three-phonon scattering N-processes in graphene monolayer thermal conductivity are accounted within Calawey model, while neglected within Debay model. It is shown that Calawey model is more successful than Debay model in explaining experimental measurements of thermal conductivity in graphene.

P.S.B.10.

Cup anemometer tribology and revised IEC standard

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In the IEC standard 61400-12-1:2017 revision, Part 12.1 Power performance measurements of electricity producing wind turbines, the cup anemometer is included as a standard instrument for horizontal wind speed measurement. In wind industry, this wind speed sensor is very popular since it operates as a vertical axis wind turbine which converts wind speed to the angular velocity of the equipment rotor. The theory of a cup anemometer considers the dynamic balance of the resulting aerodynamic, friction and output signal conversion system torques. The terms in balance equation as a function on rotor angular velocity depend on “influencing parameters” such as the temperature, pressure, flow inclination angle, turbulence, rotor bearing pair tribological characteristics etc. The anemometers are classified according to the characteristic climate and terrain at the measurement region. The revised standard proposes four instead of previous two classes. The main difference between the old and new classification is the surrounding air temperature. In new revision, the temperature range includes the area of cold climate so that the low temperature limit is 200C. In this paper we analysed the existing data of several commercial cup anemometers. The main conclusions are that some terms in equation used for the anemometer performance simulation applied in classification have to be modified, as well as some experimental methods used in classification. At low temperatures, the inclination angle characteristic is dependent on the temperature due to the rotor-bearing pair tribological properties influence. This also requires the development of a new or modified method for determination of friction and wear properties.

P.S.B.11.

Prediction of new B₆O structures and their properties using ab initio data mining approach

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Boron suboxide B₆O is the hardest known oxide with high thermal stability, high chemical inertness and high melting temperature which make it applicable for cutting, grinding, drilling and coatings. We used ab initio data mining approach to investigate B₆O system and discover new possible modifications, besides experimentally known R-3m structure (-boron structure). All modifications were optimized by two different ab initio methods using the Crystal17 code. Also, mechanical and electronic properties of experimentally known R-3m structure and new predicted modifications with the B₆O stoichiometry were explored by means of ab initio calculations. Corrections for long-range van der Waals dispersion interactions were taken into account. In this way we could predict the stability of new modifications and possibility to synthesize them using appropriate experimental technique. Obtained results gave us more insight in the B₆O system and open a possibility for ex-panding its use in device applications.

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P.S.B.12.

Impact of thickness on properties of high-entropy and conventional metallic glasses

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Properties of metallic glasses (MG) depend sensitively on the cooling rate (thus thickness for melt-spun ribbons). We present the effect of thickness on properties of high-entropy $(\text{TiZrNbCu})_{100-x}\text{Ni}_x$ ($x = 50$) and conventional binary $\text{Cu}_x\text{TE}_{100-x}$ ($\text{TE} = \text{Ti}$ or Hf , $x = 70$) and ternary $\text{Cu}_{55}\text{Hf}_{45-x}(\text{Zr},\text{Ti})_x$ ($x = 45$) glassy ribbons. Both, as-cast and relaxed (short anneal just below glass transition temperature) samples were studied. The mechanical and vibrational properties (ultrasound velocity, Young's modulus, microhardness, Debye temperature) of as-cast alloys showed clear effect of thickness superposed on that due to composition, whereas those of relaxed samples showed little effect of thickness. Properties of relaxed samples were larger than those of corresponding as-cast alloys and in ternary $\text{Cu}_{55}\text{Hf}_{45-x}(\text{Zr},\text{Ti})_x$ alloys the effect of relaxation was larger for $x=\text{Ti}$ than for Zr which may indicate the interplay between α - and β -relaxations in Cu-base MGs. The effect of cooling rate on mechanical properties provides simple criterion for glass forming ability.

P.S.B.13.

Crystal structure and X-Ray spectroscopic properties of R.E.₂Ni₁₂P₅ compounds

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We have studied experimentally and theoretically the electronic structure and x-ray absorption spectrum at the R.E.L3 - edge and x-ray emission spectra of Ni and P in the R.E.₂Ni₁₂P₅ compounds. Crystal structure of the ternary phosphate Ce₂Ni₁₂P₅ has been refined using X-ray powder diffraction pattern of the single phase sample with the same nominal composition, and the isotopic structure as for earlier known La₂Ni₁₂P₅-type has been proved: space group P21/m, formula units Z = 2, lattice parameters are a = 1.07809(2) nm, b = 0.36869(1) nm, c = 1.31490(3) nm, b = 107.776(4), residual R-values are RI = 0.0681, RP = 0.0442, RwP = 0.0603. The theoretical calculations have been carried out by means of the ab initio fully-relativistic spin-polarized Dirac linear muffin-tin orbital method. The calculations show good agreement with the experimental measurements. R.E.LIII - absorption spectra in ternary R.E.₂Ni₁₂P₅ compounds were obtained at 78K and 300K using a tube spectrometer equipped with an RKD-01 co-ordinate detector. The mixed valence state of Ce and Eu was obtained in the Ce₂Ni₁₂P₅ and Eu₂Ni₁₂P₅ compounds.

P.S.B.14.

Study of the interaction between graphene oxide and 12-tungstophosphoric acid in their nanocomposite

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The rich surface chemistry and large surface area of graphene oxide (GO) provide a platform for various functional materials that synergistically enhance charge storage properties of the composite. In present work we have investigated interaction between GO and 12-tungstophosphoric acid (WPA) in their nanocomposites as a function of different mass ratio of constituents. For this purpose, the Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectrometry (XPS), temperature programmed desorption method (TPD) and thermogravimetric/differential thermal analysis (TGA-DTA) methods were used. FTIR spectra have shown shifts and splitting of characteristic bands of WPA as a result of interactions with GO. Both XPS and TPD methods have shown an initial decrease of the total amount of surface oxygen groups of GO, with a minimum at around 10 wt.% of WPA, above which a restoration of the amount of surface oxygen groups was noticed. TGA-DTA analysis revealed an improved thermal stability of the material up to 25 wt.% of WPA; at higher loading of WPA the thermal properties of nanocomposite became alike to the ones of individual components. The obtained results suggest optimal conditions for preparation of GO-WPA nanocomposites for electrochemical charge storage applications.

P.S.B.15.

Transport coefficients of Ar⁺ in BF₃ gas

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Cold plasmas are frequently used in new technologies where they open up possibilities of non-intrusive production or modification of various substances. Transport of Ar⁺ plays significant role in various etching and deposition processes [1], in dark matter detection [2] and many more applications. In this work we present a cross section set for Ar⁺ in BF₃ gas where existing experimentally obtained data are selected and extrapolated. A Monte Carlo simulation method is applied to accurately calculate transport parameters in hydrodynamic regime. We discuss new data for Ar⁺ ions in BF₃ gas where mean energy, flux and bulk values of reduced mobility and other transport coefficients are given as a function of low and moderate reduced electric fields E/N (E-electric field, N-gas density).

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P.S.B.16.

The influence of basalt content on the properties of austenitic stainless steel 316L

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The aim of the paper is to examine the influence of basalt content on the properties of austenitic stainless steel as well as the possibility of using this composite material for wider industrial application. In the experiment, powder of commercial austenitic stainless steel (SURFIT TM 316L) of the diameter from 20 to 100 μm was used. The steel powder of the spherical shape obtained by gas atomization was mixed with the basalt from the locality "Vrelo" Kopaonik, Serbia, with particle size below 45 μm in the content of 1, 5 and 10 wt.%. The samples were pressed of about 500 MPa and then sintered into a vacuum furnace at temperatures of 1100 °C and 1200 °C. Characterization of sintered samples was performed using X-ray diffraction (XRD), scanning electron microscope (SEM), Vickers hardness as well as cavitation resistance.

P.S.B.17.

Comparative study on noble metal based nanocatalysts on different supports for low temperature fuel cells application

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Platinum based nanostructures on carbon support are state of the art materials for proton exchange membrane fuel cells application. Contemporary research directions in this field imply synthesis and characterization of novel carbon free catalysts supports to overcome disadvantages of carbon supported ones. We have recently synthesized platinum and palladium nanocatalysts onto different novel metal oxide based supports: titanium-oxide, tin oxide and tungsten oxide, doped by different metals (Nb, Ru, Sb), to achieve satisfactory conductivity. These novel nanostructures were characterized by X-ray diffraction (XRD), high resolution transmission electron microscopy (HRTEM), X-ray photoelectron spectroscopy (XPS), as well as by electrochemical techniques. The synthesized nanostructured catalysts were tested for oxygen reduction reaction. Obtained catalytic activities and stabilities were compared to the same noble metal loading catalysts on Vulcan XC-72 support. The results of comparison revealed many advantages of carbon free supported nanocatalysts, regarding both activity and stability.

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P.S.B.18.

Experimental Study of Drying Process of Porous Materials

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This work presents a study of a convection drying process of sand porous bricks under forced air with variable conditions to investigate the effect of drying conditions that is the air velocity, temperature and relative humidity on drying curves. Experimentally, a test rig constructed in the lab to study the influence of different conditions on drying curves as well as on heat and mass transfer characteristics associated with the drying process. The experimental results were presented and discussed. From the results obtained, it was found that the sand porous samples drying process is affected by drying conditions, where the drying rates increases with higher velocity and temperatures conditions.

P.S.C.1.

Production of synthesis gas by carbon dioxide over catalytically active molybdenum based carbide and nitride nanowires

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Transition metal carbides and nitrides with large surface area are attractive for various catalytic reactions. Here we present a route to synthesize Molybdenum carbide, molybdenum nitride and a heterophase including both materials from two different precursor materials. As shown by transmission and scanning electron microscopy resulting material preserves the initial low dimensional geometry of the two precursors. The prepared catalysts were characterized using powder XRD, physisorption (BET), chemisorption (H₂-TPR and CO-TPD) and microscopic techniques. With XRD and elemental analysis performed by transmission electron microscope we confirmed the composition of the material. XPS analyses were performed to follow the possible changes after the catalytic reactions. From the samples we synthesized we measured a relative conversion rate of CO₂ during the RWGS reaction in a wide temperature range. The lowest catalytic activity, throughout the temperature region was observed over pure nitride catalysts. We also found that the composite material i.e. Mo₂C/Mo₂N showed a higher conversion compared to pure Mo₂C with comparable surface area. The stability of Mo₂C/Mo₂N catalyst was tested at a temperature of 300 °C, and the catalyst showed a high stability over a long period of time (< 24 h).

P.S.C.2.

Nanofibrous polyaniline preparation by the oxidative polymerization of aniline with the oxidant in excess: Raman and FTIR spectroscopy study

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The interest in nanostructured conducting polymers, such as polyaniline (PANI), has continuously been growing over the past decade due to the improved properties, such as improved dispersibility and processability, improved performance in sensors, actuators and supercapacitors, in comparison to ordinary granular polymers. In this work nanofibrous PANI was synthesized by the oxidative polymerization of aniline using two oxidants, ammonium peroxydisulfate (APS) and a mixture of APS and hydrogen peroxide, in excess. Molecular structure of the reaction intermediates present in the reaction mixture at different reaction times, as well as of the final PANI products without their isolation was studied in detail by in situ Raman spectroscopy. In addition, FTIR was used to study molecular structure of the isolated solid final PANIs. Both techniques confirmed that PANI predominately consists of its conductive, emeraldine salt form, while the vibration bands indicative for branched and phenazine-type structures are more pronounced for reaction intermediates.

P.S.C.3.

One-pot synthesis of biocompatible NaYF₄:Yb,Er nanoparticles for cell labeling

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In modern medical research, great attention has been focused to the development of the new biomarkers which include up-converting nanoparticles (UCNPs). Their optical response is triggered by NIR radiation that achieves deeper tissue penetration when compared with traditionally used fluorophores. In this work, biocompatible NaYF₄: Yb, Er nanoparticles were synthesized by polymer assisted one-pot solvothermal processing using chitosan or poly(lactic-co-glycolic acid). X-ray powder diffraction and electron microscopy results revealed differences in crystal arrangement and morphology of the as-synthesized particles. Fourier transform infrared spectroscopy confirmed the presence of corresponding polymers moiety on UCNPs surface providing their biocompatibility and low cytotoxicity towards human gingival fibroblasts (HFG). As a consequence of efficient up-conversion, prominent green emission (between 512-533nm and between 533-560nm) as well as red emission (630-690nm) were recorded in the particles photoluminescence spectra, and these are applied further in the visualization of the HFG using the laser scanning microscopy with a NIR laser source.

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P.S.C.4.

Shape-controlled synthesis of CeO₂ nanoparticles: effects of different precursors on the formation of oxygen vacancies

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Oxygen storage in solid catalyst is very important for industrial oxidation reactions such as HCl oxidation reaction (Deacon process). Ceria nanoparticles act as promising catalysts for HCl oxidation reaction. Ceria possesses high OSC (oxygen storage capacity) which is a measure of the oxygen quantity that material can store and release. This makes ceria suitable for redox reactions which usually follow Mars-van Krevelen mechanism (surface oxygen atoms directly involved in reactions) [1]. Because of the reversible change in oxidation state from Ce⁴⁺ to Ce³⁺, neutral oxygen vacancies are formed. Giving the fact that redox reactions take place at ceria surface, it's important to investigate the type of the surface in different nanostructured ceria-based materials. As a result, different shapes show different facets of preferential orientation ((111) for octahedrons, (110) for nanorods and (100) for nanocubes) thus also showing different stability and activity [2]. An important factor that might have an impact on properties of synthesized ceria is a type of a precursor. Type of an anion in a precursor salt might have an impact on crystallization of ceria thus also on formation of oxygen vacancies. In this research, shape-controlled CeO₂ nanoparticles (nanorods and nanocubes) were synthesized by previously published hydrothermal method [3] and by two different cerium precursors (Ce(NO₃)₃ · 6H₂O and CeCl₃ · 7H₂O). Synthesized materials have been characterized by powder X-ray diffraction (PXRD), Raman spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM). Obtained results show pronounced effect of different cerium precursors on the crystallization of ceria and formation of oxygen vacancies.

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P.S.C.5.

Characterization of mechanochemically synthesized CuInS₂/ZnS nanocomposite

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Many ternary chalcogenide nanocomposites have found applications in various fields, namely in bioimaging technology. In such case, at least one component of nanocomposite must have good optical properties and cannot be toxic for living organisms. In this paper the CuInS₂/ZnS nanocomposite was synthesized by dry mechanochemical synthesis. CuInS₂/ZnS mixed nanocomposite have been prepared by a two-step solid-state mechanochemical synthesis. CuInS₂ has been prepared from copper, indium and sulphur precursors in the first step. The obtained tetragonal CuInS₂ was then mixed in the second step with the cubic ZnS synthesized mechanochemically from the zinc acetate and sodium sulphide precursors. The obtained nanocrystals were characterized from the structural point of view by X-ray diffraction analysis and Raman spectroscopy, from the microstructural point of view by high-resolution transmission microscopy and from the morphological and surface point of view by scanning electron microscopy and specific surface area measurements. Its optical properties were also studied using UV-Vis absorption and PL emission spectroscopies. The prepared CuInS₂/ZnS nanocomposite could serve as labeling medium because of its extraordinary properties.

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P.S.C.6.

Preparation and characterization of nanostructured silver supported on carbonaceous material obtained by hydrothermal carbonization process

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The wide range of carbon nanostructures and properties provides attractive opportunities for various applications: environmental protection, energy-storage and conversion, in catalysis, for sensors and actuators, etc. Due to their biocompatibility there are various applications in medicine and pharmaceutical industry. In this study the influence of nitric acid and fructose concentrations and process temperature on the size of silver nanoparticles were examined. Hydrothermal carbonization process was chosen for materials preparation. The advantages of this process besides low cost is the possibility of using cheap, readily available precursors. The obtained samples were characterized by XRD analysis, scanning electron, and atomic force microscope, EDAX, for microbial activity. Nanostructured silver supported on carbonaceous material was obtained. Results have been shown that the dependence of these process parameters on the silver particle size exist.

P.S.C.7.

Morphological, microstructural and magnetic characteristics of electrodeposited Ni-Fe-W-Cu alloy powders

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Nanostructured Ni-Fe-W-Cu alloy powders were electrodeposited from an alkaline ammonium citrate solution on a titanium cathode. Powder particles were dendrite- and cauliflower-shaped. The dendritic particles had a high density of branches made up of interconnected globules. XRD analysis showed that the powder contained an amorphous matrix and FCC nanocrystals of the solid solution of Fe, W and Cu in Ni. As the deposition current density increased, the mean nanocrystal size decreased, and the mean value of internal microstrain and the total weight percent of Fe and Ni in the alloy increased. The powders deposited at higher current densities exhibited higher magnetization. During annealing at temperatures up to 460°C, the powders underwent short-range ordering, which caused an increase in magnetization, whereas at temperatures above 460°C, the magnetization decreased due to the formation of large FCC crystalline grains.

P.S.C.8.

Adsorption of arsenic(III) from aqueous solution on carbon cryogel and carbon cryogel/ceria composite

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In this study we compared arsenic(III) adsorption on pure carbon cryogel and on carbon cryogel/ceria composite. Both materials were characterized using following methods: nitrogen adsorption-desorption measurements, field emission scanning electron microscopy (FESEM), temperature programmed desorption (TPD) and Raman spectroscopy. Also, point of zero charge (PZC) was determined. Adsorption of As(III) from aqueous solution on both synthesized materials was investigated as a function of contact time, arsenic concentration and pH of the solution. The adsorption mechanism of As(III) ions was discussed in view of arsenic speciation and adsorbent PZC.

P.S.C.9.

Peculiar optical features of molecular crystalline films

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In this paper a model of molecular crystalline ultrathin film-layers and feature research methodology of exciton system as well as analysis of dielectric properties of these spatially very restricted structures with perturbed fundamental parameters on surfaces were presented. The two-time Green's functions adapted to symmetry breaking crystalline structures were used with our own developed numerical-graphical software and the dynamic permittivity in the direction normal to the boundary surfaces was calculated. It was shown that the possible appearance of localized states in the surfaces define schedule and determine the number of the resonant absorption lines in the near infrared area of the external electromagnetic radiation. These occur in the ultrathin structure instead of continuous absorption area in the corresponding bulk. It is important fact in (nano) optical engineering as well as in nanomedicine, for the potential construction of nanomarkers, nanocarriers and nanodelivers of drugs or appropriate nanoequipment.

P.S.D.1.

Lipid production with a high palmitoleic acid content by *Debaryomyces globosus* yeast under conditions of continuous cultivation

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Palmitoleic acid (POA) is an important fatty acid for pharmaceutical applications. On industrial scale, POA is produced from animal fats, macadamia oil and sea buckthorn oil.

In this paper, the effect of the nature of the growth-limiting component (ethanol and zinc) on lipid- and POA production was studied in a constitutive lipid producer *Debaryomyces globosus* VKPM Y-953 using a chemostate regimen at $\mu=0.05 \text{ h}^{-1}$ with limitation of cell growth by nitrogen. It was found that a large amount of lipids (27.8% of the dry biomass) was synthesized under limitation cell growth by nitrogen; in this case the amount of POA consisted of 37.5% of sum of fatty acids or 10.4% of the dry biomass. The limitation of cell growth by zinc resulted in the decrease in lipid content in 3 times and POA accumulation on 22%.

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P.S.D.2.

New multifunctional materials based on steel slag

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Electric arc furnace slag (EAFS) is the by-product of steel production in an electric arc furnace. In a past two decades a special attention is paid to the valorization of metallurgical slags by alkali activation. The process involves a chemical reaction of slag with the alkaline activator followed by the condensation and hardening processes. Aluminium-containing calcium silicate hydrate gel i.e. C-(A)-S-H gel with a low C/S ratio has been identified as a reaction product of slag alkali activation.

We have synthesized the AAS using the EAFS as the precursor and Na₂SiO₃ solution as an activator. The AAS samples are characterized by XRD, SEM/EDS and FTIR analysis. Moreover, investigation of mechanical properties dilatometric and porosity analysis were performed as well so as to build up a detailed illustration of AAS properties and possible application of these materials.

The results have shown that AAS may reach the compressive strength (~ 40 MPa) which enables its application in a civil engineering. Moreover, the AAS sample exhibits improved strength (~ 50 MPa) at elevated temperatures thus potential application of these materials in a high temperature conditions should be considered. On the other hand, these materials may be used as an effective adsorbent for the Cu²⁺ removal from sulfate bearing wastewater. The Cu₂⁺ ions have been found to be attached on the surface of AAS by formation of stable hydroxocomplexes that are sorbed on the adsorbent surface via hydroxyl groups in the form of posnjakite crystal phase.

P.S.D.3.

Biological markers of the petroleum alkane fraction as a forensic tool for determining the presence of petroleum pollutants in the environment

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Normal alkanes, isoprenoid aliphatic alkanes, and polycyclic alkanes of the sterane and terpane type are biological markers of the crude oil alkane fraction. Since oil is the most mature form of the organic substance of the geosphere, these organic compounds have distributions characterized by the dominance of thermodynamically the most stable isomers. These distributions can be considered typical for oil (as "finger prints"). On the other hand, in the native organic matter of recent sediments, soils and ground and surface waters as the segments of the environment, these hydrocarbons characterize the distribution with the dominance of biolipid, isomers. They have a significantly lower degree of thermodynamic stability. Thanks to these differences, alkane biological markers could be used as a tool for determining the presence of petroleum pollutants in the environment. In this paper, an attempt was made to prove this assumption in the case of waters, coastal sediments and river sediments of the Vrbas River in the territory of the city of Banja Luka.

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P.S.E.1.

Addition of porogens improved the characteristics of biodegradable implants made of poly(-caprolactone)/calcium phosphate ceramic composites

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Metal implants are routinely used in fixations of bony fragments. However, the excessive mechanical strength causes bony atrophy and/or disuse osteoporosis because of the implants stress-shielding effects and strain-induced bone resorption. The mechanical strength of pure biodegradable polymer fixators is insufficient, and most of these materials are non-radiopaque which are difficult to evaluate the placement postoperatively and difficult to investigate the degradation of the bioabsorbable fixation devices. Therefore, we designed a new composite made of calcium phosphate ceramic (CPC, including tricalcium phosphate [TCP] and tetracalcium phosphate/dicalcium phosphate [TTCP/DCP]) and poly(-caprolactone) (PCL) to fabricate biodegradable orthopedic fixators. After implantations, for these composites dissolved slowly, some porogens had been applied to improve the characteristics of these composites. In this study, calcium sulfate (CS) and strontium (Sr) were added into poly(-caprolactone)/calcium phosphate ceramic (PCL/CPC) composite for fabricating biodegradable orthopedic fixators. The dissolution of CS and Sr can create porous structures in implants. In the meantime, CS can provide calcium ions for hydroxyapatite formations. Moreover, CS can upregulate osteoblasts and inhibit osteoclasts. The strontium has been dispensed clinically as an anti-osteoporosis regimen which improves osteoblast's functions and depresses those of osteoclast. Different weight ratios of CS or Sr are added into the PCL/CPC. We examined the mechanical properties, microstructure, degradation time, and the material mediated cytotoxicity of PCL/CPC/CS and PCL/CPC/Sr composites. The degradation pattern will be established. After the in-vitro study, the formula of PCL/CPC/CS and PCL/CPC/Sr will be selected to prepare the bone screws, which are implanted into rabbit femurs. Computed tomography and histologic examination will be applied to evaluate the in-vivo performance and osseointegration of these new implants. The results revealed that the addition of CS accelerates the biodegradation and enhanced apatite formation of the PCL/ CPC composite screw. In PCL/CPC/Sr group, the Sr-impregnated bone fixator improves osseointegration in osteoporotic animals.

P.S.E.2.

The application of hydroxyapatite as the *Bletilla striata* polysaccharide carrier for sarcopenia treatment

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Sarcopenia is a disease of muscle mass loss and muscle function decline caused by aging. There are no effective drug without side effects to treat sarcopenia. *Bletilla striata* is a chinese herb. The polysaccharide isolated from *Bletilla striata* (BSP) have wound healing and anti-inflammatory property. But BSP is easily broken down in the body, so we need drug carrier to prolong drug effect. Hydroxyapatite (HAp) is one of the components of bones and teeth in the human body, has well biocompatibility and biodegradability. This study will develop hydroxyapatite particles as drug carriers carrying BSP (HAp-BSP, BHAp); it also may provide patients with calcium ions which lack in the body and reduce the drug injection frequency. In this study, we will perform the material test, in vitro cell biocompatibility test and in vivo test. In this study, we successfully to induce muscle injury that similar to sarcopenia, and HAp-BSP could decrease the symptoms caused by induced. It was confirmed that HAp-BSP had its anti-oxidation and promoting tissue capacity.

P.S.E.3.

Hydroxyapatite/gelatin particles embedding stromal cell-derived factor-1 for bone tissue engineering

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A bone fracture is a damage in the continuity of the bone, which may be the result of high force impact or stress, osteoporosis, osteopenia, bone cancer, or osteogenesis imperfecta. Bone grafts or bone tissue engineering are the use of a combination of cells, engineering and materials methods to improve or replace biological tissues. For the bone grafts, there are three critical properties in bone tissue engineering, osteoinduction, osteoconduction, and osteogenesis. However, most of bone tissue engineering lacks osteoinduction. Stromal cell-derived factor-1 (SDF-1) is a well-characterized chemokine for attracting stem cells and thus a strong candidate for promoting regeneration. Therefore, the purpose of this study is to develop an osteoinductive bone graft, hydroxyapatite/ gelatin particles loaded with stromal cell-derived factor-1 for bone tissue engineering. In primary results, the particles synthesized by spattering in three hundred micro-meter to five hundred micro-meter, and the component was similar to the natural bone. In vitro study, there was no cytotoxicity in the particles, and stem cells differentiated or develop into preosteoblasts co-culture with particles. All the results indicated hydroxyapatite/ gelatin particles, which is osteoinductive bone grafts could use to bone tissue engineering for bone regeneration.

P.S.E.4.

A novel multilayer capsule as desensitizing agent for dental hypersensitivity

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Dental Hypersensitivity (DH) is a very common oral disease in Taiwan. According to the statistics, over 30% Taiwanese suffer the dental hypersensitivity and most of them have no cognition with the disease. However, the therapeutic of DH currently is filling the Dentin Pore with Calcium Phosphate Minerals (CPM), which is a mechanical filling and is not able to completely fit the dentin pore. In this case, we developed a new multilayer capsule for dentinal tubules filling. The material characteristics could not only evaluate the adhesion between capsules and dentin pore but enhanced the regeneration ability of dentin. The capsules filled in dentin pore could provide a microenvironment for dentin regeneration and avoid the stimulate. As the materials used in capsules fabricating are biodegradable, the capsules in dentin pore would degrade after dentin regenerate. We expect the capsules might be a long-term treatment for dental hypersensitivity.

P.S.E.5.

Electrospun silk fibroin composite scaffold for tendon repair

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Applying electrospun nanofibers to the regenerative medicine is an emerging field. Electrospinning is a remarkably simple, robust, and versatile technique capable of generating fibers with diameters down to the nanoscale. A number of approaches to fabricate scaffolds from electrospun nanofibers have been developed. We developed a new strategy for tendon repair by using electrospun silk fibroin (SF) composite scaffolds. The silk fibroin composite has 3D aligned silk fibers and high porosity. It also incorporated bioactive molecules to mimic the native tendon architecture and provide biomimic microenvironment. Experimental results demonstrated that primary tenocytes exhibited better native spindle-shaped morphology, cell infiltration and cell proliferation on the silk fibroin composite (tendon-ECM supplemented scaffold) compared with SF scaffold. In addition, SF/tendon-ECM scaffold in promoting injured tendon repair was more efficiency than SF scaffold in rat tendon injured model. All the results suggest silk fibroin composites can improve tendon tissue engineering to facilitate tendon repairing.

P.S.E.6

BMP-2 and insulin delivered from plasma synthesis of carbon-based nanocarriers for bone regeneration

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Insulin and bone morphogenetic protein-2 (BMP-2) have been widely used in the fields of tissue engineering stimulate bone formation. The aim of this study was to determine whether Insulin and BMP-2 are involved in the homing of human mesenchymal stem cells (hMSCs) for bone regeneration and to innovate strategy of developing the carbon-based nanocarriers as drug delivery systems. We evaluate the properties of carbon-activated plasma-polymerized nanoparticles (nanoP3) can be synthesized in dusty plasmas with tailored properties; this includes an examination of how the different features of carbon nanocarriers affect tissue growth, how these properties to them might be leveraged in regenerative tissue therapies and how substances jeopardize their toxicity and biological interaction. In vitro, both Insulin and BMP-2 also have been confirmed to induce the homing of hMSCs. Observations based on ALP activity, type I collagen, OC gene expression, and mineralized formation were increased in the BMP-2 and insulin-treated group compared with control group. These findings support our hypothesis that the localized release of Insulin and BMP-2 promote bone regeneration.

P.S.E.7.

Rare earth dual-doped multifunctional hydroxyapatite particles for potential application in preventive medicine

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Composite biomaterials based on nano hydroxyapatite (HAp) are the subject of numerous studies in reconstructive medicine. Multifunctional and nanoparticulate systems based on HAp and biodegradable polymers are successfully designed as systems for controlled and systemic drug delivery suitable for use in reconstructive medicine. Thanks to the stability and flexibility of the apatite structure, Ca ions can be replaced with various elements (Zn, Sr, Mg, Co, etc.). Doping the apatite structure enables potential application of this material in preventive medicine, too. Multimodal imaging (MI) is a new and promising technique for improved diagnosis and it is patient-friendly because it saves time. MI has recently attracted much attention due to the advantageous combination of various imaging modalities, such as computer tomography (CT), photoluminescence (PL) and magnetic resonance imaging (MRI). For such a promising approach, we devised new multimodal contrast agents using the doping of a HAp matrix with rare earth (RE) ions.

Pure HAp ($\text{Ca}_5(\text{PO}_4)_3(\text{OH})$), magnetic HAp:Gd ($\text{Ca}_{4.85}\text{Gd}_{0.15}(\text{PO}_4)_3(\text{OH})$), down-converting HAp:Gd,Eu ($\text{Ca}_{4.94}\text{Gd}_{0.02}\text{Eu}_{0.04}(\text{PO}_4)_3(\text{OH})$) and up-converting HAp:Gd,Yb/Tm ($\text{Ca}_{4.85}\text{Gd}_{0.03}\text{Yb}_{0.1}\text{Tm}_{0.02}(\text{PO}_4)_3(\text{OH})$) were synthesized using a hydrothermal procedure. Morphological and structural characteristics of the particles were obtained using X-ray powder diffraction (XRPD), scanning and transmission electron microscopy (SEM/TEM), energy dispersive X-ray spectrometry (EDX), photoluminescence (PL), Fourier Transform Infrared (FTIR) and diffuse reflectance spectroscopy (DRS). The results show that needle-like nano- or microparticles were obtained in all systems. Their phase composition and uniform distribution of dopants were confirmed by the structural refinement of the XRPD data, change in the band gap, and luminescence spectra recorded using different excitation sources ($\lambda = 370, 394$ and 977 nm).

P.S.E.8.

The processing and application of modified dental composites and dental inserts based on Mg-doped HAp

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Bioceramic dental inserts reduce polymerization shrinkage and improve the mechanical properties of insert-containing dental restorations. The aim of this study was to investigate the possibilities for processing of dental inserts based on Mg-doped HAp and to investigate potential application by determination of shear bond strength (SBS) between inserts and different restorative materials. The possibility for modification of dental composite with calcinated Mg-doped bioceramic fillers was also investigated. Hydrothermally synthesized HAp powder doped with Mg was calcinated in order to obtain bioactive fillers. Obtained fillers were used instead of 10 wt. % of commercial glass fillers for processing of dental composites based on Bis-GMA/TEGDMA resins. The values of hardness and flexural strength before and after storage in SBF were in the range of commercial composites. Mg-doped HAP powder was sintered in order to processed cylindrical dental inserts. Application protocols significantly affected SBS between obtained dentin substituents and different commercial adhesive materials.

P.S.E.9.

Hybrid dental composites with improved mechanical properties

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Poly(ethylene oxide)-based oral films and nanofibers, as novel oral dosage forms, exhibit better patients compliance and improved formulation properties such as high drug load, uniform drug distribution and increased dissolution rate of e.g. poorly soluble carvedilol in comparison to the pure drug. This study aimed to assess the expected carvedilol plasma concentration-time profiles following oral administration of the selected oral film and nanofibers using physiologically-based *in silico* modeling. The design carvedilol-specific absorption model was validated by comparison with the *in vivo* data from literature. The simulations revealed that orally administered carvedilol is mainly absorbed from the proximal intestine and undergoes extensive hepatic first pass metabolism, while changes in drug release rate additionally modulate drug absorption pattern. The obtained results also indicate that carvedilol administration via oral film and nanofibers would result in similar extent of drug absorption as with conventional immediate-release tablets, but with notably higher maximum plasma concentration values.

Acknowledgement: Projects No. TR34011 and TR34007, Ministry of Education Science and Technological Development, Republic of Serbia.

P.S.E.10.

Biomimetic evaluation of novel β -TCP/alginate macroporous scaffolds in perfusion bioreactors for potential in bone tissue engineering

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The aim of this work was to investigate possibilities for production of novel macroporous scaffolds based on alginate hydrogels with addition of β -tricalcium phosphate (β -TCP) and to characterize the best candidates in perfusion bioreactors for potential use in bone tissue engineering. We have examined influence of two alginate concentrations (1.5 and 2 % wt.) and four β -TCP concentrations (0.5, 0.67, 1.5 and 2 % wt.). In addition, two preparation methods were examined. Produced samples were characterized regarding mechanical properties in a bioreactor with dynamic compression (337.5 $\mu\text{m/s}$ rate, 0.42 Hz frequency, 10 % deformation). Scanning electron microscopy has shown uniformly dispersed inorganic phase in all obtained scaffolds and different macroporous structures depending on the preparation method. The best scaffolds had the dynamic modulus of ~ 230 kPa. β -TCP stayed preserved over 7 days of continuous perfusion in bioreactors while after 14 days of perfusion hydroxyapatite crystals were noticed within selected scaffolds.

P.S.E.11.

The morphology of the osteoporotic rabbit bone after implantation of strontium doped biphasic ceramic

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Introduction. Strontium (Sr) doped biomaterials influence on bone mineralization, resorption, growth and differentiation was an aim of our research.

Methods. 37 osteoporotic rabbits were used. A 4 mm bone defect of right trochanter was filled with granules of 70% hydroxyapatite (HA), 30% tricalcium phosphate (TCP) and 5% of Sr in 7 rabbits; HA(70)/TCP(30) in 7 rabbits. Following groups contained the material without Sr. Controls included sham bone, unaffected leg and intact bone. Bone were analysed by immunohistochemistry.

Results. Only the volume of intact bone statistically significantly differed from all other groups. The relative number of OC, OPG, NFkB105 and BMP2/4-containing cells was higher in the femur with biomaterial. Only OPG elevated significantly, but Runx2 showed variable expression. Conclusions. Different biomaterial and Sr implantation of 12 weeks doesn't change the osteoporotic bone volume. The Sr doped biphasic ceramic increases the suppression of osteoclastogenesis and stimulates the bone regeneration and development.

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P.S.E.12.

Spider silk coated with maghemite nanoparticles-synthesis and characterization

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Spider silk (SS) is a biopolymer that outperforms some of the strongest natural or man-made materials known. Spider silk collected from *Pholcus phalangioides* spider was used as a template for obtaining SS coated with superparamagnetic maghemite nanoparticles (γ -Fe₂O₃ NPs). As a result, strong composite fibers responsible in a magnetic field were obtained. The material was synthesized by simple one-pot precipitation technique. X-ray diffraction analysis of the sample confirmed the presence of maghemite nanocrystalline phase, and EDS measurements confirmed the presence of iron oxide in the composite. According to SEM, it could be seen that the SS fibers were completely and homogeneously covered with γ -Fe₂O₃ NPs and HRTEM was used to estimate the size of maghemite NPs. SQUID analysis were used to describe magnetic properties of the obtained composite.

P.S.E.13.

Cefazolin-loaded polycaprolactone fibers produced via blend and co-axial electrospinning

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This paper investigated the production of cefazolin-loaded polycaprolactone (PCL) fibers that can be used as antibiotic delivery system. A special precedence of this delivery system is a possibility of delivering high controlled doses of antibiotic to the exact location of the necessary application. Cefazolin-loaded PCL fibers were produced by using blend and co-axial electrospinning method. The results of the drug release profiles of the blend and co-axial electrospun fibers was about 50 % and 30 %, respectively, after a period of 15 days. Antibacterial test showed that cefazolin-loaded PCL fibers had better effects on *Staphylococcus aureus* when compared to *Escherichia coli*. According to the obtained results, the cefazolin-loaded PCL fibers could have a role as antimicrobial material, for various medical applications, such as antibacterial gauzes, catheters, the treatment of urinary tract infections, etc.

P.S.E.14.

In silico simulation of carvedilol absorption from oral films and nanofibers

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Poly(ethylene oxide)-based oral films and nanofibers, as novel oral dosage forms, exhibit better patients compliance and improved formulation properties such as high drug load, uniform drug distribution and increased dissolution rate of e.g. poorly soluble carvedilol in comparison to the pure drug. This study aimed to assess the expected carvedilol plasma concentration-time profiles following oral administration of the selected oral film and nanofibers using physiologically-based *in silico* modeling. The design carvedilol-specific absorption model was validated by comparison with the *in vivo* data from literature. The simulations revealed that orally administered carvedilol is mainly absorbed from the proximal intestine and undergoes extensive hepatic first pass metabolism, while changes in drug release rate additionally modulate drug absorption pattern. The obtained results also indicate that carvedilol administration via oral film and nanofibers would result in similar extent of drug absorption as with conventional immediate-release tablets, but with notably higher maximum plasma concentration values.

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P.S.E.15.

Stability of the magnetite particles dispersed in different surfactans using wet stirred media milling

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Magnetite (Fe_3O_4) based particles are widely studied because of their interesting magnetic properties and low toxicity. Therefore they have found applications e.g. in magnetic data storage, ferrofluids or drug delivery system research. The combination with the optically active material, e.g. zinc sulphide (ZnS), can extend their spectrum of properties. Such bifunctional composite materials with both magnetic and fluorescent properties are very desirable, mostly for their potential applications in optoelectronic and biomedicine. In a first step, the Fe_3O_4 and $\text{Fe}_3\text{O}_4/\text{ZnS}$ particles were prepared by co-milling of natural magnetite (Kiruna, Sweden) and precursors for ZnS ($(\text{CH}_3\text{COO})_2\text{Zn} + \text{Na}_2\text{S}$). Subsequently, these materials were capped by three types of non-toxic, biocompatible surfactants (non-ionic, cationic and anionic) using wet stirred media milling. The properties from the structural, morphological, optical and especially physical stability point of view were studied. The most suitable capping agent was cationic one, chitosan. In such a system, unimodal particle size distribution was obtained with the best stability properties. The size of the particles was ~ 210 nm with the high zeta potential values ~ 80 mV. Such a system could be further tested for targeted and bio-imaging applications.

P.S.E.16.

Electrochemical characterization of Mg-Zn bulk materials prepared by powder metallurgy Method

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Magnesium alloys can be used in medicine as bone implants or stents. Magnesium is nontoxic and commonly found in human body. Mechanical properties of magnesium materials and human bones are similar and because of biodegradable behaviour, magnesium facilitates treatment after insertion of implant, since no further surgery is required to remove the implant. This work deals with the study of electrochemical properties of powder materials based on Mg with 1, 5 and 10 wt. % Zn prepared by hot pressing at 300 and 400°C. The influence of chemical composition, structure and their final properties on corrosion mechanism and rates is determined by electrochemical impedance spectroscopy (EIS) and immersion test in the simulated body fluids. The corrosion resistance of prepared materials increased with zinc content and compaction temperature. In the case of materials with 1 and 5 wt. % prepared at 300°C layer mechanism of corrosion was detected, porosity of the materials and subsequent penetration of electrolyte into the pores may be the reason of this behaviour. Material with 10 wt. % prepared at 300°C corrodes uniformly over the entire surface likely due to uniform distribution of the intermetallic phase. In the case of materials prepared at 400°C the trend was the opposite. Materials with 1 and 5 wt. % Zn corrode uniformly over the entire surface and the material with 10 wt. % Zn showed layer mechanism of corrosion. This is probably due to the microgalvanic corrosion between the matrix and the intermetallic phase.

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P.S.E.17.

Improvement of biocompatibility by formation of nanotubular oxide layer on the ultrafine grained Ti-13Nb-13Zr alloy

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To improve their biological properties, biomaterials typically need some surface modification. These surface modifications can be classified into four categories: physical, chemical, mechanical and biochemical. One of the most commonly used methods is the electrochemical anodization, which is a simple process used to form nanotubular oxide layer on the metal surface by oxidation. In the present study, nanotubular oxide layer was formed on coarse-grained (CG) Ti-13Nb-13Zr alloy and ultrafine-grained (UFG) Ti-13Nb-13Zr alloy, obtained by high pressure torsion, using electrochemical anodization in the 1M H₃PO₄ + NaF electrolyte, during 60 minutes and 90 minutes. The scanning electron microscope (SEM) was used to characterize the surface and it showed that homogenous nanotubular layers were obtained by anodization during 90 minutes, while anodization during 60 minutes produced inhomogeneous nanotubular oxide layer. Also, the results show that the nanotubular oxide layer on the UFG Ti-13Nb-13Zr was more homogeneous than the one on CG material. The aim of this study is to determine the in vitro biocompatibility of the titanium alloy before and after electrochemical anodization during 90 minutes. In vitro nanotubular oxide layer examinations were performed on the human (MRC-5) and animal (L929) fibroblast cells lines. The cytotoxicity of the examined materials was measured as a percent of cell growth inhibition using in vitro colorimetric methyl-thiazol-tetrazolium (MTT) test. Results show that nanotubular oxide layer formed on the UFG Ti-13Nb-13Zr alloy during 90 minutes allow better cells contact and spreading along nanotubular surface.

P.S.E.18.

The longterm chemical degradation of magnesium alloy AZ31 and AZ61 processed by method squeeze casting in SBF solution

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The long-term chemical degradation of magnesium alloys AZ31 and AZ61 processed by method squeeze casting in simulated body fluid solution (SBF) were evaluated in depending on alloy compositions, time duration, and released amount of degradation products and pH level changes. The chemical degradation was realized during several time intervals from 24 to 1008 hours and alloys AZ31 and AZ61 were immersed in Hank's solution with various salt concentrations. The pH changes were determined electrochemically; alloys compositions and released amount of degradation products were determined using spectrometrically (GDS glow discharge emission spectrometer and AAS atomic absorption spectrometry). The results confirmed the important role of chemical heterogeneity of AZ31 and AZ61, type of SBF and time dependence of degradation.

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P.S.E.19.

Crystal structures of mixed chloride-azide zinc (II) and chloride-isocyanate cadmium (II) complexes with the condensation product of 2-quinolinecarboxaldehyde and girard's reagent

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The mixed chloride-azide $[\text{ZnL}(\text{N}_3)_{1.65}\text{Cl}_{0.35}]$ (1) and chloride-isocyanate $[\text{CdL}(\text{NCO})_{1.64}\text{Cl}_{0.36}]$ (2) complexes have been prepared in the reactions of (E)-N,N,N-trimethyl-2-oxo-2-(2-(quinolin-2-ylmethylene)hydrazinyl)ethan-1-aminium chloride (HLCl) and the corresponding Zn^{2+} and Cd^{2+} salts by adding the NaN_3 and NaOCN , respectively. The structures of complexes 1 and 2 were determined by X-ray crystallography.

In complexes 1 and 2, Zn_1 and Cd_1 ions, respectively, are five-coordinated in a distorted square based pyramidal geometry with NNO set of donor atoms of deprotonated hydrazone ligand and two monodentate ligands N_3^- and/or N_3^- and Cl^- in the case of 1 and OCN^- and/or OCN^- and Cl^- in the case of 2.

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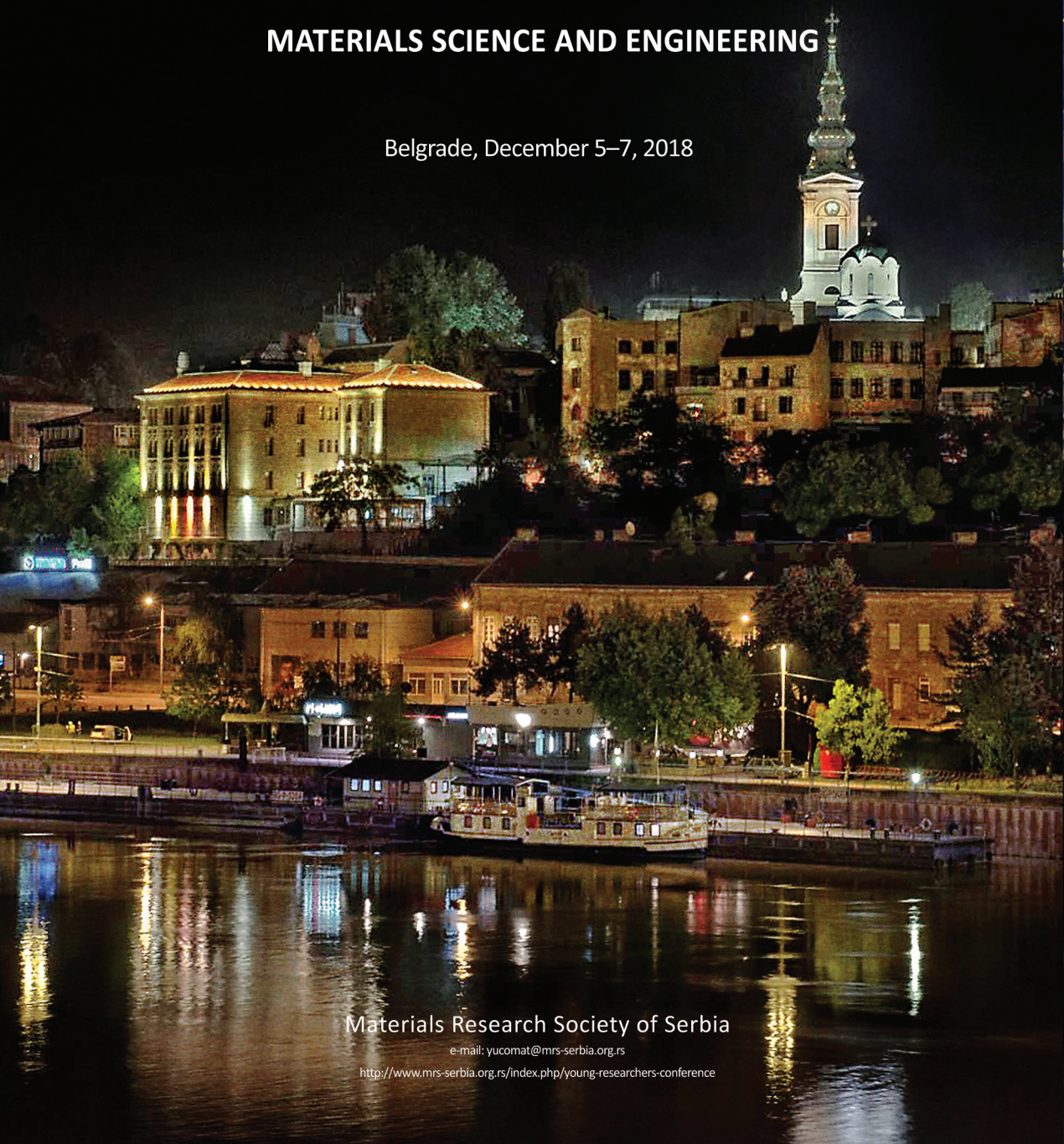
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