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**Atomistic simulations of high strain rate loading of nanocrystals**[1]

E.M. BRINGA, D. TRAMONTINA, C.J. RUESTES, Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Y. TANG, M.A. MEYERS, University of California, San Diego, N. GUNKELMANN, H.M. URBASSEK, Physics Department and Research Center OPTIMAS, University Kaiserslautern, Germany — Materials loaded at high strain rates can reach extreme temperature and pressure conditions. Most experiments on loading of simple materials use poly crystals, while most atomistic simulations of shock wave loading deal with single crystals, due to the higher computational cost of running polycrystal samples. Of course, atomistic simulations of polycrystals with micron-sized grains are beyond the capabilities of current supercomputers. On the other hand, nanocrystals (nc) with grain sizes below 50 nm can be obtained experimentally and modeled reasonably well at high strain rates, opening the possibility of nearly direct comparison between atomistic molecular dynamics (MD) simulations and experiments using high power lasers. We will discuss MD simulations and links to experiments for nc Cu and Ni, as model f.c.c. solids, and nc Ta and Fe, as model b.c.c. solids. In all cases, the microstructure resulting from loading depends strongly on grain size, strain rate and peak applied pressure. We will also discuss effects related to target porosity in nc's.

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