

### Serbian Ceramic Society Conference ADVANCED CERAMICS AND APPLICATION V New Frontiers in Multifunctional Material Science and Processing

Serbian Ceramic Society
Institute of Technical Sciences of SASA
Institute for Testing of Materials
Institute of Chemistry Technology and Metallurgy
Institute for Technology of Nuclear and Other Raw Mineral Materials
School of Electrical Engineering and Computer Science of Applied Studies

## PROGRAM AND THE BOOK OF ABSTRACTS

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properties. Such circumstance limits the use of constitutive models with linear elasticity followed by appropriate hardening law, and a more general framework is required, in which elastic properties are dependent on plastic deformation. The use of complex constitutive model which takes into account elasto-plastic coupling, makes the numerical implementation challenging as the number of parameters to calibrate significantly grows, while some of them require high pressure experiments, or experimental setups that are inducing complex state of stress, which can make the industrial application potentially difficult.

An alternative and advantageous strategy for such calibration is based on the employment of inverse analysis (IA) methodology. Advantages consist in more accurate and more economical transition from experimentally measured quantities to material constitutive parameters, which are of major interest for reliable simulation of compaction process. The IA methodology is centered on appropriate minimization of a "discrepancy function" designed to quantify the difference between measured quantities and their computed counterparts. By adopting this strategy for parameter calibration of constitutive models used for powder compaction simulations, it is possible to completely eliminate the need for performing experiments on a green body. This goal requires an adequate modification of compaction tools to stimulate the sensitivity of measurable quantities to sought parameters. The fulfillment of this objective is assured by appropriate design of experimental setup, achieved through sensitivity analysis.

The purpose of this lecture is to present some of the advancements within the above outlined technology, pointing out limitations of currently applied techniques. Results from different approaches of modeling of powder compaction processes will be comparatively presented. Particular emphasis will be given to the employment of inverse analysis methodology for the calibration of constitutive models in a given context. Results recently achieved by our research team will be shown considering the above-mentioned and related topics.

#### INV9

# Comparative fractal analysis of *Valeriana officinalis* roots shrinkage during drying

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Valerian plant roots (Valeriana officinalis)shrinkage was investigated during the convective hot air drying. Combined fractal and image analysis was performed in this study. The samples were prepared for light microscopy observation by standard paraffin wax method, sectioned by sliding microtome and stained by Alcian blue and Safranin. The fractal dimensions of sample images were calculated using the box counting method. Both polar and orthogonal meshes were used. The normalized changes of fractal dimension of the microstructural images were used to describe the shrinkage process of biomaterial. The changes of physical properties and microstructure of roots strongly depends on drying regime and drying agent properties. Comparative analysis of fresh and dry root samples shows that microstructural changes in bio material can be

correlated with drying parameters during the dehydration process. Fractal dimension was found to be a good indicator of the microstructural changes of aninvestigated bio-material.

#### INV<sub>10</sub>

## Silica particles with controlled roughness – synthesis, characterization, and use as building blocks for non-close packed arrays

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Silica nanoparticles are widely used in many applications. The reactivity and the interactions of such particles with surfaces are not only determined by their size and chemical functionalization but also by their surface roughness. Nonetheless, an exact characterization of the surface roughness of nanoparticles on a nanometer scale is challenging and different techniques lead often to significantly deviant results. Hence, a systematic investigation of this issue is highly demanded. In the present study, silica particles of 100-500 nm diameter with different surface roughnesses were prepared by a novel method yielding highly monodisperse particles on a several gram scale. Their roughness is tuned by using different tetraethyoxysilane (TEOS) to octadecyltri-methoxysilane (ODS) ratios. Other approaches for controlling the surface roughness including the approach of Hartlen et al.[1] and the use of CTAB (cetrimonium bromide) as a pore builder are also discussed.

BET was applied for the determination of the total surface area and the porosity of the particles. However, this method yields only indirect information on the extent of the outer surface area and the related surface roughness. In addition, the results are influenced by the decreasing polarity of inner and outer surfaces with increasing ODS:TEOS ratios. Atomic force microscopy (AFM), the standard technique for the determination of surface roughness was also utilized, but accurate measurements of strongly curved small objects as in the present case are challenging. Further, a novel approach based on the analysis of TEM images for determining the surface roughness is presented. The results of the different techniques are compared.

In the second part of the presentation, we show that the surface roughness of silica nanoparticles is a key issue for the preparation of non-close-packed ordered two-dimensional nanostructures. [2] Such structures are needed for a variety of technological applications and consequently, the quest for simple and reliable preparation methods for such structures is ongoing. In the present approach, positively charged amino-functionalized silica nanoparticles (118-162 nm diameter) were self-assembled from dispersion on gold surfaces using a quartz crystal microbalance with dissipation monitoring (QCM-D). The resulting arrays were imaged by scanning electron microscopy (SEM). Since the particles are exerted to a drying process after the arrangement from dispersion, the system is exposed to capillary forces. To prevent aggregation of the particles during this process, the surface roughness of the particles surface is increased. By exploiting frictional forces between both systems because of the surface roughness of the nanoparticles and the gold surface the formation of aggregates during the drying process is limited. When additionally, the chemistry of the linkage between the nanoparticles and the gold surface is optimized stable well-ordered systems result. This was achieved by replacing weak dispersive