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Non-equilibrium Molecular Dynamics Studies of Interfacial Chemistry in Shocked Ni/Al Nanolaminates[1] JASON QUENNEVILLE, Spectral Sciences, Inc., NARESH THADHANI, Georgia Institute of Technology — 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. Our results show a clear dependence of pressure and temperature on interface orientation, in agreement with continuum-scale simulations.

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