Direct Temperature Measurements in Solids via Inelastic X-Ray Scattering Under Shock and Ramp Compression

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Shock and quasi-isentropic compression of solid-state matter via laser-ablation affords the creation of high energy density states of matter, with pressures and temperatures of relevance to core conditions within planets in our own solar system and beyond. Crystallographic phase and density can be discerned via ultra-fast x-ray diffraction, whilst pressure is deduced from VISAR measurements. Temperature is more difficult to determine, but techniques based on inelastic scattering from phonons are being considered [1]. It is in this context that we present here multi-million atom molecular dynamics simulations of the phonons present in fcc crystals shocked beyond their elastic limit. Despite high dislocation densities behind the shock front, distinct phonon modes can still easily be discerned, though such defects do contribute to the quasi-elastic peak that will compete with any inelastic scattering signal in a real experiment. Changes in the dispersion curves due to compression and the high number of stacking faults can also be observed.

[1] E.E. McBride et al., Rev. Sci. Instrum. **89**, 10F104 (2018)

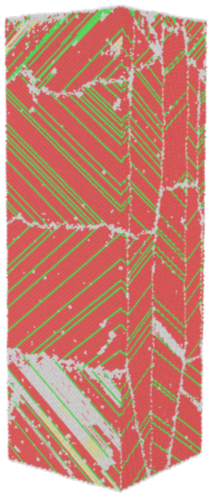

Figure: Atoms of molecular dynamics simulation of copper shocked to 70 GPa. Crystal phases highlighted my Ovito Dislocation Analysis (DXA) with FCC (green), HCP (red) and other (grey). Numerous stacking faults traverse the block of atoms.