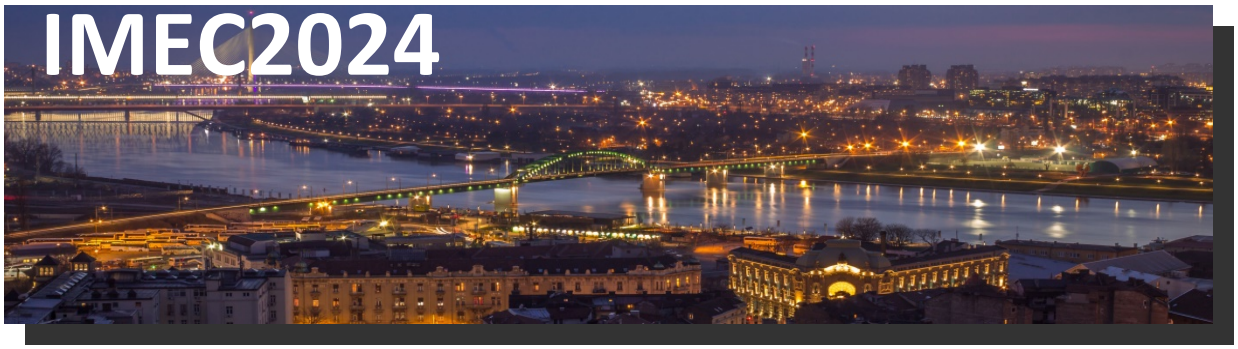
2nd International Conference on Innovative Materials in Extreme Conditions



PROGRAM

and

BOOK OF ABSTRACTS

20-22 March 2024

Belgrade, Serbia

2nd International Conference on Innovative Materials in Extreme Conditions

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Program and Book of Abstracts of the 2nd International Conference on Innovative Materials in Extreme Conditions (IMEC2024) publishes abstracts from the field of material science, physics, chemistry, earth, and computational science on the phenomena arising during the processing and/or exploitation of the innovative materials, which are presented at the international conference on innovative materials in extreme conditions.

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Preface

Dear conference participants and readers, we have the pleasure to welcome you all to Belgrade, Serbia, as the venue for the 2nd International Conference on Innovative Materials in Extreme Conditions (IMEC2024). This event is jointly organized by the Serbian Society for Innovative Materials in Extreme Conditions (SIM-EXTREME), the Center of Excellence "Center for Synthesis, Processing and Characterization of Materials for Application in Extreme Conditions - CEXTREME LAB" of the Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, and the Faculty of Mechanical Engineering, University of Belgrade.

The scope of the IMEC2024 is to become the worldwide forum for discussion of experts and young researchers on the phenomena arising during the processing and/or exploitation of the innovative materials. The IMEC2024 conference is focused on the current research in the field of material science, physics, chemistry, earth, and computational science. Experimental and computational investigations of materials obtained or operated under extreme conditions presented during the conference are highlighting recent progress in the development of the innovative materials at high pressures, under high magnetic and electric fields, over a wide range of temperatures, radiation conditions, corrosive environments, under extreme mechanical loads, and non-equilibrium thermodynamic conditions. The interrelation between external effects, microstructural characteristics, and material properties is considered on the experimental and theoretical level to obtain new or enhanced insights into the material behavior and their application.

We want to use this opportunity to thank our sponsors and co-organizers for helping us to successfully organize the IMEC2024 conference. First of all, we want to mention that the Ministry of Science, Technological Development and Innovation of the Republic of Serbia recognized our conference as an important event and gave their financial endorsement. Also, we want to thank the Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, for their strong financial support. We especially appreciate the support of the Royal Family of Serbia and the Serbian Royal Palace. In the end, we would like to thank all the members of the Conference Advisory Board, the Conference International Scientific Committee, and the Conference Organizing Committee who participated in the preparations of the IMEC2024 conference.

Editors

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PLENARY LECTURES

Rapid hot-pressed silicon carbide ceramics for ultra-high temperature applications

Pavol Šajgalík[1], Ondrej Hanzel[1], Michal Hičák[1], Alexandra Kovalčíková[1], Chengyu Zhang[2], Alexander Mukasyan[3]

[1]*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta, 9, Bratislava, 84536, Slovak Republic*

[2]*North Western Polytechnic University, Xi´An, China*

[3]*University of Notre Dame, Notre Dame IN, USA*

Freeze-granulated silicon carbide powder was densified to the full density without any sintering aids by rapid hot-pressing at temperatures from 1850 °C to 1900 °C. This densification temperature is at least 150-200 °C lower compared to the up to now known solid state sintered silicon carbide powders. This way prepared material has a high thermal conductivity of almost 200 W/mK and high electrical conductivity of 8.3×10^{2} S/m.

These additive-free *s*ilicon carbide ceramics was crept in vacuum at temperatures of 1500 °C to 1750 °C and compressive loads of 200 MPa to 400 MPa. The results showed that this way prepared ceramics had the lowest creep rate reported in the literature. The observed strain rates increased from 2.5×10^{-9} s^{-1} at 1500 °C and a load of 275 MPa to 1.05×10^{-7} s^{-1} at 1750 °C and a highest load of 400 MPa.

Static and dynamic oxidation resistance of this way prepared ceramics is excellent. The static oxidation (parabolic rate constant) at 1450 °C for 204 h was 4.9×10^{-5} mg^2/cm^4h, which is almost negligible in comparison to the parabolic rate constant 7.0×10^{-5} mg^2/cm^4h of the LPS sintered SiC materials. In the dynamic regime the ceramics sustained 1900 °C for 60 s without substantial damage, weight loss was only 0.2 %. When the oxidation was prolonged to 300 s the damage was visible but still not crucial, weigh loss was 1.6 %. It seems that this material is really suitable for ultra-high-temperature applications

Acknowledgment: This work was supported by the Slovak Research and Development Agency under the contract no. APVV-19-0497 and APVV-21-0402. The support of JRP SAV TUBITAK project No. 720464 is also acknowledged.

Hydrogen embrittlement in additively manufactured metals: A concise review

Milos B. Djukic[1*], Alireza Behvar[2], Meysam Haghshenas[2], Gordana M. Bakic[1], Dejan Zagorac[3], Aleksandar Sedmak[1], Bratislav Rajicic[1]

[1]University of Belgrade, Faculty of Mechanical Engineering, Kraljice Marije 16, Belgrade 11120, Serbia

[2]Fracture, and Fatigue Laboratory (F3L), Department of Mechanical, Industrial, and Manufacturing Engineering (MIME), University of Toledo, OH 43606, USA

[3]University of Belgrade, Vinca Institute of Nuclear Sciences - National Institute of the Republic of Serbia, Belgrade 11001, Serbia

Hydrogen embrittlement (HE) considerably influences crack initiation and propagation in additively manufactured (AM) metals exposed to static and fatigue loadings. Specifically, hydrogen during fatigue testing exacerbates the initiation and propagation of cracks in AM alloys, which are commonly characterized by AM microstructures featuring inherent defects [1]. Hydrogen within the material can expedite the initiation of cracks through various HE mechanisms. The typical HE mechanisms are plasticity-mediated HE mechanisms, i.e., the hydrogen-enhanced localized plasticity (HELP) and the hydrogen-enhanced strain-induced vacancies (HESIV), and also opposite intergranular cracking assisted by hydrogen-enhanced decohesion (HEDE) mechanism of HE [2-6]. However, the synergistic action of HE mechanisms according to the broadly accepted HELP+HEDE model for HE in metallic materials proposed by Djukic et al. [1-6] is still not widely investigated in the case of various AM alloys.

HE susceptibility to and predominant HE mechanism can vary based on the AM alloy's processing parameters and the presence of defects and residual stresses. The HE impact on crack initiation during tensile and fatigue testings is influenced by several variables, including material composition, microstructure, type of loading, and AM metal post-processing treatments. While comprehensive studies on the HE behavior of AM alloys are still relatively limited, recent literature [1] focusing on the HE behavior of AM alloys has highlighted similar microstructural effects as in the conventionally manufactured (CM) alloys on the crack initiation.

Nevertheless, still, there are conflicting conclusions that need further clarification. In this concise review article, we thematically classify the microstructure behavior and its role in HE phenomena, synergistically active HE mechanisms (HELP+HEDE mode), and crack initiation in common AM alloys [1]. Future studies focusing on the interplay between microstructure, crack initiation, and fatigue behavior of AM alloys in HE conditions will contribute to a more comprehensive understanding of the underlying mechanisms [1].

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MAX Phases: Overcoming the Challenges of Extreme Environments

Miladin Radovic
Materials Sceince and Engineerign Department, Texas A&M University, 3003 TAMU, College Station, TX 77840, USA

In the past two decades, a remarkable class of carbides, nitrides, and carbonitrides has emerged, challenging their traditional characterization as hard, difficult-to-machine materials prone to damage and thermal shock. This diverse group, comprising over 300 members, is known as the MAX phases. Defined by their common chemical formula $M_{n+1}AX_n$ (where n = 1, 2, or 3, M is an early transition metal, A is primarily group 13-16 elements, and X is either C or N), these materials have a layered crystal structure with strongly bonded MX layers interleaved by weakly bonded A layers [1-3]. The surge of interest in MAX phases stems from their exceptional and often unique blend of mechanical and thermal properties, rendering them prime candidates for structural applications at elevated temperatures. MAX phases typically exhibit high elastic stiffness, excellent thermal and electrical conductivity, resistance to chemical attacks, and relatively low thermal expansion coefficients. Remarkably, they are also comparatively soft, highly machinable, thermal shock-resistant, and damage-tolerant. Notably, certain MAX phases, such as Ti_2AlC and Cr_2AlC, exhibit outstanding oxidation resistance attributed to the formation of a protective, self-healing, and adherent alumina oxide scale. This presentation provides a comprehensive examination of the fundamental properties of MAX phases crucial for their structural application in extreme conditions, encompassing mechanical characteristics and resistance to oxidation.

This presentation first delves into the mechanical behavior of MAX phases, with a particular focus on their deformation mechanisms, including kinking and basal plane slip, stemming from their laminated crystal structure [4-6]. Anisotropic deformation and failure mechanisms in MAX single crystals and micropillars are explored in detail. Furthermore, the presentation reviews deformation and failure mechanisms below and above the brittle-to-plastic transition temperature in MAX phases, along with the influence of microstructure (e.g., grain size and secondary phases) on the observed mechanical behavior of polycrystalline MAX phases. Brief discussions also touch on possibilities for enhancing the mechanical properties of MAX phases through composition and microstructure tailoring.

Furthermore, the presentation will highlight recent advancements in understanding the kinetics of oxidation processes in MAX phases, shedding light on the intricate interplay between environmental factors and material properties [7-8]. Efects of impurities, secondary phases and grain size on the oxidation mechanism and morphology of the protective oxide layers will be discussed in mor detials. Last but not least, our recent findings on oxidation breakaway studies conducted on Ti_2AlC and C_2AlC wedge-shaped samples will be presented and analyzed

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Small-scale mechanical testing of entropy stabilized ceramics

Ravi Kumar
Laboratory for High Performance Ceramics, Department of Metallurgical and Materials Engineering, Research Center on Ceramic Technologies for Futuristic Mobility, Indian Institute of Technology Madras, Chennai 600036

Entropy stabilized ceramics of various crystal structures are being developed and some of them are processed under extreme conditions. Many times, preparing large samples are not always easy but understanding the mechanical reliability and deformation behaviour is vital for practical considerations. Small-scale mechanical testing serves the purpose but for ceramics it is always difficult. Concomitantly, developing novel testing techniques to determine specific mechanical properties is all the more challenging. Single crystal Elastic Constants (SECs) are fundamental to the understanding of the deformation behaviour of materials. SECs are also essential for micromechanical modelling of various properties, for residual stress measurements using diffraction techniques and for interpretation of seismic data in the field of geological sciences. Though the necessity for estimating SECs is well established, standard methodologies for the estimation are limited and accompanied by complexities. The most common techniques used to measure SECs are resonant acoustic spectroscopy (RUS) and the Brillouin scattering and in both these techniques sufficiently large single crystals are required. But for many of the inorganic compounds and engineering alloys, it is difficult to grow a single crystal of sufficiently large length and also of the same composition as its polycrystalline counterpart. This led to the use of computational techniques and in particular first principle density functional theory (DFT) simulations. Although DFT simulations are successful in estimating SECs for several inorganic compounds, the method fails for several new engineering alloys and also the SECs estimated using computational techniques require experimental validation. One alternate approach to estimate SECs is by *in situ* loading of polycrystalline samples in a diffractometer. Such experiments are usually carried out in synchrotron and neutron diffraction facilities. Therefore in this work, we have attempted to develop an elegant methodology wherein SECs could be determined from polycrystalline samples using a commercial laboratory X-ray diffractometer. For this purpose, a universal miniature multiaxial loading fixture was custom-built that is capable of performing *in situ* experiments by integrating it with a commercial laboratory X-ray diffractometer. Proof-of- concept experiments have been carried out using polycrystalline entropy stabilized oxide of composition (MgCuNiZnCo)O).

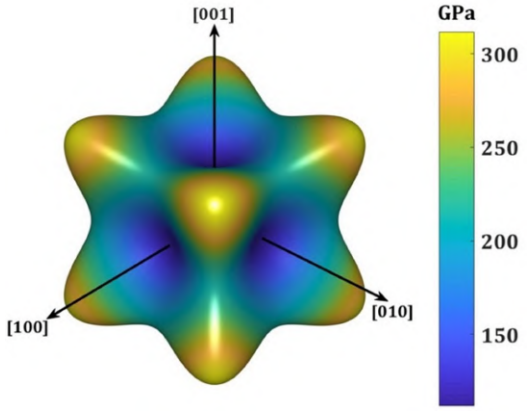

Figure 1. Orientation dependent single crystal elastic constants.

INVITED LECTURES

The high-temperature applicability of the Ti,Nb-Al-C MAX phases-based bulk materials and vacuum-arc deposited films

T.A. Prikhna[1], T.B. Serbenyuk[1], O.P. Ostash[2], V.B. Sverdun[1], A.S. Kuprin[3], B. Matović[4], I. Cvijović-Alagić[4], V.Ya. Podhurska[2]

[1]V.Bakul Institute for Superhard Materials of the National Academy of Sciences of Ukraine, Avtozavodskaya St. 2, 04074 Kiev, Ukraine

[2]Karpenko Physical-Mechanical Institute of the National Academy of Sciences of Ukraine, Naukova St. 5, 79060 Lviv, Ukraine

[3]National Science Center Kharkov Institute of Physics and Technology, Akademicheskaya St. 1, 61108 Kharkov, Ukraine

[4]Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovića Alasa 12-14, 11000 Belgrade, Serbia

The MAX phases of the Ti-Al-C system show promising characteristics for high-temperature wear-resistant applications due to their lightweight, electro-conductive behavior, and high damping and low friction abilities. During the present research the bulk Ti_2AlC, Ti_3AlC_2, and $(Ti,Nb)_3AlC_2$ were developed and their characteristics, as promising materials for the production of solid hydrogen fuel cells interconnects, pantograph, and damping substrates, were examined.

The porous Ti_3AlC_2 material was synthesized by hot pressing under low 15 MPa pressure. A significant reduction of wear of the copper substrate was achieved when Ti_3AlC_2 was applied. Namely, during friction in pair with copper its wear resistance in comparison with traditionally used Silumin was 40 times higher, and the wear of copper was 50 times smaller. Moreover, Ti_3AlC_2 demonstrated much higher arc resistance than Silumin. Moreover, the produced 5-μm-thick Ti_3AlC_2-based films, that were deposited on the Ti substrate using a vacuum-arc method from the hot-pressed target, showed extremely promising characteristics for the high-temperature applications, in particular for interconnects fuel cells and as cavitation-resistant coatings on turbines. Namely, the obtained testing results showed that after heating at 600 ^oC for 1000 h the deposited films surface electrical conductivity only slightly decreased from 0.01°Ω to 0.01-3°Ω while the surface of pure Ti after 250 h in the same regime was completely oxidized and lost its conductivity.

On the other hand, during the conducted investigation it was established that the resistance to fretting fatigue at room temperature of the samples with deposited 13.3-μm-thick coating based on the Ti_2AlC MAX phase is almost 5 times higher when compared with the samples without coating, *i.e.* 324,000 load cycles *vs* 67,000 cycles. Namely, the wear study at 500°C of the samples with a deposited coating based on the Ti_2AlC MAX phase showed significantly better wear-resistant behavior than in the case of the uncoated sample. During the mentioned testing at the initial stage the coefficient of friction, μ, increased to the same value ($\mu = 0.42$) for both sample types, however, for the uncoated sample it continued to increase over time contrary to the coated sample behavior where μ value remained stable. A significant difference was also observed in the friction track profiles: for the coated sample the friction track was quite uniform with the track depth of 3 μm, while in the case of the uncoated sample the local ridges were observed in the 7-μm-deep track. Furthermore, the specific wear rate parameter, W, turned out to be almost 2 times higher for the samples without deposited coating ($W=2.35\times10^{-3}$ mm^3/Nm) than for the samples with Ti_2AlC coating (1.27×10^{-3} mm^3/Nm).

Results of the present research indicated that the films obtained from the target with added Nb, *i.e.* $(Ti,Nb)_3AlC_2$ films, are characterized by slightly lower wear resistance than those obtained from the target based on MAX phases without Nb.

A role of micro/nano graphene platelets on strengthening and toughening mechanisms of TiB_2-SiC ceramic composites

A. Kovalčíková[1], P. Tatarko[2], Z. Chlup[3], R. Sedlák[1], E. Múdra[1], J. Dusza[1]
[1] *Institute of Materials Research Slovak Academy of Sciences, Košice, Slovakia*
[2] *Institute of Inorganic Chemistry Slovak Academy of Sciences, Bratislava, Slovakia*
[3] *Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czechia*

The role of micro/nano graphene platelets on microstructural development and mechanical properties of brittle titanium diboride-silicon carbide ceramics, mainly instrumented hardness, bending strength and chevron-notched fracture toughness was studied. TiB_2-SiC-GPs and TiB_2-GPs ceramic composites fabricated by field-assisted sintering technology at 2100°C in the argon atmosphere have been investigated.
According to the results for optimal strength and fracture toughness, the amountof microsized and nanosized oPs additive should be 2 wt. % . The increasing of GPs addition to TiB_2-20 % SiC from 1 to 10 wt. % resulted in significantly improved densification. The highest bending strength was measured for the experimental samples TiB_2-20SiC-2GPs (nanosized GPs) with the value of 729 MPa and the highest fracture toughness for the system TiB_2-20SiC-10GPs (microsized GPs) with values 6.2 MPa.$m^{1/2}$.
Fractography revealed no fracture origin in the form of processing flaws as pores or clusters after bending strength test. The toughening mechanisms on fracture lines and surface mainly in the form of crack bridging and crack branching by GPs, and pull-out of GPs were observed. Achieved results of tested mechanical properties were compared with TiB_2-SiC composites without GPLs addition and TiB_2-GPs ceramics without amount of SiC .

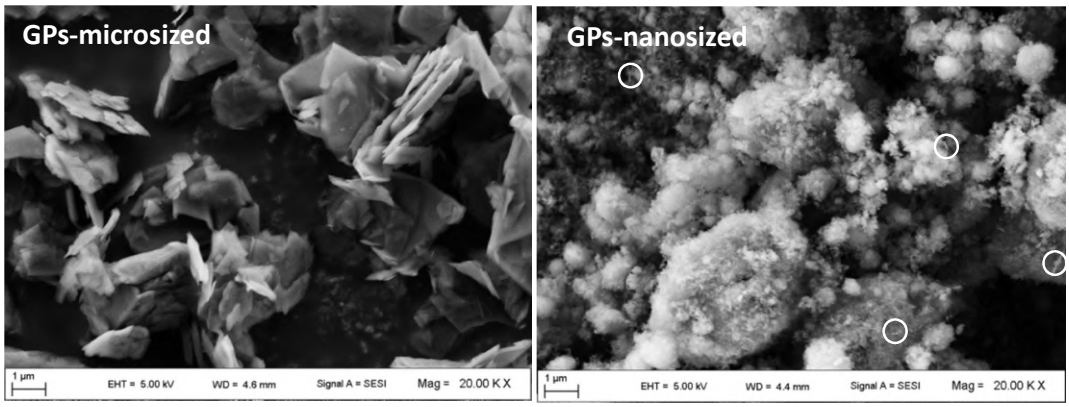

Figure 1. SEM micrograph of microsized and nanosized graphene platelets in starting powder.

Acknowledgement: This work was supported by the Slovak Research and Development Agency under the contracts no. APVV-21-0402 and APVV-22-0493.

Growth and stability of Ni_3N layers obtaiend in pure ammonia at high temperatures

Matej Fonović, Dario Kvrgić
University of Rijeka, Faculty of engineering, Vukovarska 58, Rijeka, Croatia

Nitriding is a theromchemical surface heat treatment technique, which involves inwards diffusion of nitrogen into the surface-adjacent layers of metals. For some metals this can be a desired process leading to improved properties (e.g. mechanical) of the treated material, e.g. in iron or iron-based alloys. However, in other cases, like in nickel-base superalloys, nitriding can even be regarded as a corrosion process, degenerating benificial properties [1, 2]. Various gaseous nitriding experiments on pure nickel plates were performed. Specimens were nitrided in pure ammonia (100 % NH_3), as function of time and temperature. Upon the nitriding treatment a closed Ni_3N layer is developed between 250 °C and 550 °C, which can be clearly observed after etching with the Fe^{3+} solution. A nitriding temperature of 550 °C causes a high amount of porosity in the layer, which is connected with formation of N_2 inside the solid. This process of nitride decomposition is known for occurring in iron nitrides, especially for longer periods of time, as reported in Ref. [3]. All specimens show compressive macrostresses for the Ni_3N layer. Optical microscopy investigations and measurements reveals increasing of the layer thickness with time and temperature. Similar observation of the nitrided morphology were reported before [4].

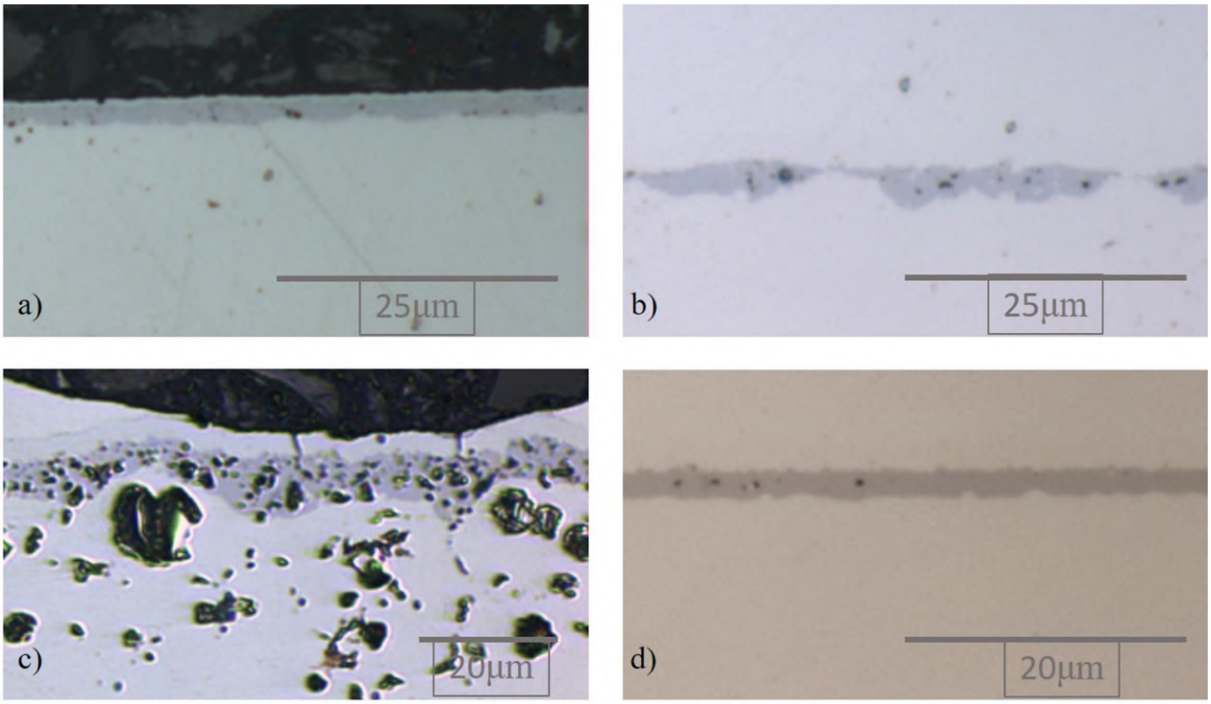

Figure 1. Light-optical micrograph showing a typical cross-sectional microstructure and morfology of developed Ni_3N upon nitriding of pure nickel in 100% ammonia at: a) 400 °C, b) 500 °C, c) 550 °C, d) 450 °C.

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Order Amidst Disorder in Multicomponent High Entropy Oxides (HEOs): Synthesis, Characterization and Applications

Subramshu S. Bhattacharya
Nanofunctional Materials Technology Centre (NFMTC), Department of Metallurgical and Materials Engineering, IIT Madras, Chennai – 600036, India

The recent interest in high entropy materials has opened up a large number of opportunities for the development of multicomponent equimolar oxide ceramics with phase-pure crystal structures. The fundamental premise appears to point to the fact that the presence of a large number of cations in a random fashion in the crystal sublattice results in its stabilization despite the high chemical disorder. Several different cases of nanocrystalline HEOs have been considered here wherein 5 or more transition metal or rare earth cations or a combination of the two have been incorporated in the crystal sublattice(s) to form a phase-pure (a) cubic rocksalt structure (transition metal based, TM-HEO), (b) fluorite structure (rare earth based, RE-HEO), (c) spinel structure (SP-HEO) and (d) perovskite structure (PE-HEO). The selection of the cations in all the cases was made on the basis of Hume-Rothery and Pauling's rules.

The phase-pure nanocrystalline powders were synthesised by wet chemical, reverse co-precipitation (RCP) processes as well as by aerosol processes (flame spray pyrolysis, FSP or nebular spray pyrolysis, NSP) using nitrate precursors. Standard characterization techniques were used to ascertain the structural and functional properties of these materials. The rocksalt type TM-HEO exhibited structural stabilisation as a single phase through the high configurational entropy. On the other hand, factors other than entropy were found to stabilize the single phase in case of the fluorite type RE-HEO. All the synthesized systems exhibited a narrow bandgap, lower than the constituent unary oxides. These studies show that multicomponent equimolar oxides form a novel class of materials that can be used in a variety of practical applications along with a wide range of tuning possibilities.

Development and Integration of Entropy Stabilized Ceramics

Peter Tatarko[1], Naser Hosseini[1], Fabrizio Valenza[2], Hakan Ünsal[1], Zdeněk Chlup[3], Alexandra Kovalčíková[4], I. Dlouhý[3]

[1]Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36 Bratislava, Slovakia

[2]Institute of Condensed Matter Chemistry and Technologies for Energy - ICMATE, National Research Council –CNR, Via De Marini 6, 161-49 Genoa, Italy

[3]Institute of Physics of Materials, Czech Academy of Sciences, Žižkova 22, 602 00 Brno, Czech Republic

[4]Institute of Materials Research, Slovak Academy of Sciences, Watsonová 45, 040 01 Košice, Slovakia

In this work, a group of High Entropy Ceramics (HEC) was developed, including High Entropy Carbides (HECC) with the compositions of (Hf-Zr-Ta-Nb-Ti)C and (Mo-Nb-Ta-V-W)C, and High Entropy Borides (HEB) with the composition of (Hf-Zr-Ta-Nb-Ti)B_2. While HECC were synthesized using a solid-state synthesis of a powder mixture of binary carbides, HEB was synthesized using boro/carbothermal reduction of oxide mixtures. All the samples showed single solid solutions after Spark Plasma Sintering in the temperature range of 1600°C - 2050°C. The hardness, Young's modulus, strength, and wear resistance of the materials were investigated.

Since the manufacturing of these materials in complex shapes with large dimensions is extremely difficult and expensive, the present work was focused on the development of an appropriate method to join these ceramics. Several different approaches were investigated, including direct bonding (without any interlayer between two substrate materials), brazing (using alloys above their melting temperatures) and solid state diffusion bonding (using a refractory high entropy alloy as an interlayer). The direct bonding led to the formation of seamless joints, but a relatively high temperature and pressure were required, which led to the deformation of some of the base high entropy materials. On the other hand, the pressureless brazing of HECC was obtained using an eutectic Ni-Ta alloy, whose composition was selected based on the wetting studies. A strong joint with a shear strength of ~ 220 MPa was obtained. High entropy alloys having the same transition metals as present in the ceramics were prepared by arc-melting approach, followed by rolling and annealing. The as-prepared HEA foil was then used as the joining filler between two HEC. Sound joints were obtained by solid state diffusion bonding in the temperature range of 1400 – 1800°C. The higher the temperature the more significant reaction between the alloy and the substrate, leading to the phase separation and loosing a high entropy composition in the interlayer. In all cases, strong joints were obtained, as the joining area was stronger than the strength of the base materials.

Acknowledgment: This work was supported by the Slovak Research and Development Agency under the contract no. APVV-SK-CZ-RD-21-0089 and APVV-21-0402. The support of LUASK22219, and VEGA 2/0161/22 projects is also acknowledged. N.H. acknowledges the financial support of doktogrant No. APP0384.

Nano and micro optics on fibre tip: A possible solution for measurements in harsh environments

Shanti Bhattacharya
Department of Electrical Engineering, IIT Madras, Chennai 600036, India

It is well known that optical fibres can withstand relatively high temperatures and pressures [1]. They also work well in corrosive environments. They are commonly used in sensing interferometers, where one arm of the interferometer accesses the hostile environment, in which measurements are to be made. In this talk, I will present work on diffractive optics that can be fabricated directly on fibre tip [2, 3], enabling shaping of the light beam as it emerges from the fibre. I will also talk about meta-optics and their role in light shaping. However, their ability to withstand harsh environments needs to be studied.

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Enhancement of weak ferromagnetism, exotic structure prediction and diverse electronic properties in bismuth ferrite and holmium-substituted multiferroic bismuth ferrite

Maria Čebela[1,2], Vitalii Turchenko[3], Milena Rosić[1], Dragana Jordanov[1], Vladimir Dodevski[1], Dejan Zagorac[1,2]

[1]Laboratory for Material Science, Institute of Nuclear Sciences „Vinča“, National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia
[2]Center of Excellence ‘‘Cextreme Lab’’, Institute of Nuclear Sciences Vinča, University of Belgrade, National Institute of the Republic of Serbia, Mike Petrovića Alasa 12-14, Belgrade, Serbia
[3]The Joint Institute for Nuclear Research (JINR), Dubna, Russian Federation
[4]Institute of Physics, University of Belgrade, Pregrevica 118, 11080, Belgrade, Serbia

Bismuth ferrite (BFO, $BiFeO_3$), exhibiting both ferromagnetic and ferroelectric properties at room temperature, is one of the most researched multiferroic materials with a growing number of technological applications. In the present study, using a combined theoretical-experimental approach, we have investigated the BFO and the influence of Ho-doping on BFO structural, electronic and magnetic properties. Well crystallized single-crystal $BiFeO_3$ and $Bi_{1-x}Ho_xFeO_3$ nanopowder has been successfully synthesized with the hydrothermal method. The phase composition of the synthesized samples was determined by the x-ray diffraction (XRD) analysis, and the results showed that synthesized material crystallizes in the space group R3c. In addition, a structure prediction has been performed and 11 additional $BiFeO_3$ modifications have been proposed. After structure prediction of Ho-doped $BiFeO_3$ using bond valence calculations (BVC) calculations six most favorable candidates were found: α-, β-, γ-, R-, T1, and T2.The magnetic behavior of the synthesized materials was investigated using a SQUID magnetometer equipped with an oven. The plethora of magnetic and electronic properties of the Ho-doped BFO that our theoretical research predicted can open rich possibilities for further investigation and eventual applications.

NMR spectroscopy as a structure elucidation tool for compounds synthesised under high temperature and high pressure conditions

Thomas Bräuniger
Department of Chemistry, University of Munich (LMU), Butenandtstraße 5-13, 81377 Munich, Germany

In this paper, it is shown how Nuclear Magnetic Resonance (NMR) spectroscopy may serve as a useful complementary technique for structure elucidation of novel compounds, which have been synthesised under extreme conditions, i.e. high temperature and high pressure. In particular, it is shown how ^{27}Al-NMR may be used to track the coordination conditions of aluminium atoms in structures related to aluminium nitride. AlN is used as a material in a variety of technological contexts, such as piezoelectric devices and nanoelectronic purposes. Under ambient conditions, AlN occurs in the hexagonal wurtzite structure, where aluminium is tetrahedrally coordinated by nitrogen.

From the materials science view, it is of interest to know about the properties of aluminium nitride with higher coordination numbers, implying synthesis under high pressure. Indeed, AlN in rock-salt structure type, where aluminium atoms are octahedrally coordinated by nitrogen, has been successfully produced by the group of *Edwin Kroke* (TU Freiberg, Germany), using shock-wave experiments with pressures exceeding 15 GPa. In our group (*Wolfgang Schnick*, LMU München, Germany), the same structural motif has been found in an imidooxonitridophosphate, $AlP_6O_{3x}(NH)_{3-3x}N_9$ ($x \approx 0.33$), synthesised under 5 GPa and 1100°C in a multianvil press. As shown by both the group of *Kroke* and us, acquisition of simple ^{27}Al-NMR spectra under magic-angle spinning (MAS) allows the unequivocal identification of the coordination sphere of aluminium by evaluating the isotropic chemical shift value. Thus, here and in many other instances, solid-state NMR has been shown to be a powerful complementary tool for structure elucidation in periodic solids.

ORAL PRESENTATIONS

Caviation Erosion Resistance Behavior of Some Refractory Ceramics

Tatjana Volkov-Husović[1], Sanja Martinović[2], Ana Alil[2]
[1]*University of Belgrade, Faculty of Technology and Metallurgy,Belgrade, Serbia*
[2]*University of Belgrade, Institute for Chemistry, Technology and Metallurgy, Belgrade, Serbia*

Cavitation erosion application could be observed as dangerous phenomena which have large influence on engineering materials behavior and life time in working conditions. This phenomenon is related to fluid flow conditions, which could cause pits and defects formation resulting in mechanical properties degradation, as well as potential risk of failure of the part. In this paper results for cordierite and alumina (low cement high alumina castable, LCC), based refractories subjected to cavitation erosion testing will be presented. Testing of the samples will be according standard method, with stationary sample in ultrasonic vibratory method. Degradation of the samples will be monitored by mass and volume loss, as well as changes in morphological characteristics. Image analysis will be applied for pits characteristics (number, average diameter, area, roundness) determination.

Keywords: cavitation resistance, cordierite, low cement high alumina castable, LCC, image analysis

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Ablation performance of rare-earth modified ZrB_2–SiC composites under oxyacetylene torch test

Hakan Ünsal[1], Alexandra Kovalčíková[2], Michal Hičák [1], Zdnek Chlup [3], Ivo Dlouhý [3], Branko Matović[4], Peter Tatarko[1*]

[1]*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dubravska cesta 9, 845 36, Bratislava, Slovakia*

[2]*Institute of Materials Research, Slovak Academy of Sciences, Watsonova 47, 04001 Košice, Slovakia*

[3]*Institute of Physics of Materials, Czech Academy of Sciences, Žižkova 22, 616 62 Brno, Czech Republic*

[4]*Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovica Alasa 12-14, 11000 Belgrade, Serbia*

In the present study, dense ZrB_2-SiC composites were fabricated using Field Assisted Sintering Technology (FAST). The composites containing 25 vol% SiC particles were prepared by in situ reaction of $ZrSi_2$, B_4C and carbon black powders, which is a method to densify ZrB_2-based composites at low temperatures. Furthermore, rare-earth (RE) additives were used to improve the mechanical properties of ZrB_2-SiC composites. Phase and morphologies of the ZrB_2 based composites were characterized by X-Ray Diffraction and Scanning Electron Microscopy. Both the room temperature (hardness, strength, fracture toughness) and high temperature (ablation resistance) properties were investigated. The results showed that homogeneous microstructure and nearly fully dense ZrB_2-25vol.%SiC composites with a relative density above 99% were obtained after sintering at the temperature of 1600°C under the pressure of 70 MPa for 10 min. During sintering, the additives were completely transformed into ZrB_2 and SiC particles, which were homogeneously distributed in the ZrB_2 matrix. The RE-based additives were also uniformly distributed at the grain boundaries of ZrB_2. The mechanical properties of ZrB_2-SiC composite, such as hardness, strength and fracture toughness, were slightly improved by the addition of RE additives. Most importantly, the ablation resistance of ZrB_2-based materials was significantly improved by the addition of RE additives, and further improved with their increasing amounts.

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Mechanical testing of brittle materials: from single crystals to ceramic systems

Manuel Gruber, Peter Supancic, Raul Bermejo
Department Materials Science, Chair of Structural and Functional Ceramics, Montanuniversität Leoben, Peter-Tunner-Strasse 5, 8700 Leoben, Austria

Ceramics and other brittle materials often exhibit outstanding functional and mechanical properties, positioning them as indispensable elements in a diverse array of technical applications. Due to their inherent lack of plasticity, these materials can fail spontaneously under the combination of tensile stresses and pre-existing defects such as pores, agglomerates, or surface imperfections like scratches. Given that tensile stresses are inevitable in nearly all technical applications, understanding the mechanical behavior of these materials becomes paramount for ensuring their reliability and structural integrity.

Various mechanical testing procedures are proposed and discussed in terms of their applicability to distinct material classes and specimen geometries. The systematic analysis of the obtained data allows for the establishment of correlations between microstructural characteristics, crystallographic orientation, fracture behavior, environmental effects, and the observed mechanical properties. The insights gained through these correlations are crucial for advancing our understanding of brittle material failure mechanisms and for informing the design and optimization of structural components in various engineering applications.

Erosion wear of HCCI alloys

Bratislav Rajicic[1], Aleksandar Maslarevic[1], Gordana Bakic[1], Vesna Maksimovic[2], Milos Djukic[1]

[1]*University of Belgrade, Faculty of Mechanical Engineering, Kraljice Marije 16, Belgrade 11120, Serbia*

[2]*University of Belgrade, Vinca Institute of Nuclear Sciences – National Institute of the Republic of Serbia, Belgrade 11001, Serbia*

Failures in industrial plants, which operate under extreme conditions, could occur after a short time of exploitation. Erosion wear of materials is caused by the relative movement of solid particles and the surfaces of components. Such erosive wear can lead to the failure of industrial components in a very short time and/or a sharp decline in the structural integrity of industrial equipment. For example, the wear of the ash disposal system in a coal-burning thermal power plant, due to impact of ash particles with a high content of mineral residues, is a very common case of failure and outages in the operation of such industrial systems.

Two high chromium cast irons (HCCI) were tested to determine the erosion wear. These alloys contain 15% Cr and 25% Cr, and it was tested in as-cast and after heat treatment (annealing). A specially designed installation was used for the gas blast sand erosion test. Type of erodent was foundry quartz sand. Erosion tests were done with high erodent particle velocity (90 m/s) and high erodent feed rate (3000 g/min). This conditions represents those similar to extreme wear conditions of some components of thermal power plants using pulverized high mineral content coals.

Microstructural characterization was done at samples before and after erosion tests, Fig. 1. The main results indicate that matrix plastic deformation and distribution of carbide phase have a significant contribution to erosion resistance of HCCI alloys in such conditions.

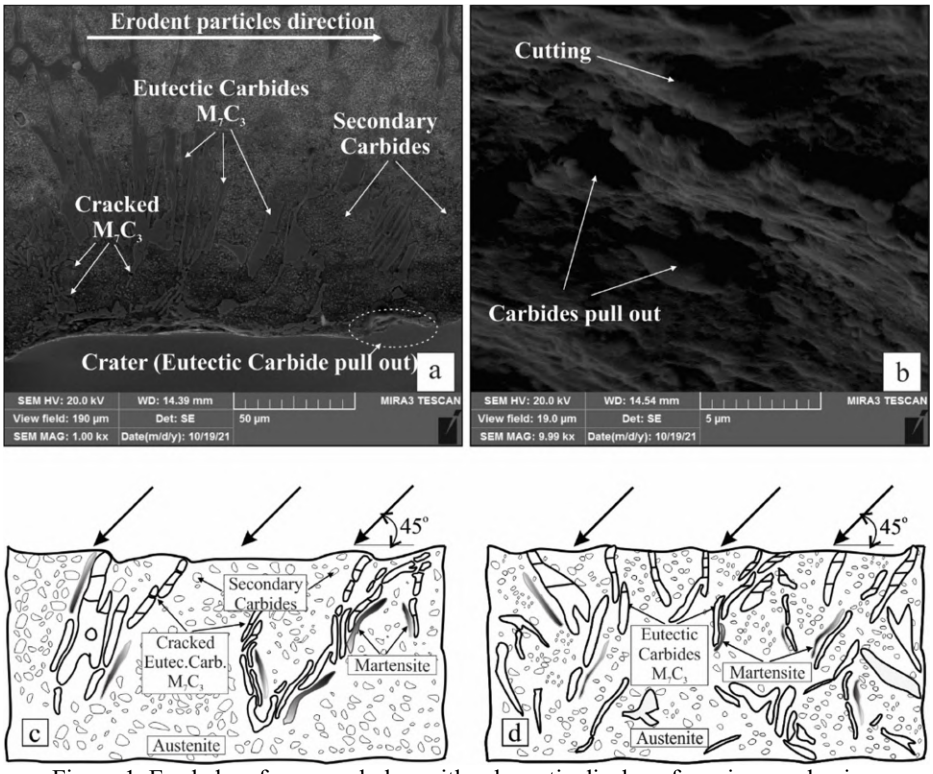

Figure 1. Eroded surface morpholgy with schematic display of erosion mechanism (a, c) HCCI-15-HT and (b, d) HCCI-25-HT

Effect of SiC whiskers on microstructure, mechanical and tribological properties of (TiZrHfNbTa)C

Lenka Ďaková[1], Monika Hrubovčáková[1], Alexandra Kovalčíková[1], Jana Andrejovská[1], Ján Dusza[1]

[1]*Institute of Materials Research Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovakia*

The investigation focused into the microstructural assessment and mechanical properties of high-entropy (TiZrHfNbTa)C carbides reinforced with SiC whiskers. HEC-SiC_w composites were prepared through the processes of ball milling and spark plasma sintering at 2100 °C for a duration of 10 minutes. Amount of SiC whiskers into the HEC matrix varied from 1 wt. % to 10 wt. %. The resulting HEC- SiC_w composites achieved a relative density exceeding 99 %, characterized by a uniformly distributed chemical composition. The measured grain size values decreased with the addition of wt.% SiC whiskers and ranged from 5 µm to 3 µm.Vickers' hardness values exhibited a range between approximately 24 GPa and 27 GPa, with indentation fracture resistance values reflecting a similar pattern, fluctuating from 2.66 ± 0.32 $MPa \cdot m^{1/2}$ to 4.59 ± 0.53 $MPa \cdot m^{1/2}$. Nanohardness values oscillated between 38 GPa and 40 GPa, while the indentation modulus of elasticity values spanned from 590 ± 16 GPa to 596 ± 15 GPa, respectively. An observation surfaced regarding the flexural strength of the composites, indicating an enhancement of approximately 25 % with the increasing addition of SiC_w. Flexural strength values ranged from 526 ± 25 GPa to 623 ± 25 GPa. Furthermore, the influence of SiC whiskers on wear resistance and wear mechanisms was thoroughly examined, describing their impact on the overall mechanical properties of the composites.

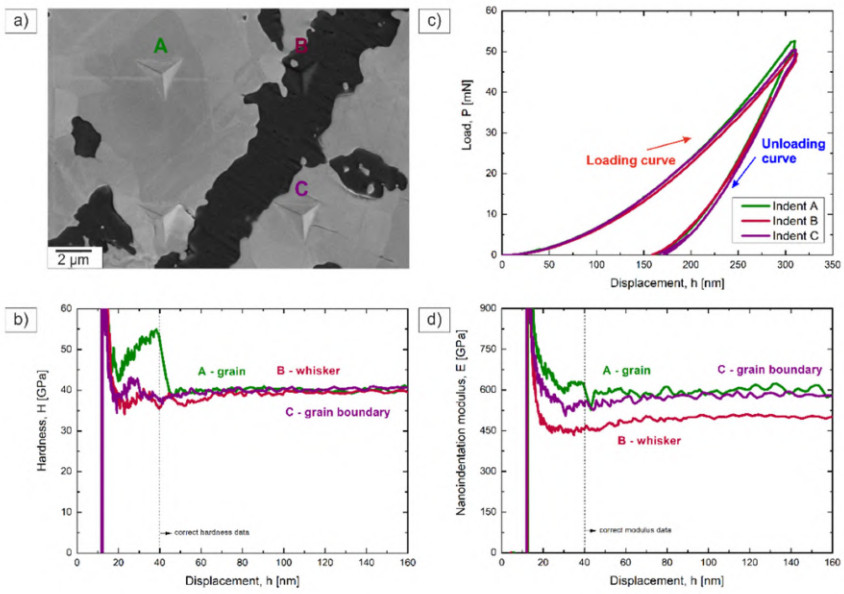

Figure 1. Imprints located in HEC-5SIC_w inside the grain (A), in whiskers (B), and at the grain boundary (C), b) hardness, c) characteristic loading/unloading curve d) nanoindentation modulus of elasticity

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Atomic layer deposition assisted graphite/ZnO composite anodes in Li-ion batteries

Alper Güneren[1*], Prangya P. Sahoo[2], Boris Hudec[3], Matej Mičušík[4], Zoltán Lenčéš[1], Karol Fröhlich[2,3]

[1]*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia*
[2]*Centre for Advanced Materials Application, Slovak Academy of Sciences, Dúbravská cesta 5807/9, 845 11 Bratislava, Slovakia*
[3]*Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 841 04, Bratislava, Slovakia*
[4]*Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, 845 41, Bratislava, Slovakia*

Graphite (Gr) is a widely-used anode material for Li-ion batteries with a specific capacity of 372 mAh g^{-1}. ZnO, with its higher theoretical capacity of 978 mAh g^{-1}, presents a viable option for high-energy demand applications. However, the use of bare/bulk ZnO is limited by volumetric expansion/shrinkage during cycling. To address these challenges, Gr/ZnO composite anodes were produced via atomic layer deposition (ALD). Anodes were prepared with milled Gr, conductive carbon, and sulfonated alginate binder in an 80:10:10 composition. ZnO films were deposited through ALD at 100 °C using diethyl zinc and deionized water as precursor and reactant, respectively. Various number of ALD cycles (10, 20, and 40) were performed to achieve different ZnO layer thicknesses. Evolution of the ZnO layers on graphite anodes was observed through scanning electron microscopy, X-ray photoelectron spectroscopy. Electrochemical performance was assessed through rate capability and long cycle tests within a Li/Li^+ voltage window of 0.01-1.5 V. Differential capacity analysis (dQ/dV) elucidated decay properties and contributions of each material to total capacities. Results demonstrate the successful enhancement of anode performance through ALD assisted Gr/ZnO composites, offering promising implications for the advancement of Li-ion battery technology.

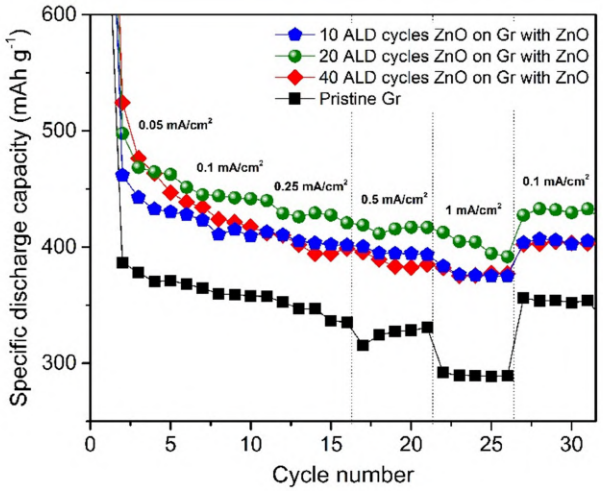

Figure 1. Rate capability of Gr/ZnO anodes.

Acknowledgement: The authors acknowledge the support from VEGA 2/0162/22, APVV-19-0461 projects and Horizon 2020 project No. 963542 (acronym SIMBA).

Physicochemical properties of bismuth vanadate photoanode irradiated by swift heavy ions

Marko Jelić[1], Ekaterina Korneeva[2], Nikita Kirilkin[2], Tatiana Vershinina[2], Oleg Orelovich[2], Vladimir Skuratov[2], Zoran Jovanović[1], Sonja Jovanović[1]

[1]*Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

[2]*Joint Institute of Nuclear Research, Dubna, Russia*

Photoelectrochemical (PEC) water splitting represent an up-and-coming method for solar energy capture and storage. Its efficiency primarly relies on the development of the photocatalyst for oxygen evolution reaction (OER). Monoclinic bismuth vanadate ($BiVO_4$, BVO) emerges as an outstanding photoanode material due to its high stability in near-neutral electrolytes, suitable band structure and cost-effectiveness. However, significant charge recombination poses a substantial limitation, emphasizing the need to comperhend contributing factors for potential enhancements. In this study, we present the results of the swift heavy ion (SHI) irradiation (Xe, 150 MeV, 1×10^{10} – 5×10^{11} ions cm^{-1}) on the physicochemical properties of hydrothermally synthesized BVO thin films. X-ray diffraction (XRD) analysis indicates that the irradiated material retains its initial monoclinic scheelite phase, displaying preferential growth along [010] direction alongside notable amorphization at the highest fluence. Scanning electron microscopy (SEM) reveals prismatic grains across all samples, averaging a size of 600 nm, with ion tracks appearing post-irradiation. A more in-depth examination of the sample irradiated with 1×10^{10} ions cm^{-2} through transmission electron microscopy (TEM) unveils the presence of amorphous ion tracks (~ 10 nm in diameter) and hillocks at the BVO surface (~ 10 nm in height). Raman spectra exhibit bands corresponding to the monoclinic scheelite phase, with new bands emerging in the 5×10^{11} ion cm^{-2} irradiated sample at 420 and 920 cm^{-1}, originating from amorphous BVO. X-ray photoelectron spectroscopy (XPS) following SHI irradiation reveals an increase in V^{4+} and oxygen vacancies, particularly at higher fluences. Diffuse reflectance spectroscopy (DRS) measurements indicate a decrease in the band gap with increasing fluence. Photocurent densities, derived from 1-hour-long chronoamperometry measurements, demonstrate that irradiation with the lowest fluence leads to a gradual recovery of PEC OER over time. Subsequent XRD, SEM and XPS analyses performed after PEC indicate variety of interesting alerations in the BVO, including material dissolution along ion tracks.

Utilization of swift heavy ions for modification of graphene oxide-based nanocomposites

Željko Mravik[1], Milica Pejčić[1], Danica Bajuk-Bogdanović[2], Nikita Kirilkin[3], Ekaterina Korneeva[3], Vladimir Skuratov[3], Zoran Jovanović[1]

[1]Center of Excellence for Hydrogen and Renewable Energy (CONVINCE), Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia
[2]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia
[3]Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, Dubna, Moscow region, Russia

Creating materials with superior properties is in modern day science often achieved by extreme conditions. This is also the case in achieving preferable properties for high capacitance electrode material for supercapacitor applications. The morphology, structure and chemistry of material is usually modified by extreme temperatures, chemical conditions, pressures, achieved by hydrothermal treatment or different forms of radiation. Ion beam irradiation can be outlined as a promising technique where introduction of the effects that are far from thermodynamic equilibrium (due to extremely short time of interaction of accelerated ion with target) can result in structures and properties that cannot be replicated by other techniques.

Graphene oxide (GO) is a widely investigated electrode material in which two-dimensional nature, defective structure, and adjustable surface chemistry dictate the applicability. Due to low electric conductivity of as-prepared GO as well as possible re-graphitization in bulk form, methods for reduction and morphology modification are developed. In this work swift heavy ions (Xe, 150 MeV) were utilized for modification of GO and its nanocomposite with 12-tungstophosphoric acid. Fluence has been varied in order to achieve different degree of modification. Raman spectroscopy was used as the main technique for monitoring of structural changes where increased defect formation is noticed with increasing fluence. Morphology was examined using scanning electron microscopy where material degradation and formation of ion tracks is evident at higher fluences (Figure 1, fluence 6×10^{11} ions/cm^2). The results show great potential of ion beams for controllable and localized modification of GO-based materials to achieve preferable properties for energy related applications.

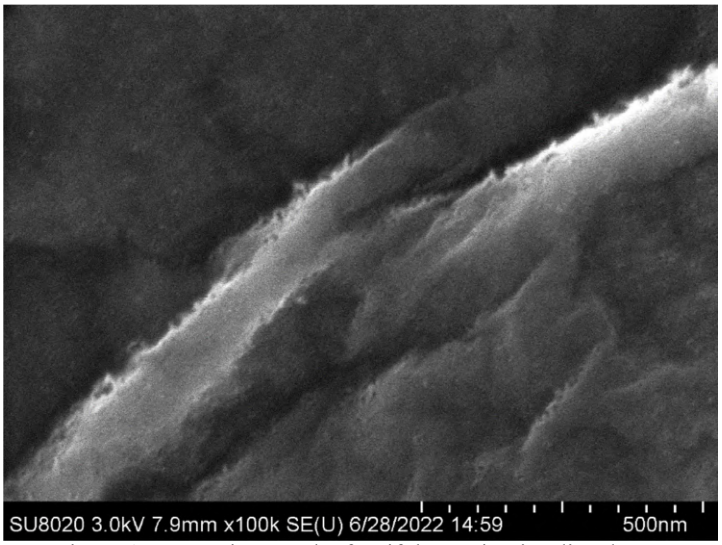

Figure 1. SEM micrograph of swift heavy ion irradiated GO.

Thermal and electrical conductivity of additive-free silicon carbide ceramics

Ondrej Hanzel, Monika Tatarková, Pavol Šajgalík
Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravska cesta 9, 845 36 Bratislava, Slovak Republic

Fully dense (t. d. > 99 %) silicon carbide ceramics without any sintering additives were succesfully prepared by combination of freeze granulation of silicon carbide powder, annealing of granulated powder and subsequent rapid hot pressing at 1900°C with dwell time from 5 to 80 minutes (Fig. 1). Thermal and electrical conductivity of prepared materials considering the ratio of SiC polytypes was investigated. Different ratio of alpha and beta silicon carbide has been achieved by adjusting dwell time during sintering. Thermal diffusivity, specific heat capacity, thermal conductivity, electrical conductivity, density, microstructure of additive-free SiC with various α/β content has been investigated. The electrical conductivity of SiC decreased from 104 S/m to 8 S/m as a content of α-SiC increased from 63 to 94 %. Opposite trend, when thermal diffusivity increased from 47.3 to 68.4 mm^2/s as a content of α-SiC increase from 63 to 94 %, was observed. In addition, such prepared materials were tested in oxyacytelene torch at 1700°C, 1800°C and 1900°C for 5 minutes. Dynamic oxidation resistance of prepared ceramics is excellent. In the dynamic regime the ceramics sustained 1900 °C for 5 minutes (Fig. 2). It seems that this material is suitable for ultra-high-temperature applications.

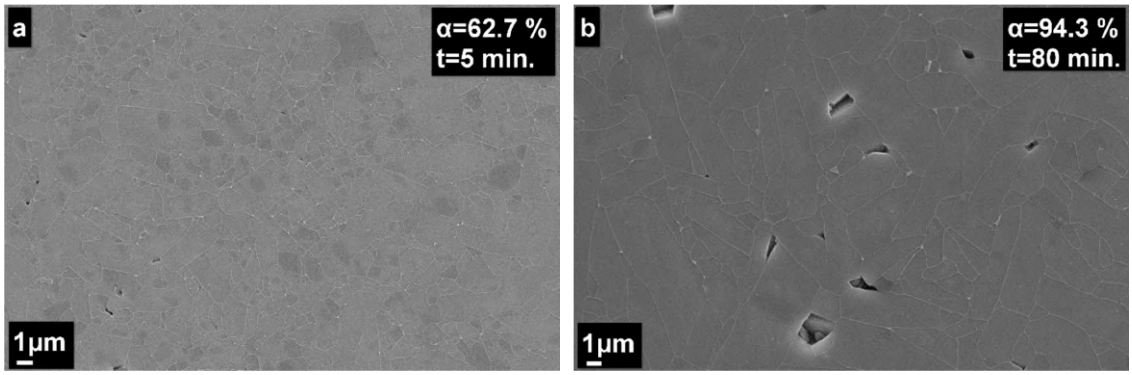

Figure 1. Plasma etched surfaces of samples with shortest and longest holding time.

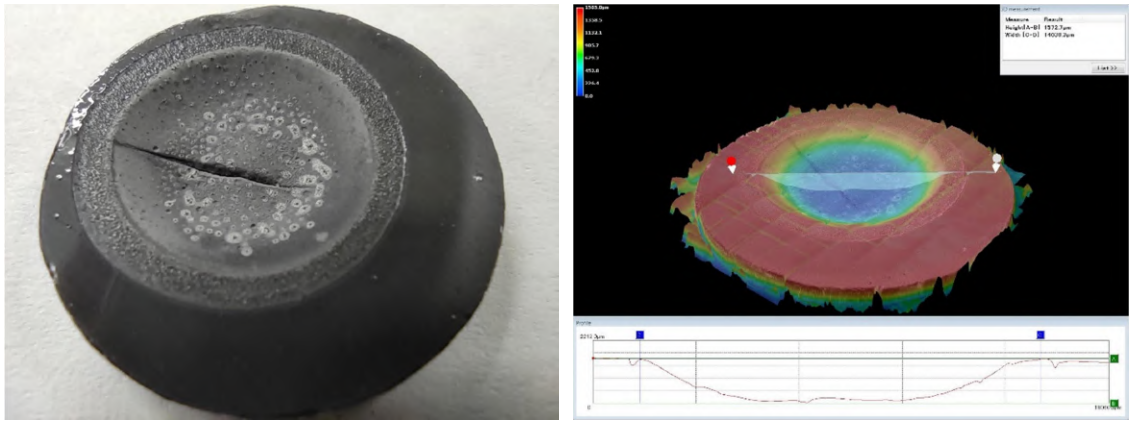

Figure 2. Additive-free silicon carbide ceramics after oxyacetylene torch at 1900°C for 5 min.

Acknowledgements: This work was supported by the Slovak grant VEGA 2/0007/21.

Synthesis and high-temperature / high-pressure exposure of compositionally complex rock-salt-type transitional metal (carbo)nitrides

Dharma Teja Teppala[1], Shrikant Bhat[2], Leonard Keil[1], Jan Bernauer[1], Johannes Peter[3], Hans-Joachim Kleebe[3], Emanuel Ionescu[1,4]

[1]*Institute for Material Science, Technical University of Darmstadt, 64287 Darmstadt, Germany*
[2]*Photon Science, DESY, 22607 Hamburg, Germany*
[3]*Institute for Applied Geosciences, Technical University of Darmstadt, 64287 Darmstadt, Germany*
[4]*Fraunhofer IWKS, Brentanostrasse 2a, 63755 Alzenau, Germany*

Transitional metal carbides and nitrides, especially of group IV and V metals, are well known in the ceramic field due to their good thermal, electrical properties, high hardness, and high temperature stability making them useful in applications that require high hardness and resistance to various corrosive atmospheres. There is abundant thermodynamic data available on binary transitional metal carbides and nitrides, such as P-T phase diagram, thermal expansion, Debye temperature and physical parameters, e.g., elastic moduli; while this is rather not the case for ternary and other high complex compositions.

Transitional metal nitrides, especially those of group IV metals, are known to form simple, high symmetry structures at ambient conditions, i.e., rock salt. However, at high pressure and temperatures, the metal nitrides were observed to undergo phase transition and these thermodynamically stable high-pressure phases were observed or predicted to be denser, harder with distinct properties compared to that of the ambient condition phase.

In the present work, two carbonitride-based complex compositions i.e $(Ti_{0.2}Zr_{0.2}Hf_{0.2}Nb_{0.2}Ta_{0.2})N_xC_{1-x}$ and $(V_{0.2}Nb_{0.2}Ta_{0.2}Mo_{0.2}W_{0.2})N_xC_{1-x}$ were synthesized via a non-oxidic sol-gel process using the respective metal amido complexes and ammonia followed by a thermal ammonolysis at 1000 °C. The obtained phase-pure carbonitrides were structurally characterized by X-ray diffraction and electron microscopy and then considered for performing experiments under extreme conditions i.e pressures up to 20 GPa and temperatures as high as 1900 ^{o}C. The experiments were performed in the large volume press facility at the beam line P61B DESY.

The in-situ x-ray diffraction study during the high-temperature high-pressure treatment revealed that the rock salt structure of the compositionally complex carbonitrides was stable under the conditions of exposure and allowed to quantify for the first time some basic physical parameters thereof, e.g., thermal expansion and bulk modulus, which were calculated by using 2nd order Birch Murnaghan equation of state.

Keywords: High entropy (carbo)nitrides, high-temperature high-pressure conditions, thermodynamics, equation of state

Experimental Investigations to Evaluate Surface Fatigue Wear in Journal Bearing by Using Vibration Signal Analysis

Amarnath M[1], Ramachandra C G[2], H. Chelladurai[3], P. Sateesh Kumar[4] and K. Santhosh Kumar[5]

[1,3,4,5]*Indian Institute of Information Technology Design and Manufacturing, Jabalpur-482005, Madhya Pradesh,* India

[2]*Presidency University, Bengaluru-560064, Karnataka, India*

Journal bearings are extensively used sliding contact machine elements to support radial / axial loaded rotors used in various applications viz. automobile crankshaft, turbine propeller shaft, rope conveyer, heavy duty electric motors. The primary reasons for failures of these bearings include unstable lubricant film, oil degradation, misalignment, etc. This paper describes the results of experimental investigations carried out to detect surface fatigue wear developed on load bearing the contact surfaces of journal bearing. The test bearing was subjected to fatigue load cycles over a period of 600 hours. The vibration signals were acquired from the journal bearing at regular interval of 100 hrs. These signals were post-processed by using the vibration analysis technique to obtain diagnostic information of wear propagated in the journal bearing system.

Keywords: Fatigue, journal bearing, sound signals, vibration signals, wear.

Experimental and simulation analysis of influence of stacking sequence on tensile and abrasion resistance of e-glass/jute fibre-based hybrid composites

Ramachandra C G[1], Lokesh K S[2], Srinivasa Mayya D[3] and Ravindra Babu G[4]
[1]Presidency University, Bengaluru-560064, Karnataka, India.
[2,3]Srinivas Institute of Technology, Mangaluru-574143, Karnataka, India.
[4]Karavali Institute of Technology, Mangaluru-575029, Karnataka, India.

The present study involves the developing synthetic and natural fibre hybrid composites in the various proportions of constituents. The reinforcements used in the present study is e-glass fibre and jute fibre reinforced stacked in different directions of 00,450,900. Developed composites through manual hand layup technique followed by compression moulding. The prepared hybrid composites are tensile tested to understand the influence of stacking sequence of hybrid reinforcements on tensile strength of the composites. Further finite element analysis has been done to find the correlation with experimental results. Hardens testing for the samples been done to assess the abrasion resistance of prepared hybrid composites. Out of all the combination composite with 00 orientation of hybrid combination perform better over other combinations.

Keywords: Hybrid composites, Analysis, Tensile Resistance Abrasion Resistance.

Study of lanthanum fluoride selenides using a combination of crystal structure prediction and DFT calculations with experimental synthesis and characterization

Dejan Zagorac[1,2], Constantin Buyer[3], Jelena Zagorac[1,2], Hagen Grossholz[3], Sarah Wolf[3], Tamara Škundrić[1,2], Milan Pejić[1,2], Dušica Jovanović[1,2], J. Christian Schön[4*], Thomas Schleid[3*]

[1]Materials Science Laboratory, Institute of Nuclear Sciences "Vinča", University of Belgrade, Belgrade, Serbia
[2]Center for synthesis, processing and characterization of materials for application in extreme conditions "CextremeLab", Belgrade, Serbia
[3]University of Stuttgart, Institute for Inorganic Chemistry, Pfaffenwaldring 55, 70569 Stuttgart, Germany
[4]Max Planck Institute for Solid State Research, Heisenberg str. 1, D-70569, Stuttgart, Germany

Lanthanum fluoride selenides (A-LaFSe, B-LaFSe and La_2F_4Se) have been synthesized through high-temperature experiments from an appropriate La/LaF_3/Se mixture and characterized using single-crystal as well as powder X-ray diffractometry and UV/Vis diffuse reflectance spectroscopy.[1] A-type LaFSe crystallizes in the tetragonal space group $P4/nmm$ with a = 413.79(3) pm, c = 715.24(5) pm and Z = 2 with the PbFCl-type structure, B-type LaFSe in the hexagonal space group $P6_3/mmc$ with a = 421.602(2) pm, c = 818.163(7) pm and Z = 2 with the CeHSe-type structure and La_2F_4Se in the trigonal space group $R\bar{3}m$ with a = 417.86(2) pm, c = 2326.78(9) pm and Z = 3 in the Ce_2F_4Se-type structure, respectively, in agreement with earlier work. The experiments are complemented by crystal structure predictions for LaFSe, which were performed using global optimization with empirical potentials and *ab initio* energy local minimizations. The results of the calculations concur with the experimentally observed structures and predict additional, so far unknown LaFSe polymorphs. In addition, detailed electronic properties were investigated both experimentally and theoretically, demonstrating possibilities for band-gap engineering in LaFSe.

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DFT study of new hybrid organic-inorganic perovskites: guanidinium-BX_3 substituted by B = (Sr^{2+}, Ca^{2+}, Mg^{2+}, Be^{2+}) and X = (Cl^-, F^-)

Dušica Jovanović[1,2], Dejan Zagorac[1,3], J. Christian Schön[4], Branko Matović[1,3], Aleksandra Zarubica[2], Jelena Zagorac[1,3]

[1]Institute of Nuclear Sciences Vinča, Materials Science Laboratory, University of Belgrade, 11000 Belgrade, Serbia
[2]Department of Chemistry, Faculty of science and mathematics, University of Nis, 18000 Nis, Serbia
[3]Center for Synthesis, Processing and Characterization of Materials for Application in the Extreme Conditions-CextremeLab, 11000 Belgrade, Serbia
[4] Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

In recent years, the development of perovskite solar cells (PSC) has attracted great attention as a "green" energy source that might even replace fossil fuels soon [1]. Conventional perovskite solar cells mostly contain toxic lead, which contributes to environmental pollution, so the solution was found to substitute lead with some non-toxic metal [2]. Our investigation of hybrid organic-inorganic perovskites aims to increase the chemical stability as well as to decrease the band gap value of crystal perovskites which enables better conductivity and shifts the absorbance range, in order to produce the most efficient perovskite solar cells. The *ab initio* calculations of GA-BX_3, where GA is the guanidinium cation $C(NH_2)_3^+$, with several different inorganic cations and anions - specifically: B = (Sr^{2+}, Ca^{2+}, Mg^{2+}, Be^{2+}) and X = (Cl^-, F^-) have been performed using Density Functional Theory (DFT), with several functionals, Local Density Approximation (LDA) and Perdew-Burke-Ernzerhof (PBE), as well as HSE06 (Heyd–Scuseria–Ernzerhof) hybrid functional. Further investigations of structural and electronic properties will provide insights into the potential applications of these new hybrid organic-inorganic perovskite structures.

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POSTER PRESENTATIONS

Novel high entropy alloys for extreme environments

Ivana Cvijović-Alagić[1], Nikola Kanas[2], Jelena Maletaškić[1], Abishek M[3], Vesna Maksimović[1]
[1]*Center of Excellence "CEXTREME LAB", Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*
[2]*BioSense Institute, University of Novi Sad, Dr Zorana Đinđića 1, 21000 Novi Sad, Serbia*
[3]*Indian Institute of Technology Madras (IIT-Madras), 600 036 Chennai, India*

Modern structural materials must withstand intense temperature variations and stresses, as well as tribologically and corrosively demanding conditions attributed to new and innovative technologies. The traditional high-strength alloys cannot fulfill all these requirements and therefore novel alloying concepts for the obtainment of compositionally complex materials (CCM), and especially high-entropy alloys (HEA), are developed. The concept of HEAs is based on the presence of five or more elements in the alloy composition in near equiatomic rations. This new class of materials is characterized by a single-phase solid solution microstructure contrary to the conventional alloys where in the microstructure the ternary or higher-order intermetallic compounds, as well as the unwanted secondary or amorphous phases, may appear as a result of the traditional alloying of the multicomponent alloys. Avoidance of the undesired phases in the alloy microstructure contributes to the enhancement of oxidation- and wear-resistance, the achievement of higher hardness and strength, and the obtainment of good thermal stability of structural materials. On the other hand, the presence of refractory elements in the HEAs composition may induce the additional enhancement of their high-temperature characteristics.

Having all this in mind the present work aimed to use the refractory IVb, Vb, and VIb group transition elements to successfully obtain the complex metallic alloy in the Hf-Ta-Zr-W-Mo system with enhanced properties suitable for application in extreme environments. In the present study, the $Hf_{0.5}Ta_{0.2}Zr_{0.1}W_{0.1}Mo_{0.1}$ alloy was successfully produced using the Field Assisted Sintering Technique (FAST) for Spark Plasma Sintering (SPS) under two different regimes to assess the influence of processing parameters on the obtained HEA characteristics. The first group of samples was produced at 1100 °C by applying a pressure of 85 MPa, while the second sample group was obtained at 1400 °C by applying a pressure of 50 MPa. In both cases, pressure was applied for 5 min in an air atmosphere. All samples were characterized in detail by scanning electron microscopy (SEM), X-ray diffraction (XRD), nanoindentation analysis, and thermal diffusivity measurements. Data collected during the research showed that even though both sample groups showed good compositional homogeneity and single-phase solid solution structure the alloy samples sintered at 1100 °C were characterized with higher density compared to the samples sintered at 1400 °C (95.2% *vs.* 91.5%), higher hardness (11.02 GPa *vs.* 7.96 GPa), and somewhat lower Young modulus (142.55 GPa *vs.* 150.79 GPa). Additional thermal diffusivity analysis showed that the $Hf_{0.5}Ta_{0.2}Zr_{0.1}W_{0.1}Mo_{0.1}$ alloy, obtained under both sintering conditions, is a good candidate for a variety of applications in extreme environments, especially for application in high-temperature conditions.

Characterization of the high-pressure sintered TiAl-TiB_2 composites

Vesna Maksimović[1], Vladimir Urbanovich[2], Jelena Maletaškić[1], Vladimir Pavkov[1], Ivana Cvijović-Alagić[1]

[1]Center of Excellence "CEXTREME LAB", Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia
[2]SSPA "Scientific-Practical Materials Research Centre of NAS of Belarus", P. Brovki Str. 19, 220072 Minsk, Belarus

Modern industrial production is in demand for innovative materials with enhanced performance and high resistance to long-term damage and failure in harsh working conditions. Intermetallic composites (IMC) of the Ti-Al-B system can provide a much-needed solution to the above-mentioned problems since these materials are characterized by advanced properties in harsh environments owned to the high-temperature properties of titanium-aluminides, and improved mechanical and tribological performance of ceramics.

The TiAl intermetallic alloy, as a new lightweight high-temperature structural material, has been applied in the aerospace and aircraft industry because of its low density, high mechanical strength, and modulus of elasticity at elevated temperatures [1,2]. The TiB_2 phase, due to its excellent high-temperature hardness, good thermodynamic compatibility, and chemical stability with the TiAl alloy, is a promising reinforcement for the TiAl alloy [1].

In the present paper the synthesis procedure, as well as the structural and mechanical characteristics of the TiB_2-reinforced TiAl-matrix composites, *i.e.* TiAl-TiB_2 composites, are reported. The TiAl-TiB_2composites were successfully prepared by applying high pressure of 4 GPa in an ambient atmosphere at temperatures ranging from 1000°C to 1400°C using a Bridgman-type toroidal apparatus. The structural characterization of the starting powders (Ti, Al, and TiB_2) and the sintered composites was performed using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy dispersive spectroscopy (EDS). The structural analysis of the obtained composite materials revealed the presence of TiAl, TiB_2, αTi, βTi, and $TiAl_3$ phases in different ratios depending on the composite sintering temperature. Obtained composites' microhardness ranged from 6.6 GPa to 9.3 GPa, also depending on the sintering temperature. Maximal microhardness was achieved for the composite with a minimal porosity of 1.8% sintered at 1400 °C.

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Boron nitride nanotubes versus carbon nanotubes: A thermal stability and oxidation behavior study

Nikolaos Kostoglou[1], Christos Tampaxis[2], Georgia Charalambopoulou[2], Georgios Constantinides[3], Vladislav Ryzhkov[4], Charalabos Doumanidis[5], Branko Matovic[6], Christian Mitterer[7], Claus Rebholz[8]

[1]Department of Materials Science, Montanuniversität Leoben, 8700 Leoben, Austria
[2]National Center for Scientific Research Demokritos, 15341 Athens, Greece
[3]Department of Mechanical and Materials Science and Engineering, Cyprus University of Technology, 3036 Lemesos, Cyprus
[4]Research School of High-Energy Physics, Tomsk Polytechnic University, 634050 Tomsk, Russia
[5]Department of Mechanical, Aerospace and Biomedical Engineering, University of South Alabama, Mobile, AL 36688, USA
[6]Vinča Institute of Nuclear Sciences, University of Belgrade, 11000 Belgrade, Serbia;
[7]Department of Mechanical and Manufacturing Engineering, University of Cyprus, 1678 Nicosia, Cyprus

Nanotubes made of boron nitride (BN) and carbon have attracted considerable attention within the literature due to their unique mechanical, electrical and thermal properties. In this work, BN and carbon nanotubes, exhibiting high purity (>99%) and similar surface areas (~200 m^2/g), were systematically investigated for their thermal stability and oxidation behavior by combining thermal gravimetric analysis and differential scanning calorimetry methods at temperatures of up to ~1300 ^oC under a synthetic air flow environment. The BN nanotubes showed a good resistance to oxidation up to ~900 ^oC and fully transformed to boron oxide up to ~1100 ^oC, while the carbon nanotubes were stable up to ~450 ^oC and almost completely combusted up to ~800 ^oC (Fig. 1). The different oxidation mechanisms are attributed to the different chemical nature of the two types of nanotubes.

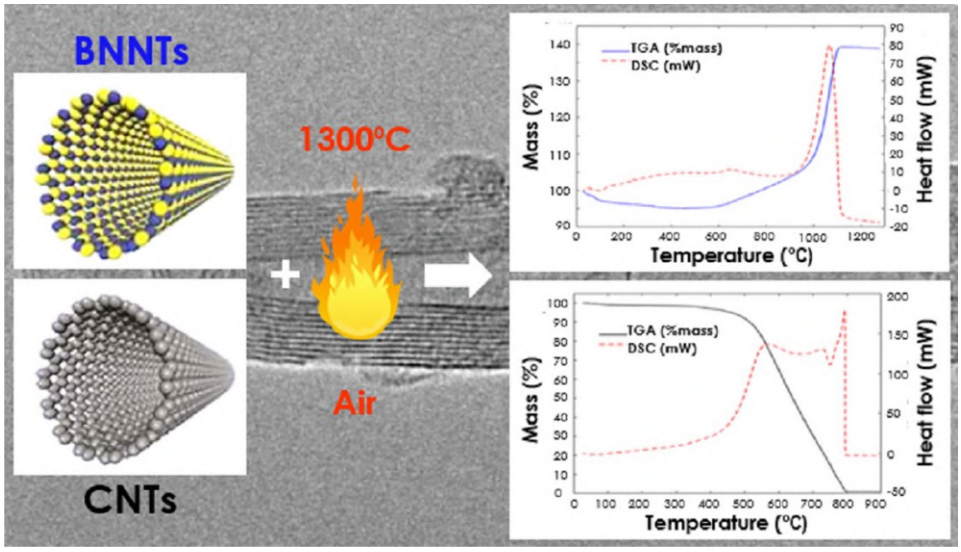

Figure 1. Combined TGA/DSC curves in synthetic air for BNNTs and CNTs.

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Purity and surface area: Key factors on thermal stability and oxidation resistance of BN nanoplatelets

Nikolaos Kostoglou[1], Sebastian Stock[2], Angelos Solomi[1,3], Damian Holzapfel[4], Steven Hinder[5], Mark Baker[5], Georgios Constantinides[6], Vladislav Ryzhkov[7], Jelena Maletaskic[8], Branko Matovic[8], Jochen Schneider[4], Claus Rebholz[1,3], Christian Mitterer[1]

[1]Department of Materials Science, Montanuniversität Leoben, 8700 Leoben, Austria
[2]Chair of Physics, Department Physics, Mechanics and Electrical Engineering, Montanuniversität Leoben, 8700 Leoben, Austria
[3]Department of Mechanical and Manufacturing Engineering, University of Cyprus, 1 Panepistimiou Avenue, 2109 Nicosia, Cyprus
[4]Department Materials Chemistry, RWTH Aachen University, D-52074, Aachen, Germany
[5]Department of Mechanical Engineering Sciences, University of Surrey, GU27XH Guildford, UK
[6]Department of Mechanical Engineering and Materials Science and Engineering, Cyprus University of Technology, Lemesos 3036, Cyprus
[7]Research School of High-Energy Physics, Tomsk Polytechnic University, 634050 Tomsk, Russia
[8]Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, 11000 Belgrade, Serbia

This study delves into the influence of purity and surface area on the thermal and oxidation properties of hexagonal boron nitride (h-BN) nanoplatelets, crucial factors in high-temperature oxidizing environments. Three h-BN nanoplatelet-based materials, synthesized with different purity levels and surface areas, were compared, including also a high-purity commercial BN reference. All materials were systematically analyzed by various characterization techniques, such as scanning electron microscopy, X-ray diffraction, Fourier-transform infrared radiation, X-ray photoelectron spectroscopy, gas sorption analysis and thermal gravimetric analysis coupled with differential scanning calorimetry. Results indicated a clear enhancement in thermal stability and oxidation resistance of the synthesized materials with increased purity. Furthermore, the reference material with its high purity and low surface area showed a superior performance, which was attributed to the minimized reactive sites for oxygen diffusion due to fewer defects, highlighting the critical roles of both sample purity and accessible surface area in h-BN's thermo-oxidative stability. These findings offer valuable insights for the development of BN-based nanomaterials, suggesting a strategic focus on purity and surface area control, while providing a pathway for optimizing their performance in applications facing extreme thermal and oxidative conditions.

Sustainable Solutions in Biomedical Substrate Design: Micro- and Nanotexturing on 3D Printed Titanium Alloys

Anna Kityk[1,2], Miroslav Hnatko[1,2], Viliam Pavlik[1], Michal Hičák[1]
[1]*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta, 9, Bratislava, 84536, Slovak Republic*
[2]*Centre of Excellence for Advanced Materials Application, Slovak Academy of Sciences, Dúbravská cesta, 5807/9, Bratislava, 84511, Slovak Republic*

Titanium (Ti) alloys play a pivotal role in the fabrication of prostheses and dental implants, due to their excellent mechanical strength, chemical inertness, and corrosion resistance. However, commercially available Ti alloy surfaces tend to be smooth, hydrophobic and bio-inert, lacking specific pretreatments. This inherent characteristic may restrict their osteogenic, osteoinductive, and osseointegration capabilities. To address existing limitations for bio-medical Ti alloys this work proposes to use new eco-friendly surface processing, which is a combination of sandblasting with the electrochemical surface treatment in deep eutectic solvents (DESs). Sandblasting, the first stage of combined processing, allows the creation of highly rough surfaces with a modified oxide layer. The second stage of processing is the short-time room-temperature eco-friendly electrochemical anodic treatment in DESs based on choline chloride. Electrochemical treatment following sandblasting can significantly improve the surface characteristics of Ti alloys: clean the surface from contamination with blasting particles, smooth out the sharp edges of the microstructure formed by sanding, and add nano-pores and nano-tubes (Fig. 1). It should be noted that electrochemical treatment in choline chloride-based DESs beneficially alters the chemical composition of the natural protective surface layer. Thus, the clean surface of Ti alloys after the proposed combined processing is characterized by improved chemical composition, a hierarchical structure consisting of micro and nano roughness, which is similar to real bone tissue, increased wettability, and bio-compatibility.

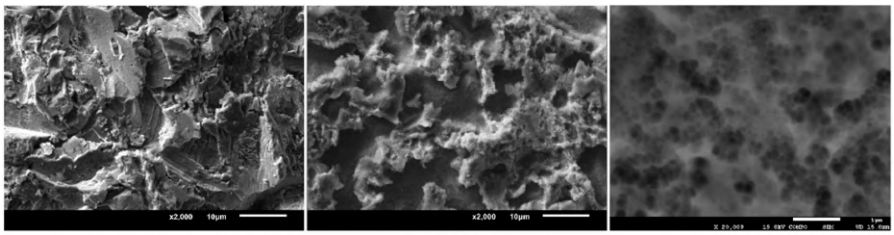

Figure 1. SEM pictures of 3D printed Ti alloy surfaces after blasting, and blasting + electropolishing.

The combination of sandblasting and electrochemical treatment in choline chloride-based DESs presents a viable strategy for surface modification, offering opportunities to fabricate titanium-based implants that exhibit superior surface properties and promote better biological integration. This advancement has the potential to contribute to the field of biomedical engineering by improving the performance and biocompatibility of titanium implants. More details about the presented work can be found in already published articles [1-3].

Acknowledgment: This work was financially supported by the Slovak Grant Agency (project APVV-20-0322), Slovak Republic and by Research & Innovation Operational Programme funded by the ERDF (ITMS project code 313021T081).

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Structure, mechanical characteristics and high-temperature stability of sintered under high and by hot pressing ZrB_2- and HfB_2–based composites

Tetiana Prikhna[1,3], Pavlo Barvitskyi[1], Branko Matović[2], Dejan Zagorac[2], Anastasiya Lokatkina[1], Bernd Büchner[3], Jochen Werner[3], Myroslav Karpets[1,4], Robert Kluge [3], Viktor Moshchil [1], Anatolii Bondar[5], Olexander Borymskyi[1], Leonid Devin[1], Semyon Ponomarov[6]

[1]V. Bakul Institute for Superhard Materials of the National Academy of Sciences of Ukraine, Avtozavodska Str., 2, Kyiv 04074, Ukraine
[2]Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovića Alasa 12-14, 11000 Belgrade, Serbia
[3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V.Helmholtzstraße 20, 01069Dresden, Germany
[4]National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute", Peremogy Avenue 37, 03056 Kyiv, Ukraine
[5]Frantsevich Institute for Problems of Material Sciences of the National Academy of Sciences of Ukraine, Krzhizhanovsky Str., 3, 03142 Kyiv, Ukraine
[6] Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine (NASU), 41, Nauky Ave., 03028 Kyiv, Ukraine

The study of the structure, mechanical characteristics and high-temperature stability in a vacuum and air (DTA and TG measurements) of sintered under high quasihydrostatic and by hot pressing ZrB_2- and HfB_2 – based materials without and with SiC and Si_3N_4 additions showed that the use of high pressures at comparatively low temperatures and short sintering time makes it possible to obtain mentioned materials with improved mechanical properties as compared to all other known methods. The pure ZrB_2 and HfB_2 and their composites with SiC and Si_3N_4 were densified using pressure of 4.1 GPa at 1800 ^oC, as well as hot pressing at 30 MPa. The results showed that the stability in the vacuum of pure ZrB_2 and HfB_2 occurred to be essentially higher than that of the materials with SiC additions. On the other side, their composites demonstrated essentially higher values for mechanical properties. In addition, high-pressure sintered materials manifested better mechanical characteristics compared to hot-pressed materials. The use of high pressures at comparatively low temperatures and short sintering time makes it possible to obtain the mentioned materials with improved mechanical properties as compared to all other known methods. The composite material prepared from HfB_2-30 wt.%SiC mixture demonstrated mechanical characteristics (density ρ = 6.21 g/cm^3, microhardness Hv(9.8 N) = 38.1±1.4 GPa, and fracture toughness K_{1C}(9.8 N) = 8.2±0.2 MH•m$^{0.5}$) which are essentially higher than that of pure HfB_2 sintered in the same conditions (ρ = 10.79 g/cm^3, Hv(9.8 N) = 21.3±0.84 GPa, K_{1C}(49 N) = 7.2±0.9 MH•m$^{0.5}$). Pure HfB_2 demonstrated Young modulus E = 984 GPa and Poisson ratio μ = 0.146.

Energy landscape exploration of the novel $CrSi_2N_4$ compound

Tamara Škundrić[1,2], Johann Christian Schön[3], Aleksandra Zarubica[4], Matej Fonović[5], Milan Pejić[1,2], Jelena Zagorac[1,2], Dejan Zagorac[1,2]

[1]Materials Science Laboratory, Institute of Nuclear Sciences "Vinča", University of Belgrade, Belgrade, Serbia
[2]Center for synthesis, processing and characterization of materials for application in the extreme conditions "CextremeLab", Belgrade, Serbia
[3]Max Planck Institute for Solid State Research, Heisenberg str. 1, D-70569, Stuttgart, Germany
[4]Faculty of Science and Mathematics, University of Nis, Serbia
[5]Faculty of Engineering, University of Rijeka – RiTeh, Rijeka, Croatia

The Cr-Si-N system holds significant importance for materials exhibiting advanced tribological and mechanical properties. Previous research has focused on Cr-Si-N coating, nanocrystalline phases, thin films, as well as theoretically predicted 1D and 2D hetero-structures, and 3D bulk Cr_2SiN_4 modifications. This particular study aims to predict potential bulk Cr-Si-N phases, specifically with the composition $CrSi_2N_4$. The research employs a multi-methodological approach, combining global optimization with data mining and the Primitive Cell for Atom Exchange (PCAE) method to explore the energy landscape of the system. Local optimization of structure candidates is conducted at the Density Functional Theory (DFT) level using the GGA-PBE and the LDA-PZ approximation. Among the discovered structure candidates in the $CrSi_2N_4$ chemical system, the ten most energetically favorable ones predominantly display monoclinic symmetry. However, these structures exhibit a range of features, from zeolite-like structures to polytypic behavior. The study also involved computing the bulk modulus and cell volume of all predicted $CrSi_2N_4$ phases under various pressures, extending up to 10 GPa. Additionally, the decomposition of $CrSi_2N_4$ into CrN, Si_3N_4, and N_2 has been investigated and the results suggested that the $TiMn_2O_4$-type modification, identified as the global minimum phase, should remain stable, particularly at lower temperatures.
Given the absence of experimental data for comparison, the study employed two different functionals to assess the robustness of the energy ranking and structural data. The good agreement observed between the two calculation levels suggests a high likelihood that the identified structure candidates represent actual (meta)stable modifications for bulk $CrSi_2N_4$. This discovery offers promising targets for future experimental synthesis, opening avenues for further theoretical studies on the electronic and magnetic properties of these materials.

Enhanced aluminum matrix composites for structural applications

Ivana Cvijović-Alagić[1], Jelena Maletaškić[1], Vladimir Pavkov[1], Slaviša Putić[2], Branko Matović[1], Vesna Maksimović[1]

[1]Center of Excellence "CEXTREME LAB", Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia
[2]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

Modern industrial practice should be in compliance with the green agenda and strongly support ecological sustainability through the achievement of zero-waste industrial production. In that regard, industrial production is nowadays focused on the reuse of industrial wastes for the attainment of new functional materials and products. Therefore, the obtainment of cost-effective and highly efficient technological procedures for the production of damage-resistant structural components with prolonged life cycles is of great importance.

Accordingly, the scope of the present research was to obtain inexpensive structural composite materials with enhanced properties through the industrial waste recycling process. Namely, to produce lightweight and highly durable structural components for application in the transportation industry the metallic waste, derived from the industrial machining of aluminum alloys, and inexpensive basalt fibers, obtained by the recycling of stone wool used as thermo-insulation materials in the building and construction industry, were foreseen as raw materials for the fabrication of aluminum matrix composites (AMCs). As the AMC matrix, the waste aluminum 2024 alloy chips were chosen and ball-milled to obtain a powder with homogeneous particle distribution. The basalt fibers from waste stone wool were used as composite reinforcements and before their mixing in a 3D tumbler mixer with Al alloy powder two different ratios, *i.e.* Al alloy : basalt fibers = 90 : 10 and Al alloy : basalt fibers = 80 : 20, were rinsed and subjected to thermal treatment. The prepared mixtures were subjected to Spark Plasma Sintering (SPS) at 500 ^{o}C under the pressure of 50 MPa and subsequent annealing at 550 ^{o}C to obtain the desired microstructure. Full characterization of the obtained AMCs was conducted using scanning electron microscopy (SEM), microhardness measurements, and X-ray diffraction (XRD) analysis. Moreover, the thermal diffusivity and thermal capacity investigations were conducted to determine the thermal conductivity of produced AMCs. The attained results showed that significant enhancement of the starting 2024 alloy's properties was achieved. In particular, it was determined that the obtained AMCs hardness and thermal conductivity are significantly improved when compared with the starting 2024 aluminum alloy.

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Two different paths to obtain pure nanosized Fe_3O_4: Morphology and Magnetic properties

Maria Čebela[1], Nataša Tomić[2], Milica Vujković[3], Milena Rosić[1], Vesna Lojpur[1]
[1]*Institute of Nuclear Sciences „Vinča", National Institute of the Republic of Serbia, University of Belgrade, 11001 Belgrade, Serbia*
[2]*The Institute of Physics Belgrade, National Institute of the Republic of Serbia, 11000 Belgrade, Serbia*
[3]*University of Belgrade – Faculty of Physical Chemistry, 11000 Belgrade, Serbia*

The nanosized Fe_3O_4 was prepared in two different ways. Firstly, the precipitation method was used with iron (II) chloride as a precursor. After calcination at T=550 ℃ the pure Fe_2O_3 phase was obtained. In order to produce Fe_3O_4 nanopowder, consequently the annealing process in a mixed atmosphere (93% Ar and 7% H_2) was conducted. This transformation was confirmed by X-ray powder diffraction (XRPD) analysis, while morphology before and after annealing was investigated by Scanning Electron Microscopy (SEM). In the second procedure, hydrothermal method was used, where iron (II) and iron (III) chloride were used as precursors in a molar ratio 1:2. The temperature was kept at T=200 ℃ for t=1h. The structural and morphological characteristics were also investigated by XRPD and SEM. Furthermore, the influence of these two synthesis methods on magnetic properties will be presented. For this purpose the measurements on SQUID will be applied. It will be pointed out which kind of route and morphology enables better performance.

Theoretical Investigations of Electronic Properties of Predicted Y_2O_2S

Dragana Jordanov[1], Dejan Zagorac[1], Klaus Doll[2], Johann Christian Schön[3], Milena Rosić[1], Maria Čebela[1]

[1]*Vinča"Institute of Nuclear Science, National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

[2]*Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany*

[2]*Nanoscale Science Department, Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany*

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. In this study we perform crystal structure prediction and investigate energy landscape of Yttrium Oxisulfide (Y_2O_2S). Global optimizations on the energy landscape of Y_2O_2S have been carried out using empirical potentials followed by, a local optimization using *ab initio* calculations [1]. Our calculations showed the *Alpha* phase in good agreement with the experimentally observed trigonal structure. Furthermore, novel *Beta* and *Gamma* modifications of pure Yttrium Oxysulfide have been discovered. Y_2O_2S is a material known as a wide-gap semiconductor. From the calculation of the bulk, it is found that the material has an indirect band gap and that the top of the valence bands shows an anisotropic character which means an anisotropic mass of the hole [2]. We included the calculation of the Density of States (DOS) for the most stable structures (*Alpha, Beta* and *Gamma*) and discuss the band gaps, also [3]. The results presented here have all been performed using the B3LYP functional and local density approximation (LDA). Our calculations are in good agreement with the literature data [4].

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Carbonate compounds formed by degassing of geothermal water from borehole B-4 at Sijarinska Banja (Serbia)

Bratislav Todorović[1], Dragan Stojiljković[1], Tanja Petrović Pantić[2]
[1]*Faculty of Technology, University of Niš, Leskovac, Serbia*
[2]*Geological Institute of Serbia, Rovinjska 12, Belgrade, Serbia*

Sijarinska Banja is located in southern Serbia. This spa has about 15 mineral water springs of various chemical composition and temperature. The B-4 borehole is a deep 1232 m with temperature 348 K, flow rate of 30 L s^{-1} and pressure in pipe installation is ≤ 8.8 bar. Also, this water shows relatively high Ca^{2+} (90 ppm) and extremely high concentration of HCO_3^- (3000 ppm) ions (Todorović et al., 2016).

When a well-head is opened, water loses its pressure, and thus loses its equilibrium. Degassing results in supersaturation of carbonate minerals because the attendant pH increase (7.6) more than compensates for decreased bicarbonate activity. Loss in pressure causes the dissolved CO_2 in water to flash into vapor. This decline in CO_2 causes the quick reaction (1) to show a tendency to the left side and thus will result in $CaCO_3$ precipitation in calcite, aragonite, and vaterite forms.

$$CaCO_3\,(s) + CO_2\,(aq) + H_2O\,(l) \rightleftharpoons Ca^{2+} + 2HCO_3^- \qquad (1)$$

Selective leaching experiments by acetate buffer have shown that a large part of the scale sample (99 %) dissolves in this fraction, suggesting that $CaCO_3$ minerals are the main components of the B-4 scale. XRD analysis of the scale has indeed proved that $CaCO_3$ minerals are the main components (99 %). $CaCO_3$ mineralogy studies have indicated that aragonite is the predominant $CaCO_3$ (95 %) mineral in the B-4 scale with lesser amount of calcite (<5 %) and minor amount vaterite. Precipitation and deposition of aragonite mineral is favored by the presence of Sr^{+2} ions (1 ppm).

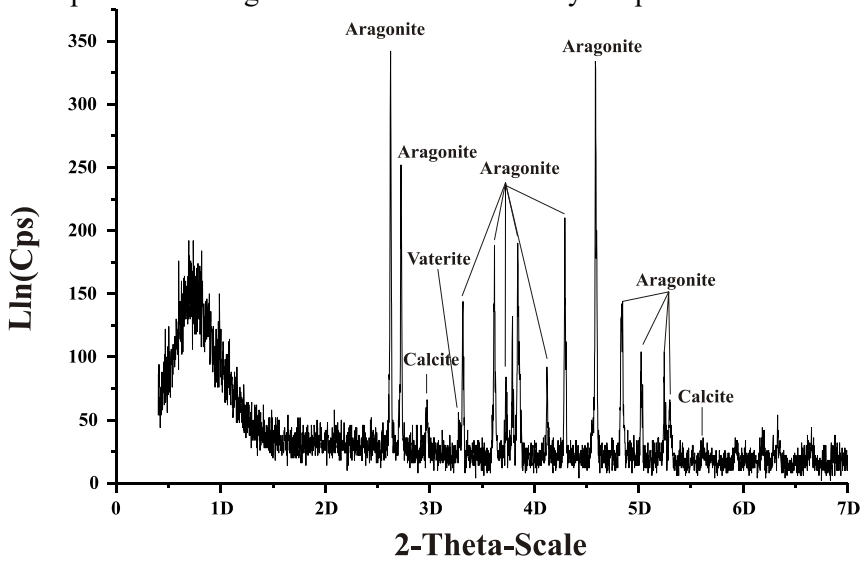

Figure 1. X-ray spectrum of sediment scale formed by B-4 water.

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Gamma Irradiation Induced Dyes Degradation: Recent Progress and Future Perspective for Wastewater Treatment

Marija Egerić[1,2], Dimitrije Petrović[1], Marjetka Savić[1], Aleksandar Devečerski[1], Srboljub Stanković[1], Radojka Vujasin[1], Ljiljana Matović[1,2,3]

[1]*Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

[2]*Center of Excellence "CEXTREME LAB", Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

[3]*College of Environmental Science and Engineering, State Key Laboratory of Pollution Control and Resource Reuse, Tongji University, Shanghai 200092, China*

Effluents generated from the textile industry contribute to the global problem of wastewater impact on the environment. It contains persistent chemicals, which are often challenging to remove using standard methods. There is an urgent need for a suitable treatment, highlighting the significance of reducing dye concentration in industrial effluents to preserve already fragile water and ecosystems. As one of the advanced oxidation process techniques, gamma irradiation has been studied as a method for the degradation of various organic molecules, including dyes. The vast literature review has shown that this technique was applied to remove dyes from single synthetic aqueous solutions and textile industry wastewater. Those highly persistent chemicals were more likely to be removed using irradiation doses in a wide range. Even though there is plenty of literature data regarding this topic, a facility for gamma irradiation treatment of wastewater contaminated by organic pollutants doesn't exist today. A mechanism of degradation was proposed: following the interaction between gamma rays and water molecules, the generation of multiple reactive species occurs. They non-specifically react with organic compounds and lead to partial or complete degradation. By-product formation is acknowledged to occur during the degradation of dyes, but their formation and persistence are not extensively studied. The efficiency of dyes' radiolytic decomposition depends on several factors, such as absorbed dose and dose rate, initial dye concentration, molecular structure of the pollutants, and pH value. Also, the synergetic effect of gamma irradiation with other chemicals and techniques has been widely studied in recent years. The application of different coupling methods influenced the reduction of gamma irradiation doses needed for partial or complete degradation of dye molecules. Promising results were achieved by coupling gamma with oxidizing agents (H_2O_2, N_2O), solid matrices and biological treatment. A synergy of multiple wastewater treatment methods opens new possibilities for designing modular or mobile plants that can meet requirements for commercial use. Research of different coupling systems helps to achieve sustainable development goals, such as better managing water resources and waste generation.

Characterization of high pressure oxygenated EuBCO and GdBCO coated conductors

Tetiana Prikhna[1,2], Aiswarya Kethamkuzhi[2], Roxana Vlad[2], Branko Matovic[3], Semyon Ponomarov[4], Robert Kluge[5], Myroslav Karpets[1,6], Viktor E. Moshchil[1], Xavier Obradors[2], Joffre Gutierrez[2], Bernd Büchner[5], Teresa Puig[2]

[1]*V. Bakul Institute for Superhard Materials of the National Academy of Sciences of Ukraine, 2, Avtozavodska Str., Kyiv 07074, Ukraine*

[2]*Institut de Ciencia de Materials de Barcelona, CSIC, Campus UAB, 08193 Bellaterra, Spain*

[3]*Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia,*

[4]*V.E. Lashkaryov Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine, 41, Nauky Ave., Kyiv 03028, Ukraine*

[5]*Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V., Helmholtzstrasse 20 01069 Dresden, Germany*

[6]*National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute", Peremogy Avenue 37, 03056 Kyiv, Ukraine*

REBCO (Re=Y, Eu, Gd) coated conductors (CC) based on biaxially textured, thick and homogeneous nanoengineered multilayer structures opened up new application opportunities, such as dissipation-free energy transmission in superconducting grids, highly efficient engines for electrical aviation or compact fusion reactors beyond ITER. However, current carrying capacities of CC could be further improved because they are still far from theoretical limits. Overdoping by oxygen the REBCO structure of CC is one of the possible robust ways to increase current carrying capacity of CC, however overdoping these materials is not easy. Here we report on the high pressure oxygenation results from EuBCO-CC (with the surface Ag layer chemically removed) and GdBCO-CC (coated with 2 μm Ag layer). Oxygen pressure were in the range from 1 - 160 bar and temperatures between 300-800 ^{o}C. The layers were characterized by XRD (estimating unit cells parameters), superconducting properties (T_c, J_c (T) and J_c(H, 77K)), and SEM, EDS and quantitative Auger spectroscopy. The highest J_c (77 K, 0 T) of 2.67 MA/cm^2 was obtained by GdBCO-CC with c= 1,17310 nm oxygenated at 100 bar O_2, 600 ^{o}C for 3 h. Its J_c (77 K, 0 T) was 4% higher than that of the initial GdBCO sample with c= 1,17351 nm. The J_c of the initial EuBCO-CC samples decreased after removing the Ag layer (J_c (77 K, 0 T)=1.38 MA/cm^2). However, among the high pressure oxygenated EuBCO-CC, the highest J_c(77 K, 0 T)=1.31 MA/cm^2 was that treated under 160 bar of O_2 at 800 ^{o}C for 3 h. The approximate composition of EuBCO matrix phase (estimated after etching of its surface by Ar ions in the chamber of microscope) according to quantitative EDX analysis was $EuBa_{2.06}Cu_{2.89}O_{7.35}Ni_{0.11}C_{1.05}$ and according to quantitative Auger analysis (which has higher locality than EDS) was $EuBa_{0.57}Cu_{0.25}O_{0.54}$. The approximate stoichiometry of the matrix phase of EuBCO initial sample was $EuBa_{2.05}Cu_3O_{7.97}Ni_{0.12}C$ (EDS) and $EuBa_{0.74}Cu_{0.22}O_{0.72}$ (Auger). This suggests that high pressure oxygenation of EuBCO may induced anion and cation diffusion. Additional treatments and experiments on charge carrier density are on-going.

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Photocatalytic application of $SrGd_2O_4$ nanoparticles doped with rare earth

Tijana Stamenković, Maria Čebela, Milena Rosić, Vesna Lojpur
Vinča Institute of Nuclear Sciences, National Institute of the Republic ofSerbia, University of Belgrade, Belgrade, Serbia

Pollution of the air and water is becoming a global concern. The process of photocatalysis provides a promising solution to these pressing problems because it is environmentally friendly, inexpensive, and sustainable. Materials exhibiting anti-Stokes and Stokes luminescence have recently come to light as potentially effective options for photocatalysis applications. Doping various Ln^{3+} ions in an inorganic host will cause irradiation to cause designable down- and up-conversion emissions that start in the UV and go up to the NIR. Photocatalytic use of the chosen samples will be investigated in this study. The sol-gel aided combustion approach was utilized to effectively prepare all of the samples. It was demonstrated by the X-ray Powder Diffraction pattern that all samples crystallize as pure orthorhombic $SrGd_2O_4$ phases. The morphology was characterized by scanning and transmission electron microscopy, which demonstrated the presence of porous, agglomerated, round-shaped particles that are suitable for photocatalytic applications. Dispersive X-ray energy Spectroscopy revealed that all of the constituent elements were evenly distributed and that dopant ions were present. The photocatalytic properties of down-converters were examined in the photocatalytic degradation of methyl orange (MO) organic dye under simulated solar light irradiation. A UV/Vis spectrometer was used to assess the decrease in MO concentration in water solutions during the experiment. Following four hours, the dye breakdown rate was successfully demonstrated by the findings of the specific time intervals in which aliquots of the working solutions were sampled. Using methylene blue (MB) as a test pollutant, the photocatalytic efficiency of up-conversion samples was examined under simulated sunshine illumination. After four hours of exposure to the simulated Sun irradiation, more than half of the initial dye concentration was mineralized, which indicated that the results were positive.

Spectroscopicand Morphological Properties of $Co_{0.9}Ho_{0.1}MoO_4$ nanopowders

Milena Rosić[1], Maja Milošević[2], Vladimir Dodevski[1], Dragana Jordanov[1], Vesna Lojpur[3], Tijana Vlašković[4], Maria Čebela[1]

[1]Laboratory for Material Science, Institute of Nuclear Sciences „Vinča“, National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia
[2]Department of Mineralogy, Crystallography, Petrology and Geochemistry, Faculty of Mining and Geology, University of Belgrade, Đušina 7, 11000 Belgrade, Serbia
[3]Department of Atomic Physics, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia
[4]Faculty of Sciences and Mathematics, University of Priština in Kosovska Mitrovica, Lole Ribara 29, 38220 Kosovska Mitrovica, Serbia

The glycine nitrate procedure (GNP) synthesized the nanostructured powder because it proved to be the most effortless and effective method acceptable for controlling the composition and morphology of $Co_{0.9}Ho_{0.1}MoO_4$. GNP is a combustion process that is a promising method for controlling stoichiometry, homogeneity, and purity. For the preparation of technologically important nanostructured $Co_{0.9}Ho_{0.1}MoO_4$, metal nitrates, and glycine were mixed in appropriate stoichiometric ratios. The samples obtained by the mentioned method were further subjected to different characterization methods such as DTA, X-ray diffraction (XRD), Fourier transform infrared spectrum (FT-IR), spectroscopy, and emission scanning electron microscopy (FESEM).The gained nanopowder showed a high level of shape anisotropy and particle size in the form of agglomerates was observed. Also, differences in the microstructures are clearly noticeable, and plate-like crystals. The synthesized sample's colour changes from darker to lighter shades upon heating treatment. The pronounced change of dominant wavelength (nm) and the purity of the colour between starting sample and the sample after the heating (1100 ^{0}C) is due to Co concentrations.

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Mechanical alloying as a crucial step in the fabrication process of Cu alloys

Marko Simić[1], Jovana Ružić[1], Dušan Božić[1], Željko Radovanović[2], Jelena Stašić[1]
[1]*Department of Materials, "Vinča" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, PO Box 522, 11001 Belgrade, Serbia*
[2]*Metallurgical Engineering Department, Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia*

Due to their exceptional combination of electrical conductivity, high strength, and thermal stability, copper based materials continue to be relevant in advanced applications discussions in industries like electrical, defence, military, nuclear and aerospace. They are particularly valuable in applications where excellent electrical conductivity combined with high strength is demanded. Moreover, their resistance to thermal fatigue and creep makes them suitable for use in high-temperature environments, such as in aerospace components and advanced cooling systems. To achieve these properties, the crucial step in the production of Cu based materials is the mechanical alloying (MA) process. The MA process involves the repeated fracturing and welding of powder particles in a high-energy ball mill (Turbula shaker mixer), which is essential for producing uniform and fine-grained microstructures. In this study, various MA parameters, including milling time (10,20,30,40h), ball-to-powder weight ratio (1:10, 1:15 ratios) and the weight ratio of the milling balls (uniform size balls (6mm), 3 different size balls (6mm, 10mm,25mm)), have been examined. The milling speed (300rpm) and the milling atmosphere (argon) were kept the same throughout the whole MA process. It was shown that the powder produced in the higher powder-ball ratio, 1:10 shows lower values of dislocation density and crystalline size compared to the 1:15 ratio. The size of milling balls has proven to be an important factor as the powders produced by uniform milling ball size, showed higher values of dislocation density compared to powders where different ball sizes were used (for the same ball-powder weight ratio). In all cases, dislocation density increases with time while crystalline size decreases due to welding as a dominant process in MA.

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Preparation of $Ca_{0.9}Er_{0.1}MnO_3$ nanopowders by combustion method

Tijana B. Vlašković[1], Bojana Laban[1], Maria Čebela[2], Vladimir Dodevski[2], Dragana Jordanov[2], Milena Rosić[2]

[1]*Faculty of Sciences and Mathematics, University of Priština in Kosovska Mitrovica, Lole Ribara 29, 38220 Kosovska Mitrovica, Serbia*

[2]*Laboratory for Material Science, Institute of Nuclear Sciences „Vinča“, National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia*

The sucrose-nitrate procedure (SNP) was used for the synthesis of $Ca_{0.9}Er_{0.}1MnO_3$ nanopowders with a perovskite-type crystal structure. During this combustion method, sucrose $C_{12}H_{22}O_{11}$ was used as fuel and complexant, and calcium nitrate tetrahydrate $Ca(NO_3)_2{\times}4H_2O$, manganese(II) nitrate hydrate $Mn(NO_3)_2{\times}H_2O$, erbium(III) nitrate pentahydrate $Er(NO_3)_3{\times}5H_2O$ as oxidants. $Ca_{0.9}Er_{0.}1MnO_3$ nanopowders synthesized in this way were calcined at a temperature between 800 - 1000 ºC. The samples were further subjected to various characterization methods such as X-ray diffraction (XRD), field scanning electron microscopy (FESEM), and Brunauer-Emmet-Teller (BET) method at room temperature. The stability of these solid solutions and crystallite growth is monitored by treatment at high temperatures (up to 1000 °C). The results show that by applying the SNP method, in a relatively short time it is possible to produce a low-cost composition of $Ca_{0.9}Er_{0.}1MnO_3$with a particle size of less than 20 nm. Therefore, this method proved to be suitable for the preparation of this composition.

Activating agricultural residues: Corn cob as a resource for adsorption-based pollution management

Ružica Mihailović [1], Aleksandra Zarubica[2], Branko Matović[1], Svetlana Butulija[1]
[1]Veterinary Specialist Institute "Kraljevo", Žička 34, 36000 Kraljevo
[2]Department of Chemistry, Faculty of Science and Mathematics, University of Niš, Višegradska 33, 18000 Niš, Serbia
[3]„VINČA" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovića Alasa 12-14, Belgrade, Serbia

In the pursuit of sustainable environmental solutions, this study investigates the transformation of corn cob, an abundant agricultural waste, into activated carbon materials. Through a cost-effective and eco-friendly approach, our research explores the adsorption capabilities of these materials for the removal of diverse pollutants from water and air. The conversion of corn cob into activated carbon not only addresses the environmental impact of waste disposal but also offers a promising avenue for developing efficient adsorbents with applications in pollution control. The syntesized material was characterized using X-ray Diffraction (XRD), High-Resolution Scanning Electron Microscopy (HRSEM), and Brunauer-Emmett-Teller (BET) analysis. This work contributes to advancing green technologies, emphasizing the potential of corn cob-derived activated carbon as a practical and effective means to tackle contemporary environmental challenges.

The influence of stainless steel particles reinforcement on the fracture toughness of glass-ceramic matrix composite

Vladimir Pavkov[1], Gordana Bakić[2], Vesna Maksimović[1], Ivana Cvijović-Alagić[1], Aleksandar Maslarević[2], Bratislav Rajičić[2], Nenad Milošević[2]

[1]*Department of Materials Science, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

[2]*Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia*

The fracture of engineering materials is always an undesirable phenomenon, which primarily can endanger human lives, create economic losses, and lead to downtime and unavailability of mechanical parts. The main drawback that still prevents the broader use of ceramic and glass-ceramic materials is the tendency to brittle fracture due to extremely low toughness. Due to the appearance of cracks, the mechanical properties and structure of the material degrade irreversibly, which can lead to catastrophic failure of the mechanical element or construction. This drawback can be overcome by synthesizing novel composite materials with glass-ceramic matrix and metal reinforcement with improved fracture toughness.

This research examined two materials: a glass-ceramic material and a composite material based on glass-ceramic-metal. The glass-ceramic material is obtained from andesite basalt powder, while the glass-ceramic-metal composite is made from the glass-ceramic matrix of andesite basalt powder and a metal reinforcement of stainless steel powder in the content of 20 wt.%. The aggregate of andesite basalt from Serbia was used as the starting natural raw material for obtaining the glass-ceramic matrix. The austenitic stainless steel powder of the commercial grade Surfit^{TM} 316L was used as a reinforcement. Both materials were obtained using powder metallurgy, which consisted of the following phases: crushing of andesite basalt aggregate, sieving of the stainless steel powder, homogenization of powder and binder, cold uniaxial pressing of the powder, cold isostatic pressing of green compact and sintering as the final phase to obtain a high-density solid sample.

The andesite basalt, and 316L stainless steel powder were characterized using a scanning electron microscope and X-ray diffraction method. The sintered samples of glass-ceramic and glass-ceramic-metal were characterized with an optical light microscope, scanning electron microscope, and Vickers hardness test.

Based on the obtained results, it can be concluded that the presence of metallic particles in the glass-ceramic matrix leads to a slight decrease in hardness while contributing to an increase in the material's fracture toughness by about 33% [1]. During crack propagation in the glass-ceramic matrix, different crack particle interactions were observed: crack stops, deflects, or bridgings when encountering the spherical metal particle. These interaction phenomena and mechanisms of crack propagation in the glass-ceramic-metal composite lead to an increase of crack propagation resistance.

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Mechanical properties of human enamel and dentin: a study by nanoindentation

Jana Andrejovská[1], Ondrej Petruš[1], Dávid Medveď[1], Marek Vojtko[1], Marcel Riznič[2,3], Peter Kizek[2,3] and Ján Dusza[1]

[1]*Institute of Materials Research, Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovak Republic*
[2]*Department of Stomatology and Maxilofacial Surgery, University Hospital, Rastislavova 43, 041 90 Košice, Slovak Republic*
[3]*Faculty of Medicine, University of Pavol Jozef Šafárik, Tr. SNP 1,04011 Košice, Slovak Republic*

As one of the most durable biocomposites found in nature, human teeth have become a type of representative biomechanical complex that have been studied extensively in the past decades [1]. Natural teeth are function–oriented unique bilayer composites, with dentin constituting the main part to support the overlying enamel. Enamel, the outer layer, can be regarded as a natural optimised coating, which protects the tooth from mechanical damage over millions of chewing cycles and cutting food in a lifespan, which is why the knowledge of the dental tissue nanohardness and elastic modulus is very important. In this study the hardness, indentation modulus and deformation characteristics of human enamel and dentin have been investigated using instrumented indentation with the aim to understand their deformation behaviour at different locations across the occlusal enamel surface, through the DEJ area to the inner area of dentin. Scanning electron microscopy was used for the characterization of the enamel and dentin and their deformation and damage behaviour. The average values of hardness and modulus for enamel in the occlusal area are 5.35 ± 0.19 GPa and 98.1 ± 1.5 GPa, in the inner area 3.68 ± 0.5 GPa and 81.8 ± 5 GPa and in the area close to the dentin enamel junction 2.83 ± 0.27 GPa and 71.4 ± 4.1 GPa, respectively. The average values of hardness and modulus of dentine in the area close to the dentin enamel junction are 0.71 ± 0.05 GPa and 21.27 ± 0.76 GPa and in the inner area 0.65 ± 0.06 GPa, 19.79 ± 0.93 GPa, respectively. The effect of the indentation location on deformation and mechanical properties were clarified. The mechanical properties and deformation behavior of enamel are the function of anisotropic properties of the enamel´s hierarchical structure, the size and orientation of enamel rods and the composition of the enamel at the tested location [2]. The factors influencing the dentinal mechanical properties include the location, density and direction of the dentinal tubules, the direction of the collagen fibers and average density of the mineral phase. In addition, dentin consists of intertubular dentin, peritubular dentin and dentinal tubules are wrapped with peritubular dentin.

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Structure-property relationship of AlN/BN mixed compounds on DFT level

Dejan Zagorac[1,2], Jelena Zagorac[1,2], Matej Fonovic[3], Tamara Škundrić[1,2], Milan Pejić[1,2], Dušica Jovanović[1,2], Milos B. Djukic[4], Branko Matović[1,2]

[1]Institute of Nuclear Sciences "Vinča", Materials Science Laboratory, University of Belgrade, Belgrade, Serbia
[2]Center of excellence "CextremeLab", Center for synthesis, processing, and characterization of materials for application in extreme conditions, Belgrade, Serbia
[3]Faculty of Engineering, University of Rijeka-RiTeh, Rijeka, Croatia
[4]University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia

In the last few decades, aluminum nitride (AlN) and boron nitride (BN) have become a point of interest to many researchers and scholars from different disciplines around the world. Due to its broad attractive properties, AlN has been successfully used in various applications, starting from advanced ceramics materials, additive for grain size control in micro-alloyed steels, through optoelectronics and microelectronics, and finally to semiconductors. On the other hand, BN has broad applications in various fields, such as 2D material, lubricant material, superhard and semiconductor material as well as many others. This study focuses on the mixed AlN/BN compounds, in particular, boron-rich AlN [1] and aluminum-rich BN [2] systems, thus having the entire range of AlN/BN compositions. The special focus was on structural, elastic, and mechanical properties investigated using DFT methods. Important mechanical properties were investigated; bulk modulus B, shear modulus K, Young's modulus E, Vickers hardness Hv, anisotropy, stiffness, Poisson's ratio, and brittleness/ductility relationship, to offer novel technological and industrial applications of mixed AlN/BN materials.

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Nanoindentation Properties of Al_2O_3 + ZrO_2 + WTiC/ZrC Ceramics Fabricated by SPS

Dávid Medveď[1], Jana Andrejovská[1], Marek Vojtko[1], Annamária Naughton -Duszová[1], Piotr Klimczyk[2]

[1]Institute of Materials Research, Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovakia
[2]Łukasiewicz Research Network – Krakow Institute of Technology, Zakopianska 73, 30-418 Krakow, Poland

The development and characterization of ceramic composites represent a key area in materials engineering, aimed at achieving materials with outstanding mechanical properties for a wide range of applications. This study focuses on the synthesis and analysis of ceramic composites based on alumina (Al_2O_3) and zirconia (ZrO_2) with the addition of tungsten-titanium carbide (WTiC) and zirconium carbide (ZrC) using the Spark Plasma Sintering (SPS) method. The composites were sintered at a temperature of 1600°C in an argon atmosphere, exploring their nanoindentation, including characteristic load-displacement curves, hardness-displacement, and modulus of elasticity-displacement.

The Al_2O_3 + ZrO_2 + WTiC composite achieved an average indentation hardness of 32.78 ± 2.45 GPa and a modulus of elasticity of 462.5 ± 27.1 GPa, while the Al_2O_3 + ZrO_2 + ZrC composite exhibited a slightly lower hardness of 27.27 ± 3 GPa and a modulus of elasticity of 379.1 ± 28.5 GPa. These results are consistent with literature data, where similar systems were evaluated based on nanoindentation, and indicate a significant potential of the added carbides in improving the mechanical properties of ceramic composites.

Comparing our results with the literature, the study by Krell and Schadlich [1] states that the hardness of alumina ceramics can be in the range of 25-30 GPa under small loads (25-50 mN), depending on the systems' microstructure. Aragón-Duarte et al. [2] report the hardness of ZTA (80 wt.% Al_2O_3 + 20 wt.% TZ−3Y) as 35 ± 1 GPa and the modulus of elasticity as 360 ± 6 GPa, which is very close to the values measured for our system. These comparisons show that the addition of WTiC and ZrC positively impacts the improvement of hardness and modulus of elasticity, which are key properties for high resistance and long life in applications.

Our findings confirm that adding WTiC and ZrC to Al_2O_3 and ZrO_2 based ceramic composites not only improves their mechanical properties but also opens new possibilities for their use in applications requiring high resistance and longevity, such as cutting tools and components for advanced engineering use.

Acknowledgments: This work was carried out within the framework of the DuplexCER project, entitled “High performance duplex ceramics for efficient machining of nickel superalloys”, co-founded by The Polish National Centre for Research and Development within the framework of the M-ERA.NET programme (Agreement No. M-ERA.NET3/2021/82/DuplexCER/2022) and by Slovak Academy of Sciences, and by projects VEGA 2/0108/24, VEGA 2/0137/22.

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Multidisciplinary approach in investigating ZnO/ZnS core/shell nanostructures

Jelena Zagorac[1,2], Dušica Jovanović[1,3], Dejan Zagorac[1,2], Tamara Škundrić[1,3], Milan Pejić[1,4], Vesna Šrot[5], Branko Matović[1,2]

[1]Materials Science Laboratory, Institute of Nuclear Sciences "Vinča", University of Belgrade, Belgrade, Serbia
[2]Center for synthesis, processing, and characterization of materials for application in the extreme conditions "CextremeLab", Belgrade, Serbia
[3]Department of chemistry, Faculty of science and mathematics, University of Nis, Nis, Serbia
[4]Faculty of Physics, University of Belgrade, Belgrade, Serbia
[5] Max Planck Institute for Solid State Research, Stuttgart Center for Electron Microscopy, Stuttgart, Germany

ZnO/ZnS core/shell nanostructures, which are studied for diverse possible applications, ranging from semiconductors, photovoltaics, and light-emitting diodes (LED), to solar cells, infrared detectors, and thermoelectrics, were synthesized and characterized by XRD, HR-(S)TEM, and analytical TEM (EDX and EELS). Moreover, band gap measurements of the ZnO/ZnS core/shell nanostructures have been performed using UV/Vis DRS. The experimental results were combined with theoretical modeling of ZnO/ZnS (hetero)structures and band structure calculations for ZnO/ZnS systems, yielding more insights into the properties of the nanoparticles.

The *ab initio* calculations were performed using hybrid PBE0 and HSE06 functionals. The synthesized and characterized ZnO/ZnS core/shell materials show a unique three-phase composition, where the ZnO phase is dominant in the core region, and, interestingly, the auxiliary ZnS compound occurs in two phases as wurtzite and sphalerite in the shell region. Moreover, theoretical *ab initio* calculations show advanced semiconducting properties and possible band gap tuning in such ZnO/ZnS structures.

Bacterial Cellulose-Cerium Oxide Hydrogel for Tailored Redox Balance in Biomedical Extremes

Svetlana Butulija[1], Jelena Filipović Tričković[1], Ana Valenta Šobot[1], Bratislav Todorović[2], Sanja Petrović[2], Bojana Ilić[1], Danica Zmejkoski[1], Branko Matović[1]

[1]„VINČA“ Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovića Alasa 12-14, Belgrade, Serbia
[2]Faculty of Technology, University of Niš, Bulevar Oslobođenja 124, Leskovac, Serbia

In recent years, there has been a growing interest in the exploration of advanced biomaterials tailored for therapeutic applications. Our study is dedicated to the development and characterization of a bacterial cellulose-cerium oxide hydrogel, specifically designed to excel in extreme environments characterized by an excessive release of free radicals. This novel hydrogel emerges as a promising solution for effectively mitigating oxidative stress across diverse biomedical scenarios. The distinctive composition of the hydrogel leverages the exceptional properties of bacterial cellulose and cerium oxide nanoparticles, creating a synergistic platform tailored for precise and targeted removal of free radicals. Notably, this biomaterial showcases outstanding biocompatibility and underscores its potential in redox regulation, particularly in the realms of wound healing and neurological recovery within extreme oxidative stress environments.

To gauge its efficacy, we conducted rigorous evaluations of redox parameters using the Pro/Antioxidant Balance (PAB) assay and Lipid Peroxidation Products assay. The results reveal a significant shift towards a more favorable redox state, underscoring the hydrogel's remarkable capability in maintaining cellular homeostasis even in the face of extreme oxidative challenges.

Our findings strongly advocate for the bacterial cellulose-cerium oxide hydrogel as a versatile tool adept at addressing oxidative stress-related complications. This research not only contributes to the evolving landscape of biomaterials designed for therapeutic interventions but also highlights a promising avenue for combating excessive free radicals in the demanding environments of various biomedical applications.

High-entropy stabilized $Zr_{0.2}Hf_{0.2}Ce_{0.2}Yb_{0.2}Gd_{0.2}O_{2-\delta}$ with fluorite structure

Marija Prekajski Đorđević[1], Jelena Maletaškić[1], Svetlana Butulija[1], Emilija Nidžović[1], Aleksa Luković[1], Ravi Kumar[2,3], Branko Matović[1]

[1]*Centre of Excellence-CextremeLab Vinca, Institute of Nuclear Sciences Vinca, University of Belgrade, Mike Petrovica Alasa 12-14, 11000, Belgrade, Serbia*

[2]*Laboratory for High Performance Ceramics, Department of Metallurgical and Materials Engineering, Indian Institute of Technology-Madras (IIT Madras), Chennai, 600036, India*

[3]*Ceramic Technologies Group-Center of Excellence in Materials and Manufacturing for Futuristic Mobility, Indian Institute of Technology-Madras (IIT Madras), Chennai, 600036, India*

High-entropy stabilized Oxides represent an advanced class of ceramic materials renowned for their exceptional functional characteristics. Employing a unique five-component oxide formulation, these materials harness configurational entropy to achieve unprecedented phase stability. The focus of this investigation centers on the successful synthesis of a groundbreaking high-entropy fluorite oxide, $Zr_{0.2}Hf_{0.2}Ce_{0.2}Yb_{0.2}Gd_{0.2}O_{2-\delta}$, using the Self Propagation Room Temperature reaction (SPRT) technique. Remarkably, comprehensive heat treatment experiments revealed that, even under elevated temperatures, all samples maintained a singular phase composition. Notably, subjecting the material to a thermal treatment at 1500°C resulted in the attainment of a fully crystallized single-phase fluorite structure. Additionally, the powders exhibited a notable absence of agglomeration, facilitating the sintered specimens to achieve substantial densification with minimal and uniformly distributed porosity.

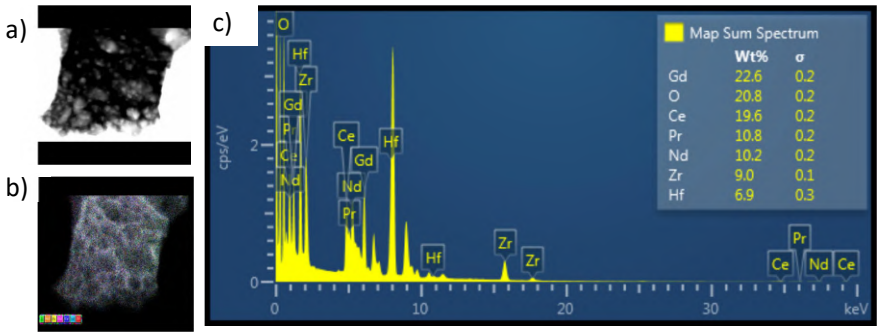

Figure 1. SEM-EDS of thermally treated sample (1500 °C): a) SEM micrograph, b) elements mapping, c) results of EDS chemical analysis.

Basaltic Glass-Ceramic Composites: Exploring Structural, Morphological, and Thermal Insights for Ballistic Protection and Radiation Shielding Applications

Aleksa Luković[1], Diana Carolina Lago[2], Jozef Kraxner[2], Dušan Galusek[2], Branko Matović[1], Danica Srećković-Batoćanin[3], Jelena Maletaškić[1]

[1]*Department of Materials, Insitute of Nuclear Sciences „Vinča", University of Belgrade, Serbia*
[2]*Department of Glass Processing, Joint Glass Centre of the IIC SAS, TnU AD and FChFT STU, Centre for Functional and Surface Functionalized Glass, TnU AD, Trenčín, Slovakia*
[3]*Faculty of mining and geology, University of Belgrade, Serbia*

The present study explores the synthesis and comprehensive characterization of basaltic glass-ceramic composites through a volume crystallization method. Utilizing basalt from the Vrelo deposit, the initial raw material underwent a meticulous processing route involving milling, melting, and annealing. The experimental design encompassed four distinct sample types: a basalt glass-ceramic without additives, a basaltic glass-ceramic with 5 wt% of iron mine tailings, a basaltic glass-ceramic with a steel wire mesh incorporated as a sandwich composite, and a basaltic glass-ceramic composite with both iron mine tailings and steel wire mesh. Advanced characterization techniques, including X-ray Diffraction (XRD), High Temperature X-ray Diffraction (HT-XRD), Scanning Electron Microscopy with Energy Dispersive X-ray Spectroscopy (SEM-EDS), X-ray Fluorescence (XRF), Differential Scanning Calorimetry (DSC), and Fourier-transform Infrared Spectroscopy (FTIR), were employed to unravel the structural, morphological, and thermal properties of the synthesized materials.

The inclusion of steel wire mesh and iron mine tailings led to unique compositional variations, impacting the properties of the synthesized glass-ceramic composites. The findings from this comprehensive characterization serve as a foundation for performance evaluation and future applications of the basaltic glass-ceramic materials, with potential applications in ballistic protection and radiation shielding.

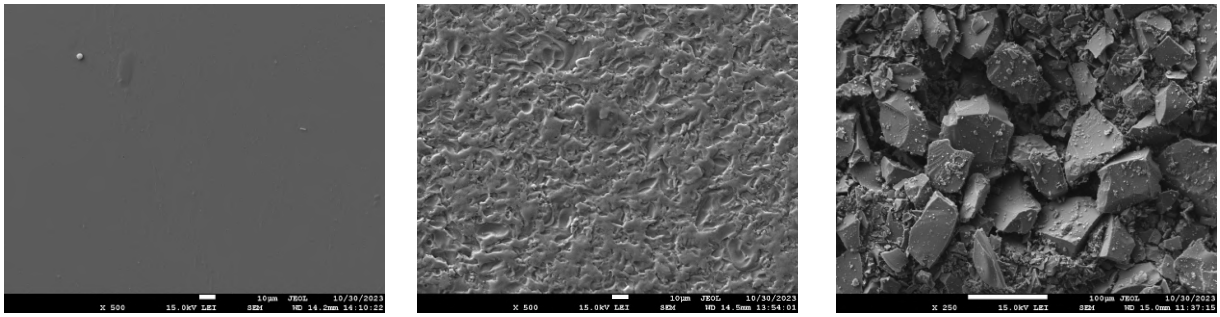

Figure 1. Scanning electron microscopy (SEM) microphotographs of basalt glass samples.

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Energy Landscape Exploration of Novel Rare Earth Chalcohalides LaXY (X=O,S; Y=I,F)

Milan Pejić[1,2], Dejan Zagorac[1,2], Jelena Zagorac[1,2], Tamara Škundrić[1,2], Dušica Jovanović[2], Branko Matović[1,2]

[1]*Materials Science Laboratory, Institute of Nuclear Sciences "Vinča", University of Belgrade, Belgrade, Serbia*

[2]*Center for synthesis, processing and characterization of materials for application in the extreme conditions "Cextreme Lab", Belgrade, Serbia*

The identification and characterization of new rare earth compounds and modifications is important for advancing diverse techological areas, including electronics, manufacturing, military applications, medicine, energy storage, biomaterials, etc. [1-4]. Traditionally, this is achieved through experimental synthesis of numerous new materials and the subsequent study of their properties. This approach is increasingly complemented by theoretical calculations which predict new compounds or modifications without experimental input. While many recent studies that focus on the chalcohalides of the rare earth elements have wide range of applications, only a few of them involve research of the lanthanum oxyiodide (LaOI) and lanthanum sulfofluoride (LaSF) chemical systems.

In this study, crystal structure candidates of LaXY systems were found using global optimization (GO) on an empirical potential energy landscape which involved use of simulated annealing combined with periodic stochastic local optimization, followed bylocal optimization of the most promising candidates on the ab initio level using density functional theory (DFT) calculations [5-7].

Energy landscapes of LaXY were explored for different numbers of formula units (N=4,6,8,12) in the simulation cell. By employing global optimization using empirical potentials, over one million local minima representing potential structure candidates were obtained for each of the LaXY systems. These candidates were then evaluated based on criteria such as ground state energy, frequency of occurrence, and symmetry, leading to the identification and selection of several hundred relevant structures. Subsequent local optimizations on the ab initio level, employing DFT calculations with different functionals, further validated and refined the predicted structures, leading to the discovery of new predicted phases.

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Synthesis and characterization of ceria doped with mercury

Tamara Minović Arsić, Jelena Maletaškić, Svetlana Butulija, Emilija Nidžović, Jelena Erčić, Marija Prekajski Đorđević, Branko Matović
Vinča Institute of Nuclear Sciences, University of Belgrade, Mike Petrovića Alasa 12-14, Vinča, Serbia

Mercury is one of the chemicals of major public health concern. People are exposed to mercury through inhalation of polluted air, ingestion of contaminated water and food, and also trans dermal and trans placental. It is very migrational element and has to be properly stored. Many materials have been developed for mercury remediation. There are many current ongoing research studies with goal to find the most inexpensive and effective material. In recent years, adsorbents with cerium as active component have been used for the removal of elemental mercury.
The aim of this study is to examine the possibility to store mercury in cristal structure of ceria. In order to do that we synthesized CeO_2 samples with 1, 3, 5, 6, 7, 8, 10 and 15 wt. % of Hg, by a self-propagating room temperature method (SPRT). Materials were characterized by X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM). Further plans are to investigate thermostability of prepared samples, also leakage of Hg, and conduct more characterization methods (Raman and X-ray photoelectron spectroscopy).

SAXS characterization of morphology controlled nano ceria

Jelena Maletaškić[1], Yulia Gorshkova[2], Sergei Yurievich Kottsov[3], G.P. Kopitsa[4], Branko Matović[1]

[1]*Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

[2]*Joint Institute for Nuclear Research, Frank Laboratory of Neutron Physics, Dubna*

[3]*Kurnakov Institute of General and Inorganc Chemistry of the Russian Academy of Sciences, Moscow, Russian Federation*

[4]*Petersburg Nuclear Physics Institute NRC KI, Gatchina, Russsian Federation*

CeO_2 nanoparticles with isometric and rod-like morphologies have been successfully prepared through a simple hydrothermal method. The morphological evolution between isometric and nanorod can be achieved by adjusting the concentration of NaOH that affects the formation and morphological evolution of CeO_2 nanoparticles. The CeO_2 structure was studied using the SAXS method.The observed SAXS pattern for all synthesized powders CeO_2-xNaOH is typical for the systems with a disordered structure consisting of randomly oriented non-spherical (anisodiametric) objects, for example, for strongly elongated (fibrils) or oblate (lamellas) particles. In summary, we have demonstrated a facile controllable approach to the synthesis of CeO_2 nanoparticles with isometric and/or rod-like morphology using simple starting materials in a hydrothermal system. The results provide an economical route for synthesis of nanosized ceria and related materials. Moreover, the clarification of the morphology evolution mechanism will open new strategies for controlled synthesis of nanostructures.

AUTHOR INDEX

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