

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

## Scientific Achievement

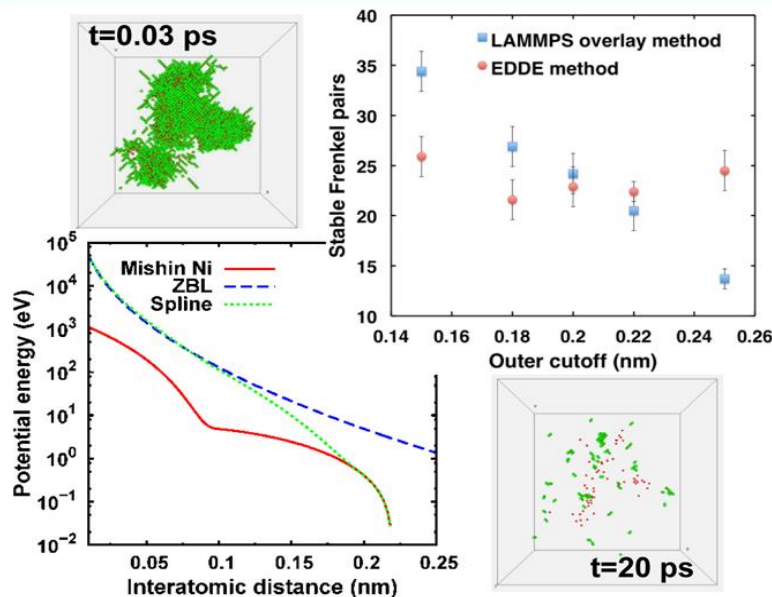
A systematic fitting procedure was developed to accurately predict short-range forces using classical force fields.

## 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.

## 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.



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.

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. Klintonberg 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



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