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Mechanism of body-centered cubic phase stabilization in Fe and He at high pressure and temperature ANATOLY BELONOSHKO, KTH Royal Institute of Technology, Stockholm, Sweden, SERGIU ARAPAN, Uppsala University, Uppsala, Sweden, LOVE KOCI, AWA Patent AB, Stockholm, Sweden, ANDERS ROSENGREN, KTH Royal Institute of Technology, Stockholm, Sweden —
We have investigated the stabilization of the body-centered cubic phase in Fe and He at high P and T by means of ab initio and classical molecular dynamics. These phases are dynamically unstable at high P and low T, however, they become dynamically stable at high T. We calculated the phonon density of states for Fe and He phases and observed that the bcc PDOS contains long-wavelength phonon states (absent in the close packed phases) that contribute to the free energy. This observation is consistent with the mechanism of stabilization proposed earlier (P. Loubeyre, J.-P. Hansen, PRB 31, 634 (1985); B. L. Holian et al., JCP 59, 5444 (1973)). Direct ab initio simulations of Fe crystallization and classical co-existence simulations for He indicate that the bcc phase is a submelting phase at high P. Previous calculations of the free energy in the bcc phase have been performed on small samples and could not adequately take the long-wavelength correlated motion into account.

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