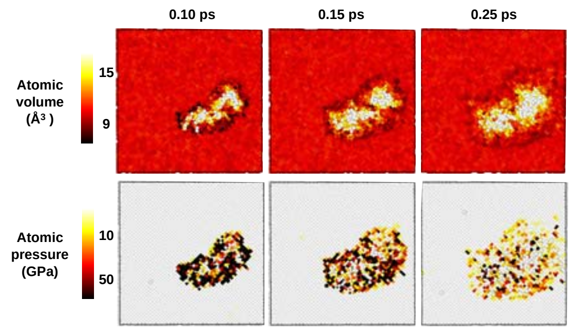
Extreme conditions revealed in radiation damage modeling

Extreme pressures and temperatures arising from high-energy recoils caused by neutron and ion irradiation are revealed by atomistic simulation. These recoils, with energies of tens of keV, generate a supersonic shockwave. The analysis shows that pressures of the order of 10-50 GPa and temperatures of several thousands of degrees Kelvin are present as the shockwave transitions to a sonic velocity. These are conditions similar to those observed in short-pulse laser ablation, high-velocity ballistic collisions and diamond anvil cells.



A typical 10 keV collision cascade in Ni creates a supersonic shockwave, involving pressures of 10-50 GPa.

Further analysis shows that the number of atomic displacements at the point in time of this supersonic-to-sonic transition is a good predictor of the number of stable defects that will be present once the shockwave is fully dissipated. The extreme pressures involved are associated with interatomic distances ranging between 0.14 and 0.2 nm, were most force fields commonly used for atomistic modeling are poorly parameterized. This result sheds doubt on the accuracy of many previous results reported in literature, and strongly motivates the development of force fields with high dependability at these short interatomic distances.

[1] Laurent K. Béland, Yuri N. Osetsky and Roger E. Stoller, "Atomistic material behavior at extreme pressures," *npj Computational Materials* **2**, 16007 (2016). doi:10.1038/npjcompumats.2016.7