Nanoscale physics

A new approach for determination of the effective diffusion coefficients in the nanostructured two-phase media

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Functional materials can have inhomogeneous structure with essentially different diffusion kinetics in their subsystems. We can distinguish two characteristic structure types in which determination of the effective diffusivities becomes a crucial issue. Firstly, it is important to describe effective diffusion permeability of nanocrystalline materials [1]. In such materials volume fraction of both grains and intergranular amorphous layers are comparable. Secondly, effective diffusion permeability in two-phase zones of ternary systems determines the morphology of the diffusion zone [2]. Traditionally, effective kinetic coefficients are defined on the basis of the Maxwell-Garnett model and some other approaches based on the modification of this model [3]. For example, Kalnin's model [4] is the most highly developed one for the description of the diffusion processes in the binary inhomogeneous medium.

A new model of effective medium is proposed for the description of the transition zone between two phases interacting by diffusion. In this model the effective diffusivity depends on the kinetic coefficients in each phase, volume fractions of phases and on the additional parameter, which generally characterizes the structure type of the two-phase zone. The Lattice Monte Carlo method was used to test the validity of different approaches in the determination of the effective diffusivity.

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