Serbian Ceramic Society Conference
ADVANCED CERAMICS AND APPLICATION IX
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

PROGRAM AND THE BOOK OF ABSTRACTS

Serbian Academy of Sciences and Arts, Knez Mihailova 35
Serbia, Belgrade, 20-21. September 2021.

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P

Development of ring-shaped specimen design using Selective Laser Sintering fabrication technique

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This paper will present the development of PRNT (pipe ring notched tension specimen) in order to create a new method for testing thin-walled pipes for which there is no standard procedure. The SLS (Selective Laser Sintering) additive production technique was used to develop these specimens. The fabrication technique was chosen because of the speed of fabrication of the specimens, while the production of a model with a relatively homogeneous arrangement of materials within the model was provided. The material from which the models are made is PA2200 (polyamide) on a FORMIGA P100 device. PRNT specimens are made in a thickness in which it is not possible to test the specimens by the standard method and have one groove with a crack. The samples were tested on a universal machine for testing the mechanical properties of materials using a specially designed tool. Based on the obtained values of tensile properties and values of fracture mechanics parameters of these specimen, it was concluded that the test process is repeatable. In addition to experimental results, numerical calculations have contributed to an easier understanding of the behavior of the specimens. The homogeneity of the obtained results was a decisive factor in the continuation of the examination of the specimens of this geometry on the samples of seam and seamless pipes.

P

Investigations of Yttrium Oxisulfide (Y_2O_2S)

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Rare-earth oxysulfides have many applications such as solar energy, wind turbines, batteries for electric vehicles and mobile phones, cathode ray tubes, metal alloys, ceramic materials and so on. Their important feature is that those materials are wide-gap semiconductors. Yttrium oxide is one of the most important compounds of yttrium and is widely used in many ceramic materials[1] RE element-doped oxysulfides has been utilized for effcient luminescent use e.g., Eu-activated Y_2O_2S emits bright red-light under cathode-ray

excitation and has been widely used for televisions[2]. In this study we perform crystal structure prediction and investigate energy landscape of Yttrium Oxisulfide (Y_2O_2S). In order to predict new crystal structures, global optimizations on the energy landscape of Y_2O_2S has been performed. Afterwards, a local optimization has been performed using ab initio calculations. In particular various quantum mechanical methods have been applied: Density Functional Theory (DFT) with Local-Density Approximations (LDA) and Generalised Gradient Approximation (GGA), and hybrid B_3LYP (Becke, three-parameter, Lee-Yang-Parr) functional.

P

Approximation and Error Prediction in Electrochemical Parameters Calculation Using Neural Networks

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Various interesting results have been achieved in calculation of electrochemical parameters in nanomaterials, using neural networks. There appear some error, during those calculations, and it varies depending on number of neurons in layers. In this research we deal with errors, calculated for neural networks with *n=1,2…10*, neurons in first or second layer. We applied mean square approximation method, in order to get explicite formula for predicton of error, for other cases.