Equation of state of beryllium from first-principles calculations
ANDREA TRAVE, LORIN BENEDICT, TADASHI OGITSU, CHRISTINE J. WU, PHILIP A. STERNE, ERIC SCHWEGLER, Lawrence Livermore National Lab — The design of experiments of materials at extreme conditions of pressure and temperature is often based on hydrodynamic simulations, which make use of equation of state (EOS) models for the description of the systems under study. The validity of these models is extremely critical, and first-principles calculations can provide consistent and accurate parameters for the determination of the EOS in a wide range of thermodynamic conditions. Extensive density functional theory calculations at zero temperature have been performed for beryllium in various solid structures, in order to obtain accurate predictions for their compression curves, and phonon and electronic densities of states. Finite-temperature simulations have been used to further improve the models to include anharmonic effects. The melting line of beryllium has been obtained with first-principles two-phase simulations, which enables the construction of a multi-phase EOS for both liquid and solid beryllium. The results of these simulations provide useful indications on the relative stability of the various solid and liquid phases of beryllium in a region of the phase diagram lacking any experimental study so far. Prepared by LLNL in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

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Date submitted: 27 Nov 2007   Electronic form version 1.4