

[PO-B2]Poster Session 2

Symposium B

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

**[P2-10]Screw dislocation-interstitial solute coevolution in W-O alloys
using atomistically-informed kinetic Monte Carlo simulations**

Yue Zhao¹, Lucile Dezerald³, Jaime Marian^{1,2} (1.Dept. of Materials Science and Engineering, University of California, Los Angeles, United States of America, 2.Dept. of Mechanical Engineering, University of California, Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France)

The interaction of interstitial impurities with in-grown dislocations in metals can lead to various processes, including solute solution hardening and/or dynamic strain aging. The coevolution of solutes and dislocations occurs on length and time scales that are very challenging to resolve experimentally. The interaction of interstitial solutes with dislocation segments is highly local, however, and models must be capable of resolving the fine details of the interaction if we are to gain any understanding from the process. Here we develop a kinetic Monte Carlo model of dislocation motion in the presence of diffusing solutes. We focus on the W-O solid solution, such that the subject of our study is screw dislocations, as they control plastic flow at low temperatures in body-centered cubic metals and alloys. Solute diffusion is affected by dislocation strain fields, which we study via the elastic dipole tensor using electronic structure calculations. As well, we calculate binding energies of O atoms to screw dislocation cores, and discuss the joint structures formed, the implications of the calculated energetics, and show the effect on the dislocation velocity of solute diffusion at several temperatures.