DETERMINATION OF EFFECTIVE DIFFUSION COEFFICIENTS FOR INHOMOGENEOUS MEDIA

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ABSTRACT

A new model of effective medium is proposed for the transition zone located between two diffusion-interacting phases. In the 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.

Key words: effective diffusivity, two-phase zone, Maxwell's model, percolation effect.

INTRODUCTION

As known, materials can have inhomogeneous structure with essentially different kinetic coefficients in subsystems. As to account of diffusion properties, one can mention two characteristic structure types where effective diffusivities determination becomes a crucial issue in describing solid state reactions. Firstly, it is important to describe effective diffusion permeability of nanocrystal materials [1], when volume fractions of both grains and intergranular amorphous layers between them are considerable. Secondly, effective diffusion permeability in two-phase zones of ternary systems determines the morphology of the diffusion zone as well as the growth rate of phase layers and two-phase zones between them [2]. Traditionally, effective kinetic coefficients are defined on the basis of Maxwell-Garnett model [3] and some other approaches (for details see [4]). Kalnin's model [5] is the most highly developed one from the viewpoint of diffusion processes description by the modified Maxwell-Garnett model. At that, when treating inhomogeneous systems with noticeable volume fractions of both phases, we face the problem of ambiguity, since systems with high-conductive matrix and almost inert inclusions and vice versa will involve different effective diffusivities at equal ratios of phase volume fractions. This means that there always exists a certain branching, like, for example, at choosing between abstract models of parallel and series connection of phases. The aim of the present work is to find a new method of defining effective diffusivities.

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METHODS OF EXPERIMENT AND CALCULATION

We aim at developing a self-consistent method for calculating the effective diffusivities in two-phase regions of ternary systems with the help of Bruggemann's approach and Kalnin's basic model for combined transition diffusion zone between two phases (*Fig.1*).

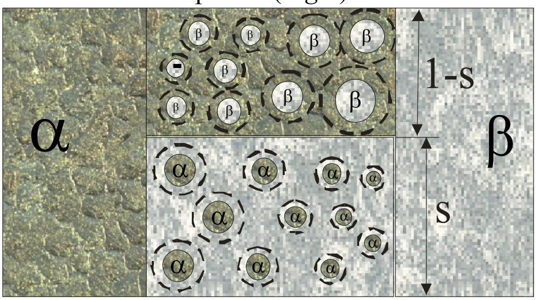


Fig. 1 – Schematic two-phase system. In the transition zone of diffusion contact the particles of α-phase precipitate in the β-phase matrix and the particles of β-phase – in α-phase

The paper provides derivation of the expression for effective kinetic coefficient in the case of transition zone between two phases containing two structure types: both the matrix of β-phase with inclusions of α-phase particles (basic structure K1) and conversely – α-phase matrix with inclusions of β-phase particles (basic structure K2).

In order to derive the formula of the combined model for defining the effective kinetic coefficients in two-phase cells Kalnin's basic models are applied:

Kalnin's model (K1) [5] for the structure, presented in Fig. 1 (left-hand side):

$$L_{eff}^{K1} = \frac{L^{\beta}}{1 - p^{\alpha} + \frac{c^{\alpha}}{c^{\beta}} \cdot p^{\alpha}} \left[1 + \frac{\dim \cdot \left(L^{\alpha} \frac{c^{\alpha}}{c^{\beta}} - L^{\beta} \right) \cdot p^{\alpha}}{(\dim - 1) \cdot L^{\beta} + \frac{c^{\alpha}}{c^{\beta}} L^{\alpha} - \left(\frac{c^{\alpha}}{c^{\beta}} L^{\alpha} - L^{\beta} \right) p^{\alpha}} \right] \tag{1}$$

Kalnin's model (K2) [5] for the structure, presented in Fig. 1 (right-hand side):

$$L_{eff}^{K2} = \frac{L^{\alpha}}{1 - p^{\beta} + \frac{c^{\beta}}{c^{\alpha}} \cdot p^{\beta}} \left[1 + \frac{\dim \cdot \left(L^{\beta} \frac{c^{\beta}}{c^{\alpha}} - L^{\alpha} \right) \cdot p^{\beta}}{(\dim - 1) \cdot L^{\alpha} + \frac{c^{\beta}}{c^{\alpha}} L^{\beta} - \left(\frac{c^{\beta}}{c^{\alpha}} L^{\beta} - L^{\alpha} \right) \cdot p^{\beta}} \right] \tag{2}$$

where c^{α}, c^{β} – concentration of component in the α-and β- phases, respectively; L^{α}, L^{β} – kinetic coefficients; p^{α}, p^{β} – volume fractions of α- and βphases, respectively, dim – model's dimension (in case of dim=3 a three-dimension system is considered), f_{11} – volume fraction of α-phase in the bottom side of the transition zone with respect to the total volume fraction of α-phase; f_{21} – volume fraction of β-phase in at the bottom side of the transition zone with respect to the total volume fraction of β-phase; f_{12} – volume fraction of α-phase in the top side of the transition zone with respect to the total volume fraction of α-phase; f_{22} – volume fraction of β-phase in the top side of the transition zone with respect to the total volume fraction of β-phase.

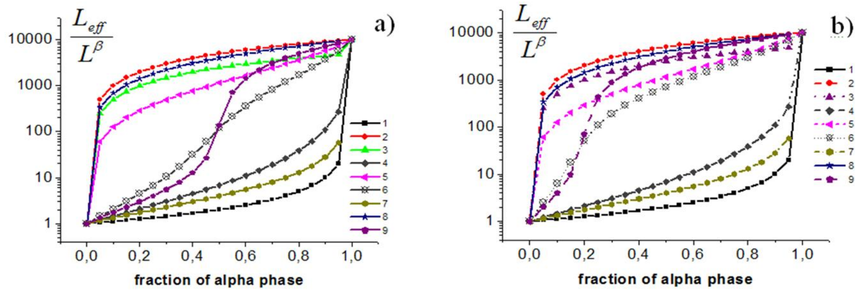
In our calculations we consider the transition zone to contain basic structures K1 and K2 in arbitrary proportion, given by coefficient s. Using the condition of the parameters unity for the effective medium for two alternative structures of the transition zone $L^1{}_{eff}, = L^2{}_{eff}$, calculate the unknown parameter f_{11}.

The obtained formula for effective kinetic coefficient of the transition zone taking into account the basic structures K1 and K2, as well as their interrelation, given by coefficient s, is as follows:

$$L_{eff}^{K1+K2}(s) = L^{\beta}\cdot s\cdot c^{\beta}\cdot\frac{s[L^{\alpha}+(\mathrm{dim}-1)\cdot L^{\beta}]+(L^{\alpha}-L^{\beta})(\mathrm{dim}-1)v^{\alpha}f_{11}}{[s(L^{\alpha}+(\mathrm{dim}-1)\cdot L^{\beta})-(L^{\alpha}-L^{\beta})v^{\alpha}f_{11}]\cdot[c^{\beta}s+v^{\alpha}f_{11}(c^{\alpha}-c^{\beta})]} \quad (3)$$

RESULTS AND DISCUSSION

In *Fig. 2* the dependencies of effective diffusivities, obtained at treating the two-phase media with essentially different kinetic coefficients in each phase, are shown. The comparative analysis confirms branching of the values of effective kinetic coefficients.



a) b)

Fig. 2 – The dependencies of effective kinetic coefficients on the volume fraction of α-phase, calculated by the models of: 1 – series phase connection, 2 – parallel phase connection, 3 – combined model of parallel connection of the basic models (those of parallel and series connection) with the weight coefficients W = 0.5, 4 – Kalnin's (K1), 5 – Kalnin's (K2), 6 – combined model based on Kalnin's models with the weight coefficients s, 7 – Maxwell-Garnett (MG1), 8 - Maxwell-Garnett (MG2), 9 – combined model based on Maxwell-Garnett models with the weight coefficient s. The calculations were done using the following parameters: $c_1 = 0.1$, $c_2 = 0.6$, $L_1 = 10^{-13}$ arbitrary units, $L_2 = 10^{-17}$ arbitrary units; a) at $s = 0.5$, b) at $s = 0.2$.

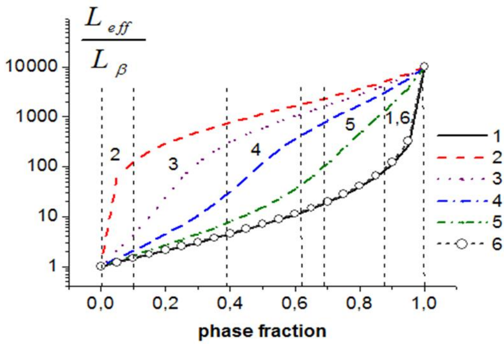


Fig. 1. – Dependencies of effective kinetic coefficients on the volume fraction of α-phase, calculated according to the following models: 1 – Kalnin's (K1), 2 - Kalnin's (K2), the model combined of Kalnin's basic models at weight coefficient 3 - $s = 0.25$, 4 - $s = 0.5$, 5 - $s = 0.75$, 6 - $s = 0.99$ using the parameters, given in *Fig. 1*

In *Fig.3* the dependencies of effective kinetic coefficients on the volume fractions of phases in the developed model of effective two-phase medium, at different values of coefficient s (describing the fraction of base structures K1 and K2 in the combined transition zone), are given.

Using different approaches to the assignment of effective diffusivities we have performed model calculations of diffusion interaction in the planar diffusion couple of a ternary system, the diffusion path crossing the two-phase region on the phase diagram. The detailed calculations are provided in [6].

CONCLUSIONS

The paper provides derivation and further analysis of the expression for effective diffusivity in the general case of transition diffusion zone at the contact of two phases in quasi-steady state conditions, grounding upon Kalnin's basic models. It is presupposed that effective diffusivity in the transition zone depends on the diffusivities of the phases brought to contact, and an additional parameter s, which allows general considering of the transition zone structure. In the developed model the general expression for effective diffusivity depending upon the additional parameter (correspondingly, depending on the volume fractions of phases and transition zone structure) between two marginal cases of Kalnin's model, is obtained.

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