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Abstract

We examine the common assumption that grain boundaries (GBs) are ideal (or perfect) sinks for point defects by comparing and contrasting its implications with an explicit model of a low-angle tilt GB described by an array of edge dislocations which annihilate point defects by climbing. We solve the resultant diffusion equation in the absence and presence of irradiation-induced point defects. The GB sink efficiency depends on the physical parameters describing the boundary geometry (*i.e.*, misorientation), material properties, and/or irradiation conditions (point defect generation and annihilation within the interior of grains). When the constituent dislocation spacing is small (large misorientation), the GB sink efficiency approaches that of the ideal sink. However, for small misorientations, the GB sink efficiency drops rapidly to zero and the ideal sink assumption for the GB fails dramatically. We derive a reduced dimension description of GBs where the influence of GB structure is captured in a single parameter in a Robin boundary condition for the diffusion equation. For the case of a low-angle tilt GB, we explicitly relate this parameter to the GB structure. We discuss the generality of this approach for cases where the low-angle GB model applies and parameterize the model so that it accurately reproduces the results of the two-dimensional dislocation model. The applicability of the approach to more general GBs is discussed as well as the implication of these results for predicting grain size effects under irradiation conditions.

Keywords: Grain boundaries; Point defects; Sink efficiency; Dislocation climb; Irradiation