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Orientation-dependent response for Tantalum single crystals with dislocation sources[1] EDUARDO BRINGA, DIEGO TRAMONTINA, Instituto de Ciencias Básicas, Universidad Nacional de Cuyo, Mendoza M5502JMA, Argentina — Defective Tantalum single crystals are expected to display a particularly rich behavior when subjected to shock waves. Using non-equilibrium molecular dynamics simulations, we model Ta single crystals containing pre existing defects, which acts as sources for heterogeneous nucleation of defects, including point defects, dislocations and twins. We use a recent embedded atom model interatomic potential specially suited for high pressure simulations [Ravelo et al., Phys. Rev B, (2013)]. Differences on the Hugoniot Elastic (HEL), dislocation densities and twin fractions for shocking along several crystalline directions have been found, resulting in a variety of microstructures [Tramontina et al., High Energy Density Physics, (2014)]. Increasing the rise time of the loading ramp typically decreases dislocation densities. Survival of defects after unloading and Taylor-wave loading lead to a significant decrease in the final dislocation densities and twin fractions, giving results comparable to recent recovery experiments.

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