Defect Evolution and Interactions During Radiation Damage Cascades in Iron: Does Magnetism Matter?

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Current understanding of the evolution of the structure and defect generation in radiation damage cascades in structural materials – specifically Fe and Fe-based alloys – is largely based on molecular dynamics (MD) simulations using classical potentials. A major reason for this is that the systems sizes required (tens of thousands to millions and larger) for realistic simulations of radiation damage cascade evolution are beyond those accessible by standard *ab initio* electronic structure methods. In this presentation I shall discuss progress towards the development of *ab initio* methods that are capable of addressing system sizes used in classical MD. I will show results for Fe that address the importance of the disruption of the magnetic state of Fe during displacement cascades that are based on large scale (~10,000 atom) models and order-N electronic structure methods. I will also show how these approaches can be extended to even larger system sizes (>1,000,000-atoms) using a novel “representative-atom” coarse graining approach.

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