Anomalous Brittle Failure of Superhard Boron Carbide

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Superhard boron carbide (B_4C) has important engineering applications in body armor, high temperature semiconductors, and more. However, their extensive engineering applications are seriously hindered by the intrinsic brittleness originating from the strong chemical bonding. The complex structures and chemical bonding pose great challenges to developing accurate inter-atomic potential for B4C and related icosahedral materials. In this talk, we illustrate the abnormal brittle failure of B_4C and its shock response from a quantum mechanics (QM) based framework integrating density functional theory (DFT) and machine learning force field (ML-FF). Firstly, we applied the DFT and ML-FF simulations on single crystal B_4C and show that its intrinsic brittle failure arises from the formation of higher density amorphous bands due to fracture of the icosahedra, a unique feature of B_4C. Then we investigate the shock response of nanocrystalline boron carbide (n-B_4C) using large-scale molecular dynamics simulations with the ML-FF. We identify three deformation mechanisms in shocked n-B4C: grain boundary (GB) sliding, intergranular amorphization, and intragranular amorphization, indicating the importance of GB in the deformation process. The mechanism of stress-induced amorphization suggests that it can be mitigated via atomic doping (e.g. P and Al). Particularly, the deformation mechanism transforms from amorphization to dislocation nucleation and motion by microalloying Al into B_4C. Al doping weakens the bonding characteristics of C-B-C chains in B_4C, and the chain bonds are easily broken, which serves as the main source of dislocation nucleation and drives dislocations to glide.

References:

1) Q. An, W.A. Goddard III, T. Cheng, Atomistic explanation of shear-induced amorphous band formation in boron carbide. Physical Review Letters 113 (9), 09501 (2014). https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.113.095501
2) Q. An, Mitigating amorphization in superhard boron carbide by microalloying-induced stacking fault formation. Physical Review Materials 5 (10), 103602 (2021) https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.5.103602
3) Q. Yang, C.J. Marvel, Y. Shen, et al., Activating dislocation mediated plasticity in boron carbide through Al-doping. Acta Materialia, 118412 (2022). https://www.sciencedirect.com/science/article/abs/pii/S1359645422007893
4) J. Li, Q. An, Quasiplastic deformation in shocked nanocrystalline boron carbide: Grain boundary sliding and local amorphization. Journal of the European Ceramic Society, 43, 208-216 (2023). https://www.sciencedirect.com/science/article/abs/pii/S0955221922007816