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Strain-Rate Dependence of Deformation-Twinning in Tantalum[1]

JAYALATH ABEYWARDHANA, Computational Science University of Texas, El Paso TX, TIM GERMANN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, RAMON RAVELO, Physics Department, University of Texas, El Paso TX — Large-Scale molecular dynamics (MD) simulations are used to model quasi-isentropic compression and expansion (QIC) in tantalum crystals varying the rate of deformation between the range $10^8 - 10^{12} s^{-1}$ and compressive pressures up to 100 GPa. The atomic interactions were modeled employing an embedded-atom method (EAM) potential of Ta. Isentropic expansion was done employing samples initially compressed to pressures of 60 and 100 GPa followed by uniaxial and quasi-isentropically expansion to zero pressure. The effect of initial dislocation density on twinning was also examined by varying the initial defect density of the Ta samples ($10^{10} 10^{12} cm^{-2}$). At these high-strain rates, a threshold in strain-rate on deformation twining is observed. Under expansion or compression, deformation twinning increases with strain rate for strain-rates $> 10^9 s^{-1}$. Below this value, small fraction of twins nucleates but anneal out with time. Samples with lower fraction of twins equilibrate to defect states containing higher screw dislocation densities from those with initially higher twinning fractions.

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