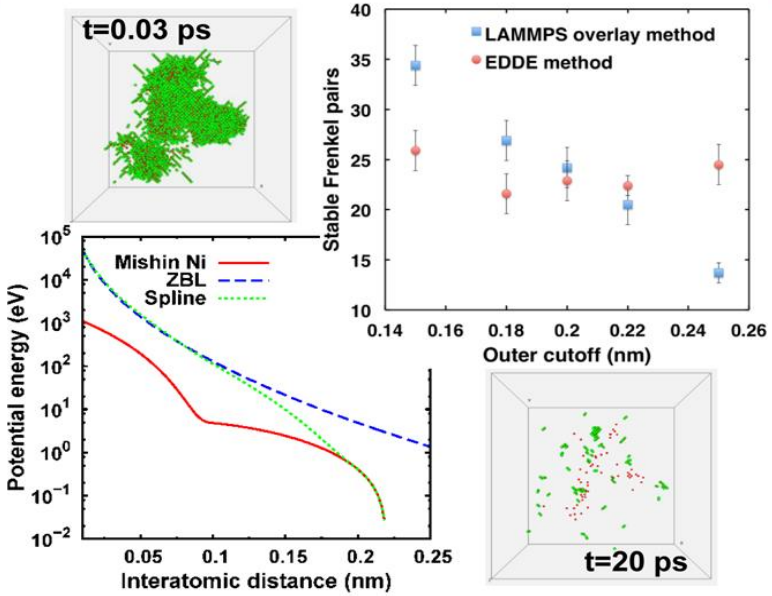
Solving the problem of short-range forces in radiation damage modeling

Scientific Achievement

A systematic fitting procedure was developed to accurately predict short-range forces using classical force fields.

Significance and Impact

The magnitude of short-range forces occurring during high-energy collision cascades is a key parameter that quantitatively controls primary damage production.



Accompanying two snapshots of the displacements caused by high-energy cascades, a representation of the force-field under consideration is plotted, as well as quantitative evidence that EDDE's refitting procedure leads to more robust outcomes than other currently used methods.

Research Details

- A number of *ab initio* approaches were tested and validated to calculate short-range interatomic forces, including those arising under extreme pressures.
- A refitting procedure for classical force-fields using this *ab initio* data was developed and shown to lead to more robust results than other currently used approaches to generate short-range forces.

R.E. Stoller, A. Tamm, L.K. Béland, G.D. Samolyuk, G.M. Stocks, A. Caro, L.V. Slipchenko, Y.N. Osetsky, A. Aabloo, M. Klintenberg and Y. Wang, "Impact of Short-Range Forces on Defect Production from High-Energy Collisions", Journal of Chemical Theory and Computation (2016). doi:10.1021/acs.jctc.5b01194