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Simulation of shock-recovered samples: dislocations, twins, porosity and phase transformations[1]

EDUARDO BRINGA, CONICET and FCEN-UNCuyo

Atomistic molecular dynamics (MD) simulations of shock compression of metals often display tremendous plastic activity in the material, including immense dislocation densities during loading, of the order of 1e16-1e17m^{-2}. These high densities are in stark contrast with dislocation densities in recovered samples, measured by electron microscopy to be the order of 1e13-1e14m^{-2}. This large disparity sometimes generated lack of confidence in simulation results as representative of experimental results, but the outlook has changed in the last few years thanks to novel experiments estimating dislocation densities during loading, and thanks to new simulations trying to mimic recovery of shocked samples. Experiments measuring instability growth, or using dynamic X-Ray Diffraction seem to agree with the immense dislocation densities predicted by MD. Simulated recovery has been shown to provide significant reduction of dislocation densities in fcc samples. Here it will be shown that this is also true in bcc Ta samples, where low dislocation mobility might have been expected to reduce dislocation disappearance. In addition to dislocations, recovered samples might display twins and porosity. Twinning has been observed in many loading simulations, but it might be reversed upon unloading. On the other hand, unloading itself might cause twinning, as it will be discussed for the case of polycrystalline Fe. Regarding porosity, it might appear due to different scenarios. For instance, dislocation recovery in fcc Au leads to vacancy clusters which would then decay into the stacking fault tetrahedra (SFTs) observed experimentally in recovered samples. Finally, phase transformations might occur during loading, including solid-solid transformations and melting. Recovery might revert those phase transformations, as it has been shown for Fe, or it might lead to further transformations and changes in the microstructure, as it will be shown for additional examples.

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