Chapter 26
Diffusion Process in Quasi-One-Dimensional Structures as Elements of Novel Nanodevices

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Abstract The effective diffusion coefficient in two-phase one-dimensional model with the periodical distribution of inclusions in the effective medium approximation is calculated and generalization about a quasi-one-dimensional case is formed.

Keywords Effective diffusion • Effective medium • Method

26.1 Introduction

In several papers the expression for the effective diffusion coefficient in the scope of generalized Maxwell-Garnett theory has been considered [1, 2]. Different concentrations of diffusing particles in matrix and inclusions require corresponding conditions on the boundary matrix-inclusion.

It has been ad-hoc assumed that a concentration jump is equal to the average concentration ratio. Further in the text we show that this result strictly follows from the effective medium approximation and that one-dimensional approach can be used in solving quasi-one-dimensional problems after performing some computer simulation.

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Y.N. Shunin and A.E. Kiv (eds.), *Nanodevices and Nanomaterials for Ecological Security*, NATO Science for Peace and Security Series B: Physics and Biophysics, DOI 10.1007/978-94-007-4119-5_26,

26.2 Effective Medium Approximation in One-Dimensional Diffusion Model

Let us consider one-dimensional heterogeneous medium: periodically distributed regions with the diffusion coefficient D_1 in matrix and the diffusion coefficient D_2 in inclusions. In the effective medium approximation we replace one-dimensional sample by a representative element consisting of a matrix and one inclusion, which are embedded into the effective media with the diffusion coefficient D_{eff} (Fig. 26.1).

The corresponding concentrations are c_{eff}, c_1, c_2 and c_3.

The external concentration field $c_{eff} = -gx$ with a constant gradient g is applied in the sample. Applying the solution of the stationary one-dimensional diffusion equation gives

$$\begin{aligned} c_{eff} &= -gx, \\ c_1 &= \alpha_1 x + \beta_1, \quad (region\, I) \\ c_2 &= \alpha_2 x + \beta_2, \quad (region\ II) \\ c_3 &= \alpha_3 x + \beta_3 \quad (region\ III). \end{aligned} \tag{26.1}$$

We choose the boundary conditions in the form

$$\begin{aligned} c_{eff}\big|_{x=x_1} &= \frac{1}{\chi} c_1\big|_{x=x_1}, \\ c_1\big|_{x=x_2} &= \frac{1}{\alpha} c_2\big|_{x=x_2}, \\ c_2\big|_{x=x_3} &= \alpha c_3\big|_{x=x_3}, \\ c_3\big|_{x=x_4} &= \chi c_{eff}\big|_{x=x_4} \end{aligned} \tag{26.2}$$

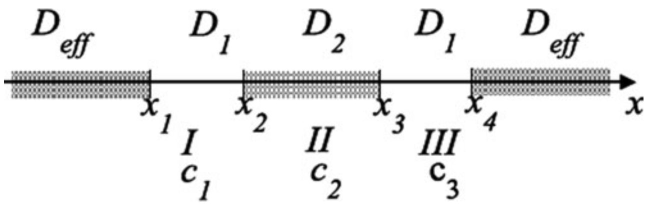

Fig. 26.1 Representative element (I-II-III) in one-dimensional effective media

and

$$\begin{aligned} D_{eff}\frac{\partial c_{eff}}{\partial x}\bigg|_{x=x_1} &= D_1\frac{\partial c_1}{\partial x}\bigg|_{x=x_1}, \\ D_1\frac{\partial c_1}{\partial x}\bigg|_{x=x_2} &= D_2\frac{\partial c_2}{\partial x}\bigg|_{x=x_2} \\ D_2\frac{\partial c_2}{\partial x}\bigg|_{x=x_3} &= D_1\frac{\partial c_3}{\partial x}\bigg|_{x=x_3} \\ D_1\frac{\partial c_3}{\partial x}\bigg|_{x=x_4} &= D_{eff}\frac{\partial c_{eff}}{\partial x}\bigg|_{x=x_4}. \end{aligned} \tag{26.3}$$

The coefficient αin Eq. 26.2 characterizes the concentration jump on the boundary inclusion–matrix and the coefficient χdenotes that there also exists a concentration jump on the boundary matrix–effective medium. D_{eff} can be determined from the systems of equations (26.2) and (26.3) inserting into them (26.1) and demanding the existence of nontrivial solution.

To simplify this equation, we assume that $x_4 - x_1 = 1, x_3 - x_2 = f, x_2 = (1 - f)/2$ and $x_3 = (1 + f)/2$. The obtained result is then

$$D_{eff} = \frac{D_1\chi}{\left((1-f)+f\frac{D_1}{D_2\alpha}\right)} \tag{26.4}$$

with

$$\chi = \frac{1}{((1-f)+\alpha f)} \tag{26.5}$$

In order to determine the coefficient α, one additional equation is needed. We get this equation on the condition that the average particles concentration in the representative region should be equal to the average particles concentration in the effective medium of the same length. Thus we have

$$\overline{c}_{eff} = \int_{x_1}^{x_4} c_{eff}dx = \int_{x_1}^{x_2} c_1dx + \int_{x_2}^{x_3} c_2dx + \int_{x_3}^{x_4} c_3dx = \overline{c_1} + \overline{c_2} + \overline{c_3}. \tag{26.6}$$

Inserting c_1, c_2 and c_3 from (26.1) into (26.6), we receive

$$\alpha = \frac{\overline{c_1}}{\overline{c_2}}. \tag{26.7}$$

Equation 26.6 has been postulated in our papers [1, 2].

Finally, for the effective diffusion coefficient D_{eff} we have

$$D_{eff} = \frac{D_1}{\left(1 - f + \frac{\overline{c_2}}{\overline{c_1}} f\right)\left((1 - f) + \frac{D_1 \overline{c_1}}{D_2 \overline{c_2}} f\right)}. \tag{26.8}$$

If $\overline{c_1} = \overline{c_2}$, we get a well known result

$$D_{eff} = \frac{D_1 D_2}{D_1 f + D_2 (1 - f)}. \tag{26.9}$$

26.3 Quasi-One-Dimensional Diffusion Example

We consider there quasi-one-dimensional diffusion in the model sample of channels and spikes with the diffusion coefficient D (Fig. 26.2).

One representative element is shown in Fig. 26.3.

A particle diffusing through the sample takes a long time in spikes. If the height of the spike grows, the diffusing particle will be trapped in the spike for an extended time. It is obvious that the effective diffusion coefficient will decrease because of spikes. We can approximate the particle diffusion in the spike (as soon as we are interested in the one-dimensional diffusion through the sample) as one-dimensional diffusion with the different diffusion coefficient, which we denote D_2. The diffusion coefficient in the channel is denoted further by D_1. Thus, we replace the representative element by some effective quasi-one-dimensional media (Fig. 26.3).

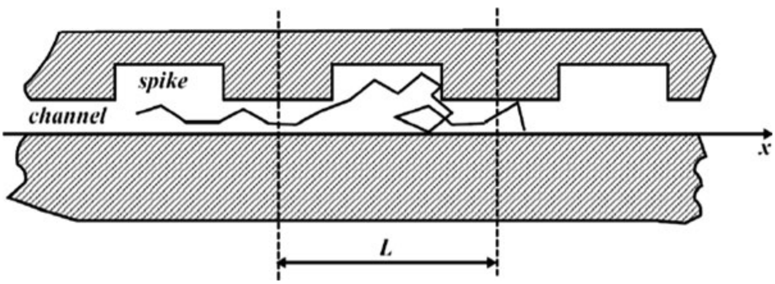

Fig. 26.2 Quasi-one-dimensional sample. L period

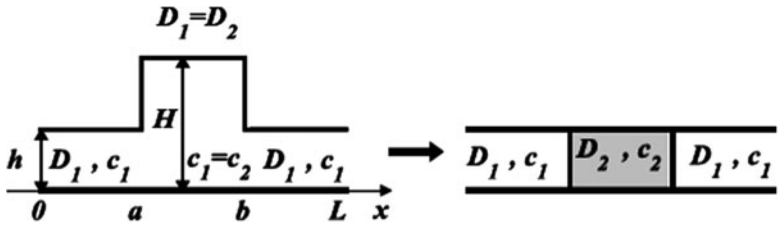

Fig. 26.3 On the *left* – representative element; the spike begins at *a* and ends at *b*. *H* the height of spike, *h* channel height, *L* the length of representative element. On the *right* – equivalent quasi-one-dimensional model

The concentration of diffusing particles in the region (*a, b*) will differ from that in the channel. We denote this concentration by c_2. (Henceforth, we denote average concentrations as c_1 and c_2.)

Now we can calculate effective diffusion coefficient through the sample as

$$\frac{D_{eff}}{D_1} = \frac{1}{\left(1 - f + \frac{c_2}{c_1} f\right)\left((1 - f) + \frac{D_1 c_1}{D_2 c_2} f\right)}, \tag{26.10}$$

where $f = (b - a)/L$. We can assume that $c_2/c_1 = H/h$, then D_{eff} depends on H and h, D_{eff} also depends on the form of spike. A computer simulation is a possible way to obtain the D_{eff} and D_2 values. The results received in the computer simulation, may be used for the estimation of effective diffusion coefficients in practical cases.

We have simulated the diffusion of particles through a quasi-one-dimensional sample using the Monte Carlo method. The simulation has been carried out in the representative element with the periodic boundary conditions along the x axes. Inside the representative volume, particles are reflected from the channel and spike borders. The mean free path of particle l has been chosen $l = 0.2$. The particle performs two-dimensional random walking with the equal probability to jump to any direction. D_{eff} is calculated by formula

$$D_{eff} = \frac{<x^2>}{2N\tau}, \tag{26.11}$$

where $<x^2>$ is the mean square displacement of a diffusing particle, N – the number of jumps, τ-jump time, $D_1 = l^2/(4\tau)$. The number of diffusing particles is 10,000, and one particle history has been varied from 50,000 to 600,000 jumps long. The estimated error is 3%. The results of computer simulation are presented in Fig. 26.4.

It is seen from Fig. 26.4, that D_{eff} and D_1 are strongly correlated.

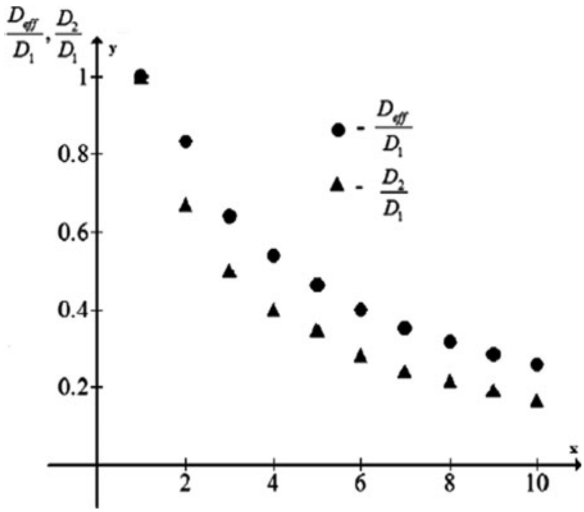

Fig. 26.4 Results of computer simulation. D_{eff}/D_1 (*circles*) and D_2/D_1 (*triangles*) dependence on H/h. $h = 1, f = 0.4, a = 3, b = 7, L = 10$

26.4 Conclusions

A closed formula for the effective diffusion coefficient in the heterogeneous media with the periodically distributed inclusions has been developed. It has been shown that the previously [1, 2] accepted ad-hoc assumption about concentrations on the boundary matrix-inclusion follows in a self consistent way from the effective medium approximation. Simple quasi-one-dimensional models can be considered as one-dimensional in an effective manner. Simple computer simulation can help to determine the necessary parameters for the construction of practically usable effective diffusion coefficients.

References

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