Abstract Submitted
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Calculated temperature dependence of elastic constants and phonon dispersion of hcp and bcc beryllium[1] STEVEN HAHN, Ames Laboratory and Iowa State University, SERGIU ARAPAN, Uppsala University, BRUCE HARMON, Ames Laboratory and Iowa State University, OLLE ERIKSSON, Uppsala University — Conventional first principle methods for calculating lattice dynamics are unable to calculate high temperature thermophysical properties of materials containing modes that are entropically stabilized. In this presentation we use a relatively new approach called self-consistent *ab initio* lattice dynamics (SCAILD) to study the hcp to bcc transition (1530 K) in beryllium. The SCAILD method goes beyond the harmonic approximation to include phonon-phonon interactions and produces a temperature-dependent phonon dispersion. In the high temperature bcc structure, phonon-phonon interactions dynamically stabilize the N-point phonon. Fits to the calculated phonon dispersion were used to determine the temperature dependence of the elastic constants in the hcp and bcc phases.

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