Title: Shock compression and spallation of tantalum: Molecular dynamics simulations

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Shock compression and spallation of tantalum: Molecular dynamics simulations

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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 (100), (110) and (111). Hugoniot states are obtained from direct shock or Hugoniotstat 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.