

Abstract Submitted
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Ion-Irradiation Induced Vacancy and Interstitial Clusters in Fe Investigated by X-Ray Diffuse Scattering and Molecular Dynamics Simulations¹ BENNETT LARSON, Oak Ridge National Laboratory, JON TISCHLER, APS-ANL, YURY OSETSKIY, ROGER STOLLER, ORNL, YANFEI GAO, UT-Knoxville/ORNL, YANWEN ZHANG, ORNL — The size and nature of vacancy and interstitial clusters in 15 MeV Ni-ion irradiated Fe have been investigated using x-ray diffuse scattering combined with scattering cross-sections based on continuum elasticity and molecular dynamics (MD) simulations. X-ray diffuse scattering measurements performed at the Advanced Photon Source within the so-called asymptotic regime near the (002) reflection of <001>-oriented single crystal Fe have been analyzed using diffuse scattering cross-sections based on continuum elasticity and MD simulated lattice displacements around <111> and <100>-surface-normal interstitial and vacancy loops. To assess the sensitivity of diffuse scattering measurements to loose vacancy clusters or voids, molecular dynamics based cross-sections were calculated for 3D vacancy structures as well as for planar vacancy loops. The diffuse scattering measurements for ambient temperature Ni-ion irradiations of Fe corresponding to 1 displacement per atom (DPA) will be presented, and the results of the analysis of the diffuse scattering measurements in terms of vacancy and interstitial cluster type, surface-normal orientation, and size distributions will be discussed.

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