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Physics of Shock Compression and Release: NEMD Simulations of Tantalum and Silicon ERIC HAHN, MARC MEYERS, SHITENG ZHAO, Univ of California - San Diego, BRUCE REMINGTON, LLNL, EDUARDO BRINGA, UN Cuyo, Argentina, TIM GERMANN, RAMON RAVELO, JAMES HAMMERBERG, LANL — Shock compression and release allow us to evaluate physical deformation and damage mechanisms occurring in extreme environments. SPaSM and LAMMPS molecular dynamics codes were employed to simulate single and polycrystalline tantalum and silicon at strain rates above 10^8 s^{-1}. Visualization and analysis was accomplished using OVITO, Crystal Analysis Tool, and a redesigned orientation imaging function implemented into SPaSM. A comparison between interatomic potentials for both Si and Ta (as pertaining to shock conditions) is conducted and the influence on phase transformation and plastic relaxation is discussed. Partial dislocations, shear induced disordering, and metastable phase changes are observed in compressed silicon. For tantalum, the role of grain boundary and twin intersections are evaluated for their role in ductile spallation. Finally, the temperature dependent response of both Ta and Si is investigated.

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