Bridging Experiment and Simulation: Multiscale Analysis of Nanoindentation in Pristine and Irradiated Iron

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We investigate the influence of self-irradiation on the nanomechanical response of high-purity iron. A combined approach utilizing nanoindentation experiments, large-scale molecular dynamics (MD) simulations, and crystal plasticity finite element method (CPFEM) analysis is employed. The MD simulations model overlapping collision cascades to achieve an irradiation dose and defect density comparable to the experiment. Subsequent simulations of the nanoindentation process on the irradiated material show qualitative agreement to transmission electron microscopy (TEM) analysis of irradiated regions at various depths below the nanoindentation imprint. A further analysis by CPFEM is carried out using MD simulations data, which provides a crucial link between the material's behavior under compressive tensile deformations. We find that irradiated samples require higher critical load for the transition from elastic to plastic deformation due to interaction of dislocation lines with the dislocation loops and point defects formed during the irradiation, leading to hardening. Moreover, traces of C in the pure Fe specimen, which may pin dislocations and unnaturally elevate H values.

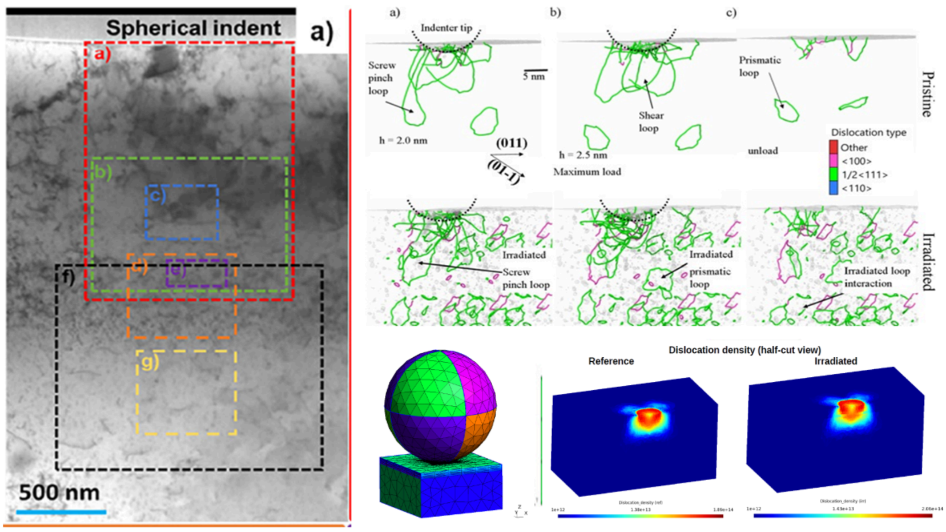

Figure 1: *Schematics of the experimentally guided multiscale modeling of nanoindentation of Fe samples.*

References

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