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The Role of Anharmonicity in the Beryllium Equation of State
LORIN X. BENEDICT, ANDREA TRAVE, CHRISTINE WU, TADASHI OGITSU, PHIL STERNE, ERIC SCHWEGLER, Lawrence Livermore National Lab, H-DIV COLLABORATION — We discuss the construction of a multiphase equation of state for Be from first principles, aimed at understanding the material's properties at extreme conditions. In addition to the usual computation of cold, quasiharmonic ion-thermal, and (negligible here) electron-thermal contributions, we consider the effects of strong anharmonicity in the bcc phase, and argue that the inclusion of such effects may greatly perturb the picture (in particular, the phase diagram) derived from assuming quasi-harmonic lattice dynamics. Our analysis involves studying the mean displacement from equilibrium of Be atoms in the lattice by DFT-molecular dynamics methods and comparing the results to those of the quasiharmonic theory.

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