FIRST PRINCIPLES-BASED EQUATIONS OF STATE FOR FUNCTIONALLY GRADED MATERIALS

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SUMMARY: Equations of state for mixture of solids are obtained from abinitio techniques or quantum mechanical method and compared with the available experimental data.

INTRODUCTION

Many kinetic energy projectiles are designed to penetrate through granular materials like concrete targets before the initiation of the reaction of energetic materials housed in the projectile. Critical loading conditions for the design of such projectiles are not the aerodynamic forces but the loading environment during penetration through granular materials. At high striking velocities, in the range of 1200 – 1500 m/sec, sharp noses of steel projectiles are subjected to a severe shock environment and nose tips are blunted while the pay load in the shank of the projectile are subjected to shock loads. The material is eroded from the nose of the projectile. In the case of the steel projectiles, melted and refrozen steel are observed on the shank of the projectile. Sections of the steel projectiles, recovered following penetration tests through concrete have displayed heat-affected zones, evidence of phase transformation including melting. Undesirable effects of the nose erosion are the deviation of the trajectory through the concrete from the intended trajectory and performance of the projectile including the penetration depth. The trajectory deviations are attributed to nose shape changes, compressive loads on the projectile and the asymmetric formation of micro cracks in the targets. The effective compressive loads and micro crack formation are also functions of the change of nose shape.

To minimize the nose erosion while the payloads, housed in the projectile, are protected from shock loads resulting from impact at high striking velocities, one choice is to design the projectiles by the use of functionally graded materials. The functionally graded materials can consist of mixtures that are excellent heat resistant materials at the nose tip to shock resistant energetic materials like the mixture of inter-metallic materials in the shank of the projectile. From the point of view of mechanics, the challenge is to formulate constitutive equations for the mixture of materials to evaluate their performance during impact. The constitutive equations are assumed to be represented by a combination of equations of state and the behavior of the contribution of the stress deviators. The mixture can contain varying ratios of different materials and thus it is very expensive to conduct a series of gas or powder gun tests for each representative mixture.

ABINITIO TECHNIQUES FOR EQOATION OF STATE FOR MIXTURES

Thus, in this paper, thermodynamically complete equations of state (EOS), which characterizes the material thermo-mechanical behavior under hydrostatic pressure and is expressed as the dependence of pressure on the specific volume and temperature, are predicted by using quantum mechanical methods. EOS is a part of the constitutive relations used in shock analysis. 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. Especially at the design stage of new materials, the measuring of EOS involves a tremendous effort at high cost. Therefore, using first principles calculations to obtain EOS of new materials seems very appealing. It saves not only the time of synthesizing materials but also the high cost for measurement. The most important 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. For the energetic intermetallic mixture like the Al-Ni mixture (payload) and refractory mixture at the nose tip, we use the following procedure to obtain the EOS of the mixture by ab initio quantum mechanical calculations. First, the EOS is obtained for each individual component from first-principle calculations. Ab initio 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 of consideration is up to 300 GPa and 1000K. As known, the melting temperatures of aluminum and nickel at the ambient pressures are about 933 K and 1728 K, respectively. Also aluminum was theoretically predicted to undergo the pressure-induced crystallographic phase sequence from fcc→hcp→bcc, at predicted phase transition pressures; 205±20GPa and 565±60 GPa. In this work, the possible polymorphic phase transitions are not considered. The single-phase EOS agrees well with the experimental shock Hugoniot. The EOS of the mixture is approximated using appropriate mixture theories, namely homobaric mixture theory and uniformly blended mixture theory.

RESULTS

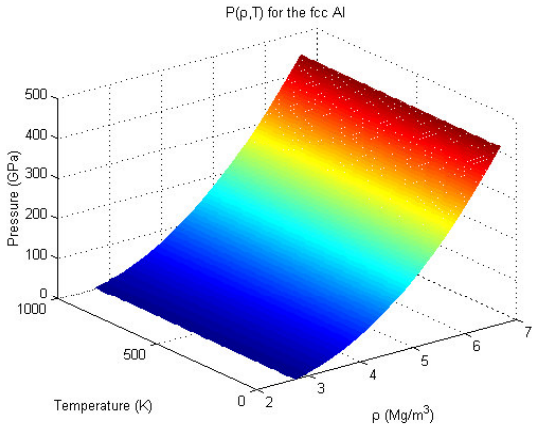
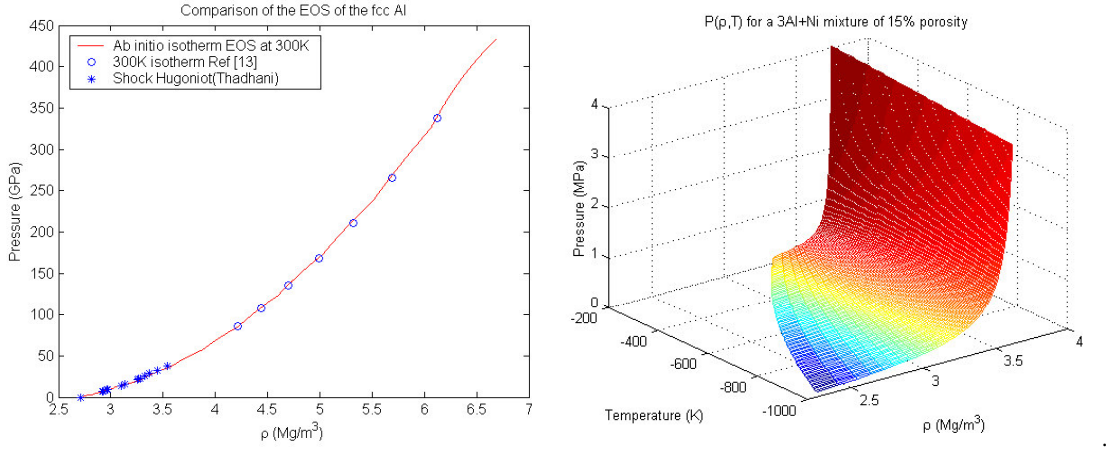


Figure 1 The thermodynamically complete equation of state of Al.



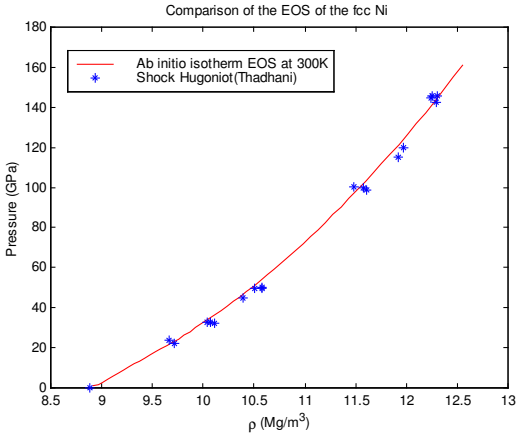


Fig.2-4: Comparison of EOS for Al & Ni with available Exptl. Data; EOS for the Mixture