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First Principles-Based Equations of State for Functionally Graded Materials

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Thermodynamically complete equations of state (EOS), which characterize the material thermo-mechanical behavior under hydrostatic pressure and are expressed as the dependence of pressure on the specific volume and temperature, are predicted by using quantum mechanical methods. EOS for mixtures is needed in the shock-induced impact analysis of kinetic energy projectiles with functionally graded mixture of materials. Traditionally, EOS has to be obtained by experimental measurement. The complete EOS requires a large amount of measurements at different state points. However, the extreme difficulty of the temperature measurement in shocked systems unavoidably leads to an incomplete EOS. The most important contribution from, the use of abinitio technique, is that it can provide the thermodynamically complete EOS. There exist some literature on the use of the first principles to calculate EOS of solids including semiconductor material silicon and some metals but not for mixtures. For the mixture of materials, first, the EOS is obtained for each individual component from first-principle calculations. Abinitio methods are based on the psuedopotential plane-wave methods. The generalized gradient approximations and the ultrasoft psuedopotential are utilized. The prediction of the EOS consists of two parts: the static-lattice EOS and thermal effects. The range of the pressure and the temperature varied for the specific mixture that is considered. In this work, the possible polymorphic phase transitions are not considered. The single-phase EOS agrees well with the experimental data. The EOS for the mixture is then obtained from the homobaric mixture theory.

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