LARGE SCALE DISLOCATION DYNAMICS SIMULATIONS OF PLASTICITY AND POINT DEFECT EVOLUTION IN PERSISTENT SLIP BANDS

Jafaar El-Awady

Johns Hopkins University, jelawady@jhu.edu

Abstract

One of the common dislocation microstructures forming during cyclic loading of face centered cubic metals are persistent slip bands (PSBs). Over the years, many experimental, theoretical, and computational studies have led to significant understanding of plasticity in PSBs, however, many open questions still remain in the prediction of the formation and evolution of these complex dislocation structure. In this work, large scale three-dimensional (3D) discrete dislocation dynamics (DDD) simulations are performed to study dislocation plasticity and point defect evolution in PSBs in single-slip oriented nickel single crystals. In these simulations partially developed PSB structures are introduced into the simulation cell and fully reversible loading is imposed. The maximum stress of the hysteresis loops and the local dislocation density in the channels/walls are shown to increase with increasing loading cycle. The dislocation interactions in the channels and the 3D contours of the local shear stress within the channels as a function of distance from the PSB walls are characterized to reevaluate the composite model proposed by H. Mughrabi and the bowing and passing model by L.M. Brown. In addition, the spatio-temporal point defect (vacancies and interstitials) generation and evolution is quantified as a function of the dislocation density in the PSB channels and walls. The results are discussed in view of a point defect diffusion model to study their migration rates to the surface. Finally, the PSB interaction with the free surface and the surface roughness evolution are also quantified.