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Molecular dynamics simulation of dynamic response of beryllium[1]

AIDAN THOMPSON, Sandia National Laboratories, MATTHEW LANE, MICHAEL DESJARLAIS, MICHAEL BASKES — The response of beryllium to dynamic loading has been extensively studied, both experimentally and theoretically, due to its importance in several technological areas. Compared to other metals, it is quite challenging to accurately represent the various anomalous behaviors of beryllium using classical interatomic potentials. A new parameterization of the MEAM interatomic potential has been obtained, which reproduces ambient elastic and lattice constants, the melting temperature, and the static compression curve up to 200 GPa, and is free of obvious pathologies. Hugoniostat and direct molecular dynamics simulations using this parameterization, as well as one due to Dremov et al. have been used to predict the dynamic response of HCP beryllium up to and including melting.

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Aidan Thompson
Sandia National Laboratories

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