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Developing New Interatomic Potentials for Advanced Ceramics Using Machine Learning and Molecular Dynamics

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Abstract

Advanced ceramics such as Boron Carbide (B4C) and Titanium Diboride (TiB2) offer great potential for applications in extreme conditions, such as cutting tools, wear resistant coatings, and body armor due to their high strength, low density, chemical and thermal stability, wear and abrasion resistance, and high melting temperature. Despite their great potential, many questions remain about how the microstructures of advanced ceramics produce these desirable properties. A major hurdle preventing the clear determination of microstructure-property relationships is the relative inaccuracy of interatomic potentials used in molecular dynamics (MD) simulations compared to density functional theory. Additionally, the complex lattice unit cell of B4C, which is composed of a 12 atom icosahedral cage surrounding a 3 atom linear chain linking the icosahedra along the (111) rhombohedral axis, is difficult to simulate. This research program employs machine learning-based (ML) methods to develop more accurate interatomic potentials for advanced ceramics that can capture complex microstructural dynamics relevant to material failure. ML potentials can provide more accurate results when compared to the traditional interatomic potentials since they benefit from high-dimensional representation of underlying potential energy surfaces. Moreover, incorporating physical constraints into the ML regression (physics-informed ML) has been shown to lead to higher precision and better extrapolation from the training data. When completed, the results of MD simulation with the new potential can be used in multi-scale modelling of the dynamic failure of ceramics. This talk will discuss ongoing MD simulation of the B4C supercell regarding equilibrating the structure, obtaining the equilibrating parameters, and understanding the deficiencies of the current ReaxFF potential. In addition to MD simulation, the process of generating a ML potential for ceramics will be discussed.