Nanoscale physics

The effective diffusivity in nanostructured two-phase systems: effective medium approximations and Lattice Monte Carlo method

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The nanostructured functional materials might have inhomogeneous structure with essentially different diffusion kinetics in their subsystems. The importance of determining the effective diffusivity inside inhomogeneous media could be demonstrated by considering two characteristic structures: nanocrystalline material [1] and the two-phase zone [2]. In nanocrystalline material, volume fractions of grains and interfaces between them are comparable. Usually, effective kinetic coefficients are defined on the basis of the Maxwell-Garnett model and some approaches based on the modification of this model [3]. For example, Kalnin's model [4] describes the diffusion processes in the inhomogeneous medium with spherical inclusions in the host matrix.

In this work a new model of the effective medium is developed for the description of the transition zone between two phases interacting by diffusion. In this model, the effective diffusivity depends on the growth kinetic coefficients of each phase, 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 compare the different phenomenological approaches in calculating of the effective diffusivity inside nanostructured systems with different morphology of the two-phase zones.

[1]. *Belova I.V., Murch G.E.* The effective diffusivity in polycrystalline material in the presence of interphase boundaries // Phil. Mag. – 2004. - **84**, № 1 – P. 17-28.
[2]. *Lyashenko Yu.O., Gladka L.I.* Modeling diffusion interaction in two-phase systems using different types of effective kinetic coefficients// *J Nano- Electron Phys. – 2012.* – **4**, № 1 – P. 03010-9.
[3]. *Snarskii A.A., Bezsudnov I.V., Sevryukov V.A.* Transport processes in macroscopically inhomogeneous media. Moscow: URSS; 2007.
[4]. *Kalnin J.R., Kotomin E.A., Maier J.* Calculations of the effective diffusion coefficient for inhomogeneous media // J Phys Chem Sol.-2002.– **63**. – P. 449-456.