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Direct Numerical Simulation of shock propagation in polycrystalline tantalum

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In this presentation, I describe our efforts to model the propagation of intense shock waves in polycrystalline metals with particular focus on tantalum. The main objective is to simulate the shock-response of polycrystalline tantalum accounting for the influence of the anisotropy of elastic and plastic deformation at the grain level as well as at the level of grain interactions, which enables to ascertain the role of these grain interactions in the overall response. The necessary ingredients enabling this type of simulations are described in some detail, including: appropriate nonlinear elastic models of cubic anisotropic behavior under large deformations, the calibration of these models to elastic constants obtained by ab-initio quantum mechanics calculations, their integration with multiscale models of b.c.c. crystal plasticity, the numerical need for especialized shock-capturing methods and, finally, the need for a framework for conducting high-resolution, large-scale calculations of the resulting initial boundary value problem. I will present simulation results corresponding to intense planar shocks propagating in tantalum and comment on our efforts to validate these simulations against experimental data.