The Segregation Effect for Grain Boundary Diffusion in Isotropic Materials

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Three principal Harrison grain boundary kinetics regimes (Types A, B and C) have been fully investigated in [1-3] for the case of self-diffusion and for grains of approximately the same size. In [4] the segregation effect for the grain boundary impurity diffusion problem was investigated for the case of the model where grains are represented by parallel slabs. In the present paper, for the first time, we analyse the grain boundary impurity diffusion problem for the closed grain model. This analysis is done by making use of an analytical approach [5] and by means of Lattice Monte Carlo (LMC). This recent technique has been successfully used on numerous occasions [1-4] for the purposes of systematic studies of the grain boundary transition regimes that occur between the principal well-defined Harrison grain boundary kinetics regimes (A, B and C – types). The segregation effect in the cubic grain model is analysed and compared with the simple parallel slab grain model. Significant differences in the resulting profiles and consequently in the resulting grain boundary diffusion properties are found.


