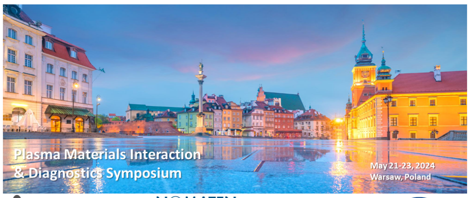

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Bridging the gap between atomistic defect evolution and continuum elasticity with an Object kinetic Monte Carlo approach

Since the degradation of macroscopic properties of irradiated materials occurs over relatively long irradiation times, the Object kinetic Monte Carlo method, which only follows the evolution of off-lattice defects, seems to be appropriate as it allows reaching physical times close to those achieved experimentally. In the absence of external forces and in an ideal perfect crystal lattice,
defects can be considered as independent random walkers. However, in any realistic material, the host lattice is often locally distorted by the presence of external loads, dislocation lines, grain boundaries, small precipitates or other defects. This elastic distortion might bias the direction of the jumps depending on the elastic interaction energy of the defect when moving in different directions.
Here, we propose a general novel computational method to include elastic interactions in OkMC simulations considering anisotropic elastic behavior and any defect distribution, curved dislocations and phases with different elastic properties. The approach does not rely on the dipolar approximation but instead is based in obtaining numerically the elastic fields of the defect map using a micromechanical FFT approach combined with defect eigenstrains or static
field dislocation mechanics. The method developed will be used to analyze the evolution of <111> prismatic dislocation loops in Fe in the presence of other defects and immobile dislocations. The dislocation loops appear as consequence of the irradiation of steels under harsh environments such as those found in fission or in future fusion reactors and are responsible of the change of mechanical properties of steels.

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