Abstract Submitted
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Atomistic simulation of shocks in single crystal and polycrystalline Ta[1] E.M. BRINGA, CONICET & Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, Argentina, A. HIGGINBOTHAM, Department of Physics, Clarendon Laboratory, University of Oxford, N. PARK, A.W.E., Aldermaston, Reading, RG7 4PR, UK, Y. TANG, Department of Mechanical Engineering, University of California San Diego, M. SUGGIT, G. MOGNI, Department of Physics, Clarendon Laboratory, University of Oxford, C.J. RUESTES, Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, Argentina, J. HAWRELIAK, P. ERHART, Lawrence Livermore National Laboratory, M.A. MEYERS, Department of Mechanical Engineering, University of California San Diego, J.S. WARK, Department of Physics, Clarendon Laboratory, University of Oxford — Non-equilibrium molecular dynamics (MD) simulations of shocks in Ta single crystals and polycrystals were carried out using up to 360 million atoms. Several EAM and FS type potentials were tested up to 150 GPa, with varying success reproducing the Hugoniot and the behavior of elastic constants under pressure. Phonon modes were studied to exclude possible plasticity nucleation by soft-phonon modes, as observed in MD simulations of Cu crystals. The effect of loading rise time in the resulting microstructure was studied for ramps up to 0.2 ns long. Dislocation activity was not observed in single crystals, unless there were defects acting as dislocation sources above a certain pressure.

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