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Shock compression and spallation of tantalum: Molecular dynamics simulations S.N. LUO, Los Alamos National Laboratory, Q. AN, California Institute of Technology, R. RAVELO, T.C. GERMANN, D.L. TONKS, Los Alamos National Laboratory, W.A. GODDARD III, California Institute of Technology — We perform large-scale molecular dynamics simulations of shock wave compression and spallation of Ta single crystals with different potentials including embedded-atom method (EAM), first-principles-based EAM (qEAM) and reactive forcefield (ReaxFF). Shock loading is applied along $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$. Hugoniot states are obtained from direct shock or Hugoniostat simulations. Anisotropic behaviors are observed in plasticity (including twinning) during compression/tension and in spallation. We present detailed analysis of dislocations, twins and void nucleation and growth, and their implications for the mechanisms of plasticity and spall damage in Ta.

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