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Predicting Dislocation Climb and Creep from Explicit Atomistic Details MUKUL KABIR, TIMOTHY T. LAU, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, DAVID RODNEY, Science et Ingénierie des Matériaux et Procédés, Institut Polytechnique de Grenoble, CNRS/UJF, 38402 Saint Martin d'Hères, France, SIDNEY YIP, Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, KRYSYTN J. VAN VLIET, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — We report kinetic Monte Carlo (kMC) simulations of dislocation climb in a heavily deformed body-centered-cubic Fe comprising a supersaturation of vacancies. This approach explicitly incorporates the effect of nonlinear interactions between these point and line defects on vacancy migration barriers, and enables predictions of diffusivity and climb over relevant timescales at elevated temperatures. Vacancy migration barriers rapidly decrease inside the dislocation core and thus self-diffusivity locally increases. For a given uniaxial stress, We employ kMC to calculate climb velocities and thereby the macroscopic creep rates. The extracted stress exponent for steady-state creep and its variation with temperature agree well with experiment. Finally, these atomistically informed kinetic simulations demonstrate the stress dependence of creep activation energy in such metals that is attributable to complex point-line defect interactions.

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