

Abstract Submitted
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Thermal conductivity of ultra high temperature ceramics (UHTC) ZrB_2 and HfB_2 from atomistic simulations JOHN LAWSON, NASA Ames Research Center, MURRAY DAW, Clemson University, CHARLES BAUSCHLICHER, NASA Ames Research Center — Ultra high temperature ceramics (UHTC) including ZrB_2 and HfB_2 are characterized by high melting point, good strength, and reasonable oxidation resistance. These materials are of interest for use as sharp leading edges for hypersonic vehicles among other applications. Progress in computational modeling of UHTCs has been limited in part due to the absence of suitable interatomic potentials. Recently, we developed Tersoff style parametrizations of such potentials for both ZrB_2 and HfB_2 appropriate for atomistic simulations. As an application, Green-Kubo molecular dynamics simulations were performed to evaluate the lattice thermal conductivity for single crystals of ZrB_2 and HfB_2 . The atomic mass difference in these binary compounds leads to oscillations in the time correlation function of the heat current, in contrast to the more typical monotonic decay seen in monoatomic materials. Results at room temperature and at elevated temperatures will be reported.

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