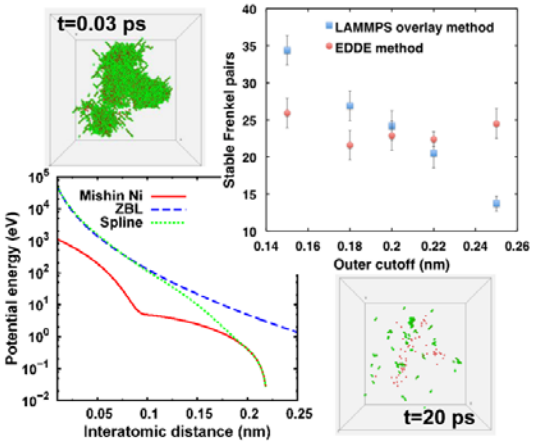
Solving the problem of short-range forces in radiation damage modeling

A recent analysis of high-energy displacement cascades revealed that neutron and ion-irradiated materials are subject to extreme pressures involving tens of GPa and short interatomic distances, which are typically inaccurately modeled.[1] This is a serious problem for quantitative comparison of primary defect production between alloys, especially if they have similar composition. Given the interest of EDDE into radiation effects in high-entropy alloys, this is a crucially important issue.



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.

The EDDE team and its collaborators have thoroughly investigated this problem in pure Ni [2]. They have tested and benchmarked several *ab initio* based methods to calculate short-range interactions of atoms, including those in high-pressure states. Using this information, they have introduced a novel framework to refit classical interatomic force-fields and shown the robustness of this new method, relative to the *ad hoc* procedure typically used by the community.

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

[2] 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 12 (2016) 2871-2879. doi:10.1021/acs.jctc.5b01194