Abstract Submitted
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Radiation Induced Defect Clusters in Fe and Fe-alloys Investigated by X-Ray Diffuse Scattering Measurements and Molecular Dynamics and Monte Carlo Simulations[1] BEN LARSON, Oak Ridge National Laboratory, JON TISCHLER, Argonne National Laboratory, HONGBIN BEI, ROGER STOLLER, HAIXUAN XU, Oak Ridge National Laboratory, YANWEN ZHANG, Oak Ridge National Laboratory/ Univ. TN-K — We have initiated fundamental investigations of 15 MeV Ni-ion induced defect clusters in single crystal Fe and Fe-Cr using diffuse scattering measurements near Bragg reflections combined with molecular dynamics (MD) and self-evolving atomistic kinetic Monte Carlo (SEAK-MC) simulations. Synchrotron x-ray diffuse scattering measurements performed near the (002) reflection of <001>oriented Fe and Fe(30%)Cr single crystals are analyzed within the so-called asymptotic regime using scattering cross-sections based on MD simulated local lattice distortions and SEAK-MC generated interstitial and vacancy cluster configurations. Measurements for Ni-ion irradiations of Fe and Fe-Ni with doses corresponding to 0.2 and 1 displacements per atom (DPA) at ambient temperature will be presented and discussed in connection with the local Bragg scattering interpretation of defect cluster diffuse scattering in ion-irradiated Cu. Methods for calculating diffuse scattering cross sections directly from MD simulations of atomic displacements around vacancy and interstitial loops within the single defect approximation will be considered and the importance of such approaches for complex defect clusters will be addressed.

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