Atomistic Modeling of Grain Boundary Segregation

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Point defect sinks, such as individual dislocations or grain boundaries (GB), play a crucial role in embrittlement, swelling, or non-equilibrium solute segregation driven by the point defect fluxes. These phenomena are especially important in irradiated materials. Usually, theoretical determination of grain boundaries (GB) sink strength is based on the dislocation representation of GB and, consequently, on the consideration of elastic interaction between the latter and point self defects. This approach is hardly applicable to an arbitrary GB geometry that can be found in real materials.

Recently we proposed a new modelling technique [1], Atomic Fraton Theory (AFT), that naturally incorporate structural and elastic properties of system and allows to model the most challenging cases of atomic structure in complex systems. In this paper, we present the simulation results of solute segregation and vacancies absorption at tilt grain boundaries using AFT approach [2-3]. We show that the GB sink strength for vacancy annihilation strongly depends from the GB tilt angle. An AFT model is also developed to investigate the voids formation at GB during irradiation. The effect of vacancy concentration and vacancy generation rate on the voids size, shape and nucleation sites is studied.

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