Multiscale modeling of ultra high temperature ceramics (UHTC) ZrB2 and HfB2: application to lattice thermal conductivity

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We are developing a multiscale framework in computational modeling for the ultra high temperature ceramics (UHTC) ZrB2 and HfB2. These materials are characterized by high melting point, good strength, and reasonable oxidation resistance. They are candidate materials for a number of applications in extreme environments including sharp leading edges of hypersonic aircraft. In particular, we used a combination of ab initio methods, atomistic simulations and continuum computations to obtain insights into fundamental properties of these materials. Ab initio methods were used to compute basic structural, mechanical and thermal properties. From these results, a database was constructed to fit a Tersoff style interatomic potential suitable for atomistic simulations. These potentials were used to evaluate the lattice thermal conductivity of single crystals and the thermal resistance of simple grain boundaries. Finite element method (FEM) computations using atomistic results as inputs were performed with meshes constructed on SEM images thereby modeling the realistic microstructure. These continuum computations showed the reduction in thermal conductivity due to the grain boundary network.