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Coarse graining approach to First principles modeling of radiation cascade in large Fe super-cells KHORGOLKHUU ODBADRAKH, DON NICHOLSON, AURELIAN RUSANU, Oak Ridge National Laboratory, YANG WANG, Pittsburg Supercomputing Center, ROGER STOLLER, XIAOGUANG ZHANG, GEORGE STOCKS, Oak Ridge National Laboratory — First principles techniques employed to understand systems at an atomistic level are not practical for large systems consisting of millions of atoms. We present an efficient coarse graining approach to bridge the first principles calculations of local electronic properties to classical Molecular Dynamics (MD) simulations of large structures. Local atomic magnetic moments in crystalline Fe are perturbed by radiation generated defects. The effects are most pronounced near the defect core and decay with distance. We develop a coarse grained technique based on the Locally Self-consistent Multiple Scattering (LSMS) method that exploits the near-sightedness of the electron Green function. 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. Atoms in the rest of the system are modeled by representative atoms with approximated properties. 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.

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