Sep 27, 2018

Deformation Mechanisms in Ultrahard Ceramics: A Comprehensive Experimental,DFT and MD Investigation

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ABSTRACT:

The hardest know materials for engineering applications include diamond (HV>100 GPa), cubic-boron nitride (HV=60-75 GPa), boron carbide (HV=30=35 GPa), and boron suboxide (HV>40 GPa). While the former two materials have diamond structure with a density of around 3.5 g/cm3, the latter two have icosahedral structure with a density of around 2.5 g/cm3. These icosahedral solids also exhibit high compressive strength (in excess of 5 GPa) and better thermal and chemical stability than diamond-like structures. These properties favors them in applications including protective armor, abrasives and wear resistant materials, machine tool bits, etc. However, these boron-rich solids undergo a deleterious deformation mechanism referred to as 'amorphization' when subjected to high pressure loads such as those encountered in ballistic impact. This mechanism has been attributed to reduced hardness and nonrealization of the intrinsic hardness of the crystalline phase. The present study is a coordinated experimental and computational effort on the mechanical behavior of boron-rich icosahedral ceramics with the goal of optimizing their crystal structure for enhanced performance. The pressure dependent response of the amorphized zone and its evolution beneath an indentation in boron carbide (B4C) and boron suboxide (B6O) were investigated using TEM and Raman spectroscopy. The consequences of amorphization are addressed with regard to volumetric change in the amorphized material and the stress state in surrounding regions. To determine the origin of the amorphization process, density functional theory (DFT) density functional perturbation theory (DFPT) and molecular dynamics (MD) simulations were performed. The simulated Raman spectra were compared with experiments to offer insight into the kinetics of amorphization under hydrostatic compression (up to 100 GPa) and homogeneous shear. This analysis has provided new insight into their bonding behavior, Raman spectral characteristics, Hugoniot response and thermodynamics of amorphization process. Finally, new avenues are proposed to improve the stability, amorphization resistance, and mechanical performance of boron carbide. Overall, these results provide new insight into the links between polymorph crystal structure, deformation response, and Raman spectra while simultaneously laying the foundation for polymorph-level design of boron carbide. In case of B6O, novel strengthening mechanisms such as nanotwinning (twin spacing of nm size) were attributed to reduced amorphization and increased hardness. We will rationalize these observations and provide mechanistic arguments towards development of structural ceramics with hardness in excess of the current thresholds.

BIOGRAPHY:

Professor Subhash obtained his MS and PhD degrees from University of California San Diego and conducted post-doctoral research at California Institute of Technology, Pasadena, CA. He joined the faculty of Michigan Technological University (MTU) in 1993 and then moved to University of Florida (UF) in 2007. He has received numerous honors and awards for excellence in teaching, research and professional service, including the '2018 Frocht Award', Society for Experimental Mechanics (SEM), 'Best Paper'-Journal of Engineering Materials and Technology (Nov 2016), 'Significant Contribution Award' American Nuclear Society- Materials Science and Technology Division (2014), Fellow of ASME, 'Fellow of SEM', 'Technology Innovator Award' -University of Florida (2014 and 2016), ASME Student Section Advisor Award', 'SAE Ralph R. Teetor Educational Award', 'ASEE Outstanding New Mechanics Educator'. He has served as the National Academies Panel Member on Ballistic Science and Engineering at the Army Research Laboratory (2015-2018) and as an Associate Editor for five international journals including Mechanics of Materials, Journal of the American Ceramic Society, Experimental Mechanics, ASME Journal of Engineering Materials and Technology and Journal of Dynamic Behavior of Materials.