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Title: First principles magnetic and electronic structure in large non-periodic dislocation models

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Classical Molecular Dynamic (MD) simulations characterizing dislocations and radiation damage typically treat 10^5-10^7 atoms. First principles calculations employed to understand these defect systems at an atomistic level cannot, and should not be dealt with such large numbers of atoms. We present an efficient coarse graining approach to calculate local electronic properties of large MD-generated structures from the first principles. Local atomic magnetic moments in crystalline Fe are perturbed by the presence of dislocations, and radiation generated vacancies and interstitials. The effects are most pronounced near the defect cores and decay slowly as the strain field of the defects decrease with distance. We used the Locally Self-consistent Multiple Scattering (LSMS) method for two types of iron defect structures 1) screw-dislocation dipoles and 2) radiation cascades. The atomic positions were determined by MD with an embedded atom force field. The local moments in the neighborhood of the defect cores are calculated with first-principles based on full local structure information, while atoms in the rest of the system are modeled by representative atoms with approximated properties. The calculations result in local moments near the defect centers with first-principles accuracy, while capturing coarse-grained details of local moments at greater length scales. This coarse graining approach reduces computational costs significantly. Acknowledgements: This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.