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Molecular Dynamics Simulation of Dislocation Emission from Shocked Aluminum Grain Boundaries C. POZZI, Politecnico di Torino, R.G. HOAGLAND, T.C. GERMANN, Los Alamos National Laboratory — A molecular dynamics (MD) simulation was performed to examine the behavior under shock loading conditions of the $\Sigma 11$, $\langle 110 \rangle$ $\{252\}$ $\{414\}$ asymmetric grain-boundary (GB) in Aluminum, with particular regard to the possibility of deformation twinning. Under different shock velocities, and with different embedded atom method (EAM) potentials, we observe the emission of both perfect and partial dislocations from the GB and, in some cases, the formation of nanotwins. These features and their nucleation mechanisms, as related to the shock velocity, the GB energy, and the size of the model (i.e. shock loading timescale), are discussed on the basis of our MD simulation results.

Timothy C. Germann
Los Alamos National Laboratory

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