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Ab Initio Studies of Shock-Induced Chemical Reactions of Inter-Metallics ROUSSISLAVA ZAHARIEVA, Georgia Institute of Technology, SATHYA HANAGUD, Georgia Institute of Technology — Shock-induced and shock assisted chemical reactions of intermetallic mixtures are studied by many researchers, using both experimental and theoretical techniques. The theoretical studies are primarily at continuum scales. The model frameworks include mixture theories and meso-scale models of grains of porous mixtures. The reaction models vary from equilibrium thermodynamic model to several non-equilibrium thermodynamic models. The shock-effects are primarily studied using appropriate conservation equations and numerical techniques to integrate the equations. All these models require material constants from experiments and estimates of transition states. Thus, the objective of this paper is to present studies based on ab initio techniques. The ab initio studies, to date, use ab initio molecular dynamics. This paper presents a study that uses shock pressures, and associated temperatures as starting variables. Then intermetallic mixtures are modeled as slabs. The required shock stresses are created by straining the lattice. Then, ab initio binding energy calculations are used to examine the stability of the reactions. Binding energies are obtained for different strain components super imposed on uniform compression and finite temperatures. Then, vibrational frequencies and nudged elastic band techniques are used to study reactivity and transition states. Examples include Ni and Al.

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