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Homogenized descriptions for the elastoplastic response of polycrystalline solids: mean-field approximations vs. full-field simulations for neutron-irradiated bainitic steels

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Nuclear reactor pressure vessels are mainly made of bainitic steels. These steels can undergo microstructural changes due to the neutron radiation that impact their elastoplastic response and concomitant fracture toughness. Crystal plasticity laws have been recently proposed that express microscopic plastic slip rates within crystals in terms of key microstructural features such as densities of forest dislocations, dislocations loops, and solute clusters. The laws encode information from lower length-scale simulations generated by molecular and dislocation dynamics. Macroscopic elastoplastic deformations are determined here by homogenizing such crystal plasticity laws via mean-field approximations and full-field simulations. The mean-field approximations are generated by homogenizing elastic and plastic deformations separately, assuming piecewise uniform dislocation densities, and employing various schemes of increasing complexity such as the elementary schemes of Taylor and Sachs or the more recent self-consistent schemes based on the concept of linear-comparison media. The full-field simulations, in turn, are generated with a Fast Fourier Transform algorithm implemented in the computer code CraFT. Several ways of accounting for local hardening in the mean-field approximations are presented and discussed. Sample results are provided for untextured samples subject to uniaxial tension. The elementary schemes of Taylor and Sachs predict quantitatively different responses, while the so-called Fully Optimized Second-Order (FOSO) scheme and the full-field simulations predict very similar responses for both non-irradiated and irradiated samples. Similar agreement is found between predictions for dislocation densities and their evolution with applied load. Overall, the FOSO scheme is found to provide the best compromise between precision and mathematical complexity to generate homogenized descriptions for the elastoplastic response of polycrystalline media governed by complex crystal plasticity laws.