Abstract Submitted
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Million atom DFT calculations using coarse graining and petascale computing[1] DON NICHOLSON, KH. ODBADRAKH, G.D. SAMOLYUK, R.E. STOLLER, X.G. ZHANG, G.M. STOCKS, Oak Ridge National Laboratory — Researchers performing classical Molecular Dynamics (MD) on defect structures often find it necessary to use millions of atoms in their models. It would be useful to perform density functional calculations on these large configurations in order to observe electron-based properties such as local charge and spin and the Helmann-Feynman forces on the atoms. The great number of atoms usually requires that a subset be "carved" from the configuration and terminated in a less that satisfactory manner, e.g. free space or inappropriate periodic boundary conditions. Coarse graining based on the Locally Self-consistent Multiple Scattering method (LSMS) and petascale computing can circumvent this problem by treating the whole system but dividing the atoms into two groups. In Coarse Grained LSMS (CG-LSMS) one group of atoms has its charge and scattering determined prescriptively based on neighboring atoms while the remaining group of atoms have their charge and scattering determined according to DFT as implemented in the LSMS. The method will be demonstrated for a one-million-atom model of a displacement cascade in Fe for which 24,130 atoms are treated with full DFT and the remaining atoms are treated prescriptively.

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Don Nicholson
Oak Ridge National Laboratory

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