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Twentieth Annual Conference

YUCOMAT 2018

Herceg Novi, Montenegro, September 3–7, 2018

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YUCOMAT 2018

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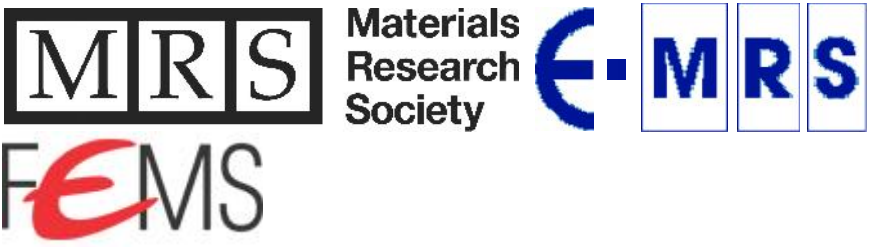

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O.S.I.2.

Synthesis and densification of monolithic nanocrystalline SiC ceramics

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

O.S.I.3.

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

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