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Molecular dynamics simulation of shock-induced melting and alloying[1] SHIJIN ZHAO, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, TIMOTHY C. GERMANN, Applied Physics Division, Los Alamos National Laboratory, Los Alamos, NM 87545, ALEJANDRO STRACHAN, School of Materials Engineering, Purdue University, West Lafayette, IN 47907, LOS ALAMOS NATIONAL LABORATORY TEAM, PURDUE UNIVERSITY COLLABORATION — We observe sequent shock-induced melting processes occurring in Ni/Al nanonaminates by means of molecular dynamics simulations. We find a nice collaboration between the melting and alloying: the heat released from the exothermic alloying reactions facilitates the local melting in the respective Ni/Al bilayer; the liquid films from the local melting accelerate the exothermic alloying reactions. On the other hand, we uncover a keen competition between the melting and alloying from the overall pressure variation: the structural expansion upon melting leads to an increase of the pressure while the alloying reactions tend to decrease the pressure.

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