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Equations of State of Dual Functional Mixtures Of Structural Energetic Materials SATHYA HANAGUD, RUSISLAVA ZAHARIEVA, Georgia Tech, XIA LU, University of Florida — Currently, the electronic structure and the equation of state of metals can be determined by the use of the density functional theory. However, the subject is still an active research field for disordered materials like alloys. This paper, however, is concerned with mixtures like aluminum, nickel and nickel oxide and not alloys. In general the mixture can be disordered and the ratio of the constituents can vary to accommodate the needed application and the associated structural design. In this paper, thermodynamically complete equations of state of mixtures are obtained from first principles calculations. Specifically mixtures of aluminum and nickel or nickel oxide, titanium and silicon, with binders and porosity, are considered. First, EOS of individual components is determined. Then, a super cell is constructed by the use of other disordered theories but noting the fact that we are considering mixtures and not alloys. Methods similar to the direct sampling method, quasi-random structures method and virtual crystal approximation are used to represent proper mixture architecture, with porosity. The results are then bridged to continuum though statistical mechanics techniques and compared with the results obtained from continuum mixture theories. To determine thermal effects, lattice thermal contributions and electron thermal contributions are included. The transition states are also discussed.

Sathya Hanagud
Georgia Tech

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