Effective diffusion coefficient in one-dimensional heterogeneous solids: a comparison of continuous and discrete lattice models

J.R.Kalnins[1], E.A. Kotomin[2], V.N. Kuzovkov[2]*

[1]Ventspils Engineering Research Institute (VIRAC), Ventspils University College, Ventspils, Latvia
[2]Institute of Solid State Physics, University of Latvia, Riga, Latvia
*kuzovkov@latnet.lv

Description of transport in heterogeneous media (solids with grain boundaries, matrices with inclusions, etc) is of great importance for many applications in physics and chemistry of real materials. It was shown in our recent papers (e.g. [1]) that the effective diffusion coefficient D_{eff} in a continuous heterogeneous media (matrix with periodically distributed inclusions) using one-dimensional model in the framework of extended effective medium theory [2-3] contains an important parameter--a ratio of particle concentrations on the boundary matrix- inclusion. This concentration jump was introduced as a phenomenological ad hoc parameter. Here we present a simple derivation for D_{eff} based on the random walk arguments, and establish relation with results [4] based on the reaction rate theory [5]. This connection allows us to formulate the concentration jump in terms of reaction rates and corresponding particle hopping probabilities on the boundary matrix –inclusion as well as generalise reaction rate relation for D_{eff} for the different hopping lengths in matrix l_1 and inclusion l_2.

It will be demonstrated how for the one-dimensional discrete lattice model (Fig.1)

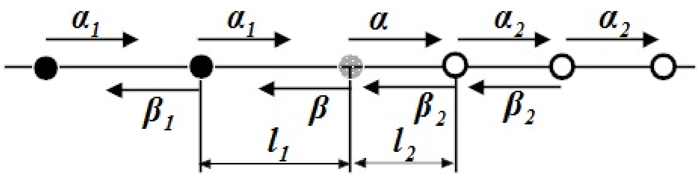

Figure 1. Transition rates on the boundary matrix (indexes 1) and inclusion (indexes 2)

we derived the following relation

$$D_{eff} = \frac{D_1}{\left(1 - f + \dfrac{\alpha\alpha_2 l_1}{\beta\alpha_1 l_2} f\right)\left(1 - f + \dfrac{\beta l_1}{\alpha l_2} f\right)}, \tag{1}$$

where f is the volume fraction of inclusion in one period representing element, D_1 matrix diffusion coefficient $D_1 = l_1^2(\alpha_1 + \beta_1)/2$.

References

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