Abstract Submitted
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Non-equilibrium Molecular Dynamics Studies of Interfacial Chemistry in Shocked Ni/Al Nanolaminates[1] JASON QUENNEVILLE, Spectral Sciences, Inc., NARESH N. THADHANI, Georgia Institute of Technology, TIMOTHY C. GERMANN, Los Alamos National Laboratory — The response of Ni/Al composite materials to shock loading has been studied using non-equilibrium molecular dynamics and an EAM force field. The simulation cells consist of layered Ni and Al laminates with at least 3 million particles in a 1:1 mole ratio. The main thrust of our research is to gain a better understanding of the chemistry that occurs at the Ni/Al interface when the real material is shocked. Initial geometries were chosen so as to identify the factors important to reaction in the complex macro-scale material. Specifically, we vary the orientation of the interface with respect to the shock wave and the geometry of the interface (*i.e.*, deviation from planarity) to study how mixing and reactivity of Ni and Al are affected. Preliminary results show that peak pressure is greater when the shock direction is parallel to the Ni/Al interface plane, in agreement with results from continuum-scale simulations. Comparison of our computational results with experimental observations is an important part of this collaborative effort and is discussed in the paper.

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Jason Quenneville
Spectral Sciences, Inc.

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