Nanoscale physics

Determination of the effective diffusion coefficients for inhomogeneous media and computer modeling of the diffusional phase interaction in the nanostructured two-phase systems

Yu.A. Lyashenko

Physics Department, Cherkasy National University, Shevchenko, 81, Cherkasy, Ukraine.
E-mail: urico@ukr.net

Various functional materials have inhomogeneous structure with essentially different diffusion kinetics in their subsystems. The importance of determining the effective diffusivity may be demonstrated by considering two characteristic structures: nanocrystalline materials [1] and the two-phase zones [2]. In nanocrystalline materials [1] volume fractions of grains and interfaces, which are formed between them are comparable. 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] describes the diffusion processes in the inhomogeneous medium.

A model of the effective medium is developed for the description of the transition zone between two phases, which interact by diffusion. The effective diffusivity depends on the growth kinetic coefficients of each phase, the volume fractions of phases and on the additional parameter that generally characterizes the structure type of the two-phase zone. A model describes the two-phase zone evolution based on the diffusion fluxes through both phases and their percolation behavior. The Lattice Monte Carlo method was used to test the validity of different phenomenological approaches in calculating the effective diffusivity in the nanostructured systems comprising the two-phase zones with different morphology.

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