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**Coarse graining approach to First principles modeling of structural materials** KHORGOLKHUU ODBADRAKH, DON NICHOLSON, AURELIAN RUSANU, GERMAN SAMOLYUK, ORNL, YANG WANG, Pittsburgh Supercomputing Center, ROGER STOLLER, XIAOGUANG ZHANG, GEORGE STOCKS, ORNL — Classical Molecular Dynamic (MD) simulations characterizing extended defects typically require millions of atoms. First principles calculations employed to understand these defect systems at an electronic level cannot, and should not deal with such large numbers of atoms. We present an efficient coarse graining (CG) approach to calculate local electronic properties of large MD-generated structures from the first principles. 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 multiple scattering equations are solved at fewer sites using the CG. 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. This CG approach reduces computational costs significantly and makes large-scale structures amenable to first principles study. Work is sponsored by the USDoE, Office of Basic Energy Sciences, "Center for Defect Physics," an Energy Frontier Research Center. This research used resources of the Oak Ridge Leadership Computing Facility at the ORNL, which is supported by the Office of Science of the USDoE under Contract No. DE-AC05-00OR22725.

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