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Magnetic Evolution of the <100> Interstitial Loop Formation Process in bcc Iron[1] HAIXUAN XU, ROGER STOLLER, G. MALCOLM STOCKS, Oak Ridge National Lab — Interstitial loops are a signature of radiation damage in materials and are only observed in systems far from equilibrium state due to their high formation energies (approximately 4eV). Unlike other bcc metals, in which the interstitial loops are almost exclusively $\frac{1}{2}$ <111> type, two types of loops, <100>and $\frac{1}{2}$ <111> are identified in bcc iron. Although $\frac{1}{2}$ <111> loops can be formed directly by atomic displacment cascades, the mechanism of <100> loop formation had remained undetermined since they were observed fifty years ago. Recently, the formation mechanism has been discovered using self-evolving atomistic kinetic Monte Carlo (SEAKMC) simulations. Here we describe the influence of magnetism in the corresponding loop formation process using the *ab initio* locally self-consistent multiple-scattering (LSMS) method. Significant magnetic moment changes during the loop formation process are observed and their effect on the loop stability are evaluated. In addition, the effects of <100> loop formation on the microstructural evolution and material properties will be discussed.

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