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Interatomic Potentials for Ultra High Temperature Ceramics (UHTC): ZrB₂ and HfB₂ JOHN LAWSON, NASA Ames Research Center, MURRAY DAW, Clemson University, CHARLES BAUSCHLICHER, NASA Ames Research Center — Ultra high temperature ceramics including ZrB₂ and HfB₂ 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. We present a Tersoff style parametrization of such potentials for ZrB₂ and HfB₂ appropriate for atomistic simulations. Parameters are fit to data generated from DFT based ab initio calculations. The accuracy of the potentials is assessed against further ab initio data.

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