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ATOMIC-SCALE DISLOCATION DYNAMICS IN THE ENVIRONMENT OF RADIATION-INDUCED DEFECTS

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Accumulation of radiation damage in structural materials leads to degradation of their mechanical properties which may also lead to their failure. A specific microstructure formed under irradiation includes clusters of vacancies and self-interstitial atoms (SIAs), secondary phase precipitates, etc. These defects, being obstacles for dislocation motion, cause strengthening, loss of plasticity, increase of ductile-to-brittle transition temperature and plastic instability. Modern predictive models are based on multiscale approach in modeling of materials behavior under irradiation conditions by decomposing the whole phenomenon into a set of simpler phenomena at particular scales each to be studied by the appropriate modeling or/and theoretical techniques. In this approach dislocation-obstacle interactions are in the basis of mechanical properties of materials. The present paper reports recent progress in atomic-scale dislocation dynamics achieved by exploring large-scale simulation of realistic dislocation and radiation-induced defects density. We have considered edge and screw dislocations the Burgers vectors _<111> in bcc (Fe) and _<110> in fcc (Cu) metals and a wide range of radiation-induced defects such as voids, SIA clusters and Cu-rich precipitates in Fe and voids, SIA clusters and stacking fault tetrahedra (SFTs) in Cu of up to 12nm in size in the temperature range from 0 to 600K. A variety of different reactions have been observed, such as dislocation climb, cross-slip and formation of superjogs at the dislocation line and ledges on the SFT and phase transformations in coherent Cu-precipitates. These cannot be rationalized without taking into account specific atomic-scale structure of dislocations and SFTs. The atomic-scale mechanisms observed are discussed and tentative interpretation of experimental results is given.

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