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Bonding structure and deformation mechanisms in ultra-hard ceramics

Ultrahard ceramics mainly stem from two structural forms: diamond-like and icosahedral. While diamond-like structures (e.g., naturally occurring diamond and c-BN) hold the microhardness record at over 100 GPa, icosahedral boron-rich solids have attracted considerable attention in recent years due to their strong thermal/chemical stability and an excellent combination of high hardness (~40 GPA) and low mass density (~2.5 g/cm^3). Boron carbide (B_4C) and boron suboxide (B_6O) are two popular ceramics in this class of materials and are preferred candidates for impact and wear resistance applications. While their structure mainly consists of a 12-atom icosahedron and few atoms that bond to the icosahedron, the arrangement of these atoms and their chemical nature controls their deformation mechanisms. For e.g., B_4C has a 3-atom chain attached to the equatorial atoms of the icosahedron, B_6O does not have a chain but one oxygen atom bonded on each side of the icosahedron. Due to the closeness in atomic radii of boron and carbon, B_4C exhibits polymorphisms where a carbon can substitute for boron and potentially yield more than 200 polymorphs. On the other hand, B_6O has no polymorphs. Thus B_6O is structurally more homogeneous than B_4C. These structural differences influence their properties and deformation mechanisms. Both materials have high hardness (>30 GPa), low density (2.52 g/cm^3 for B_4C and 2.6 g/cm^3 for B_6O), high compressive strength (up to 5 GPa), moderate fracture toughness (3.4 MPa·m$^{1/2}$ for B_4C and 4.2 MPa·m$^{1/2}$ for B_6O) and exhibit amorphization (localized crystal structure collapse) under high pressure loads. But, amorphization in B_4C can be detected in Raman spectroscopy (through appearance peaks beyond 1200 cm^{-1}), B_6O does not show any new peaks due to amorphization. While the 3-atom chain bending has been proposed as the main mechanism for amorphization in B_4C, the lack of chain structure in B_6O raises new questions as the root-cause of amorphization in this material. Similarly, B_4C has been found to occasionally undergo deformation twinning but B_6O has been shown to undergo 'nanotwinning' (twin spacing of nm scale) even in virgin state and has been theorized to provide extremely high hardness if the entire specimen undergoes nanotwinning at critical twin spacing of two atomic planes. In this research, a coordinated experimental, spectroscopic, microscopic, and quantum mechanical investigations are performed to provide fundamental insight into the above issues. Finally, implications of these structural, behavioral and bonding differences during high pressure dynamic deformation will be discussed. The long-term goal of this research is to identify novel avenues for designing of ultrahard materials with tailored properties.

Biography

Ghatu Subhash conducts multidisciplinary research at the intersection of solid mechanics, materials science, and biomechanics.Subhash's research has resulted in invention disclosures and provisional patents for a novel method for rapid testing of flexible package sealing, impact absorbing cushions for preventing head injury, rapid processing of UO_2 fuels, and development of ultra-hard boron carbide which has numerous applications as armor, hard abrasive, and thermoelectric.

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