Kinetic Monte Carlo enabled modeling of diffusion assisted plastic deformation
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ABSTRACT
Phenomena such as solute strengthening in alloys as well as embrittlement of bimaterial interfaces and grain boundaries by impurities are controlled by quantum mechanical interactions of solutes or defects – dislocations, grain boundaries, vacancies, or cracks. The local stresses driving these atomic-scale processes are determined by behavior occurring at much larger spatial and temporal scales. We describe a new model that provides a general purpose approach to couple the disparate temporal scales in a concurrent multiscale simulation using Kinetic Monte–Carlo (KMC) as a buffer between a Molecular Dynamics (MD) region and a Finite Element (FEM) region. We start by describing the temporal scale coupling between FEM and KMC and then that between KMC and MD. We finally present results for vacancy assisted dislocation motion in a simulation where far-field concentrations are solved using FEM; the dislocation is represented with atomistic resolution in an MD region using a KMC band to couple to the FEM outer region.