

Abstract Submitted
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A molecular dynamics study of the role of pressure on the response of reactive materials to thermal initiation N. SCOTT WEINGARTEN, WILLIAM D. MATTSON, BETSY M. RICE, U. S. Army Research Laboratory, ANTHONY D. YAU, High Performance Technologies, Inc., TIMOTHY P. WEIHS, Johns Hopkins University — Reactive materials have the potential for implementation into a wide variety of commercial and military applications. However, the fundamental physical and chemical processes that control the energy release are not well understood. To elucidate the mechanisms of energy release, we simulated the exothermic alloying reactions of a Ni/Al bilayer with initial temperatures of 1100 K and 1500 K using both microcanonical (NVE) and isoenthalpic (NPH) molecular dynamics simulations with an embedded atom method (EAM) potential. The mechanism of the mixing is the same for all simulations: as mixing and reaction occurs at the interface, the heat generated first melts the Al layer, and subsequent mixing leads to further heat generation after which the Ni layer melts, leading to additional mixing until the alloying reactions are completed. The results indicate that pressure has a significant influence on the rates of atomic mixing and alloying reactions. In addition, two-phase coexistence simulations were used to determine the melting temperatures of pure Al and pure Ni at various pressures using this potential, and these values are discussed within the context of the Ni/Al bilayer results.

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