Accelerated atomistic simulation of radiation events in metal

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Atomistic modeling of irradiation damages through displacement cascades is deceptively nontrivial. Due to the high energy, high velocity nature of the atom collisions, individual cascade simulations can become very computational expensive and ill-suited for size and dose upscaling. In order to examine microstructural evolutions, and mechanical property changes due to defect accumulation, accelerated methods of modeling irradiation defects needs to be adopted. Originally developed for application in ceramic materials, the Frenkel Pair Accumulation (FPA) method[1] generates point defect pairs by directly displacing atoms from its initial lattice site. The applicability of method is somewhat limited to metallic/dense materials, as it does not capture the important cascade process known as the thermal spike[2]. The presence of the thermal spikes has shown to be influence both point defect clustering[3] and sequential cascade overlaps[4]. Instead, using FPA as the basis and incorporating the additional thermal spikes, a new accelerated model of irradiation damage is developed. By adopting the athermal recovery corrected (arc) formalisms[2], the new arc-FPA method is able to predict and replicate irradiation events across a wide range of cascade energy. Using Cu and Nb as case studies, the method is verified against standard displacement cascades. Example applications for simulating dose accumulation are also provided for demonstration.

[1] Chartier, A., et al. "Early stages of irradiation induced dislocations in urania." *Applied Physics Letters* 109.18 (2016): 181902.
[2] Nordlund, Kai, et al. "Improving atomic displacement and replacement calculations with physically realistic damage models." *Nature communications* 9.1 (2018): 1084.
[3] Calder, A. F., et al. "On the origin of large interstitial clusters in displacement cascades." *Philosophical Magazine* 90.7-8 (2010): 863-884.
[4] Sand, A. E., et al. "Defect structures and statistics in overlapping cascade damage in fusion-relevant bcc metals." *Journal of Nuclear Materials* 511 (2018): 64-74.