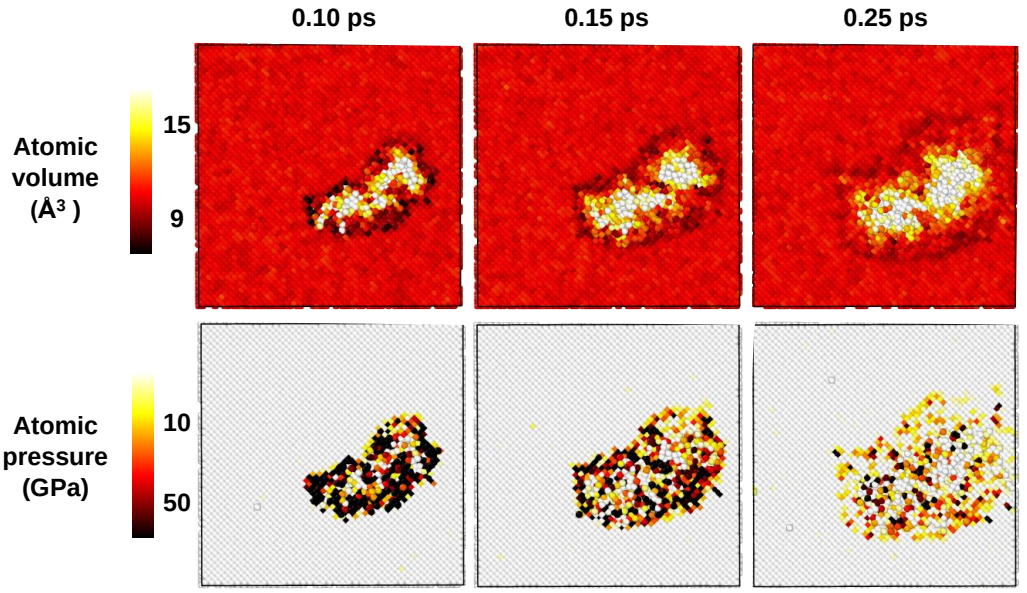
Extreme conditions revealed in radiation damage modeling

Scientific Achievement

Atomistic simulations reveal that high-energy recoils during neutron and ion irradiation produce 10-50 GPa pressure waves, the energetics of which largely determine defect generation.

Significance and Impact

Most interatomic potentials employed in radiation damage studies fail to properly describe these high pressure zones. Careful study reveals that this can lead to large inaccuracies.



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

Research Details

- The high pressures are observed when the shockwave transitions from a supersonic to sonic speed. One can predict the number of final stable defects remaining after dissipation of the shockwave by characterizing the displacements at this transition point.
- These pressures correspond to short interatomic distances where most interatomic force fields are poorly parameterized.

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.