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The lattice shift generated by two dimensional diffusion process

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ABSTRACT

The Poisson equation is used to calculate the drift velocity in the two-dimensional diffusion couple. This approach is based on the bi-velocity (Darken) method which combines the Darken and Brenner concepts that the volume velocity is essential in defining the local material velocity in multicomponent mixture at non-equilibrium. As an example the arbitrary binary system is considered. It is shown that (1) the two dimensional calculations should be applied with the stochastization method and (2) the drift term in mass conservation law does not affect the calculations.

1. Introduction

Modelling of interdiffusion phenomena is far from being unified. The specificity of different approaches lies in the arbitrary choice of the drift (convection) velocity. In computational solid mechanic it is defined as being equal to the mass average velocity [1]. Such a method allows for simplified formulation of an interdiffusion strain rate tensor and allows the Lagrangian approach for modeling interdiffusion phenomena in solid metals. In gases and fluids the drift is defined basing on the volume average velocity [2,3]. In material science the drift definition base on the Darken method [4]. This method is not widely accepted in physics and consequently it is common to postulate drift as an average mass velocity [1] or neglect drift (convection) entirely and assume simple Fick'ian diffusion only [4]. Such simplified approach to the mass transport was used in three-dimensional model of interdiffused quantum dots where an automatic solution to the Fick's diffusion equation was implemented. Obviously it does not allow considering the interdiffusion effects [4].

The entirely new concept concerning the mass transfer started with Darken method. His basic assumption was the postulate of drift velocity in binary solid solution [5]. The drift velocity, in fact is the vacancy velocity generated during interdiffusion process caused by difference in the intrinsic diffusion coefficients. Darken determine the drift velocity from mass conservation laws of A and B component as:

$$\upsilon^{drift} = (D_A - D_B)\frac{\partial N_A}{\partial x}.$$

Thus, the overall velocity in binary mixture was divided in two parts (1) the diffusion velocity, υ_i^d determined by Nernst–Planck flux equation and (2) drift velocity υ^{drift}.

The drift velocity concept nowadays is still generalized. It allows to estimate: (1) the interdiffusion process in multicomponent and multiphase systems [6], (2) the Kirkendall phenomena (the position of the kirkendall planes) [7], (3) the interactions between the self stress and interdiffusion [8–10], (4) the influence of the external pressure field and entropy during diffusion process [11], (5) a mathematical model was developed to simulate the morphological change of the sintering neck by its growth and the Kirkendall void formation in the Cu–Ni alloy [12] and many others.

In 2012 we have shown how to calculate the entropy and entropy production during diffusion process [13,11]. This concept was further used to calculate the interdiffusion process in multiphase binary and ternary couples. The use of the entropy production rate in multiphase calculations is an additional factor which allow to calculate the evolution of the phases in multicomponent systems was recently demonstrated [14].

The practical applicability causes that in spite of mathematical and numerical difficulties the three dimensional interdiffusion problems are still of interest. Recently Gusak et al. suggested 3D generalization of Martin–Erdelyi–Beke model of simultaneous interdiffusion and ordering in binary diffusion couples [15]. The objective of this work is to analyze the diffusion is solid solutions (binary alloy) and show the differences between the one- and two-dimensional interdiffusion calculations. The presented

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approach base on the bi-velocity method where the volume velocity is essential in defining the local material velocity at non-equilibrium [8,16]. The model is formulated for an arbitrary, three-dimensional system. Discussion here is limited to the two-dimensional binary solution.

2. The two-dimensional bi-velocity method

In this paragraph the two dimensional generalized Darken method will be formulated. The main law is the mass conservation law for each reacting component in the diffusion couple in the sub-set of the volume occupied by the mixture $|\Omega| \subset X$:

$$\int_{|\Omega|}\left[\frac{\partial c_i}{\partial t}+\mathrm{div}J_i\right]dx=0 \quad i=1,2,\ldots,r. \tag{1}$$

Above equation was derived from the Liouville theorem. The flux, J_i is defined after Darken as a sum of the diffusion j_i and drift fluxes, j^{drift}. The c_i denote the concentration of the ith element in the mixture. All of the above variables are a functions of the position in three dimensional space and time.

The diffusion flux can be defined from Nernst–Planck flux equation [17,18]:

$$j_i=-\frac{D_i}{kT}\ \mathrm{grad}\ \mu_i, \tag{2}$$

where the D_i and μ_i denote the diffusion coefficient and diffusion potential of the ith component, respectively. In this work for simplification we will apply the ideality sweeping statement (i.e. $a_i = c_i$). Thus the diffusion flux can be rewritten as follow:

$$j_i=-D_i\ \mathrm{grad}\ c_i, \tag{3}$$

After Darken the drift velocity will be calculated from the mass conservation laws of each component. The sum of Eq. (1) give the following expression:

$$\int_{|\Omega|}\left[\sum_{i=1}^{r}\frac{\partial c_i}{\partial t}+\mathrm{div}\sum_{i=1}^{r}J_i\right]dx=0 \tag{4}$$

assuming that the overall concentration, c is constant and that the overall flux is a sum of the diffusion and drift fluxes, $J_i = j_i + j^{drift}$ the following relation holds:

$$\int_{|\Omega|}\mathrm{div}\sum_{i=1}^{r}\left(j_i+j_i^{drift}\right)dx=\int_{|\Omega|}\mathrm{div}\sum_{i=1}^{r}(j_i+c_i\upsilon^{drift})dx=0 \tag{5}$$

The above set of the equations allows to calculate the interdiffusion process in two dimensional domain.

3. Solution

To solve above model two independent solvers should be applied. Mainly, e.g. the lines method [19] to solve the problem in space and Runge–Kutta–Fehlberg method to solve the ordinary differential equations in time. First, the uniform grid, contained M and N mesh points along the x and y direction respectively, was generated and the concentrations and drift velocity were defined at points $x_{k,l}$. The equations was discretize in space to obtain the ordinary differential equation. The discretized overall flux of the ith component can be written as follow:

$$J_i(t) := j_i(x_{k,l},y_{k,l},t)+j^{drift}(x_{k,l},y_{k,l},t) \approx \begin{bmatrix} -{}^{k,l}D_i\frac{{}^{k+1,l}c_i-{}^{k-1,l}c_i}{x_{k+1,l}-x_{k-1,l}}+{}^{k,l}c_i\frac{{}^{k+1,l}u_i^{drift}-{}^{k-1,l}u_i^{drift}}{x_{k+1,l}-x_{k-1,l}}, \\ -{}^{k,l}D_i\frac{{}^{k,l+1}c_i-{}^{k,l-1}c_i}{y_{k,l+1}-y_{k,l-1}}+{}^{k,l}c_i\frac{{}^{k,l+1}u_i^{drift}-{}^{k,l-1}u_i^{drift}}{y_{k,l+1}-y_{k,l-1}} \end{bmatrix}, \quad i=1,2,\ldots,r \tag{6}$$

the u_i^{drift} denote the drift potential. To estimate the drift velocity the Poisson equation must be solved:

$$\mathrm{div}(\upsilon^{drift})=\mathrm{div}(\mathrm{grad}\ u^{drift}+\mathrm{rot}\ u^{drift})=-\sum_{i=1}^{r}\mathrm{div}(\Omega_i c_i \upsilon_i^d) =f(x,t) \tag{7}$$

where u^{drift} denote the unknown drift potential.

In order to solve the problem numerically we need to replace the second order partial derivatives with second-order finite difference approximations:

$$\frac{u_{k-1,l}^{drift}-2u_{k,l}^{drift}+u_{k+1,l}^{drift}}{\Delta x^2}+\frac{u_{k,l-1}^{drift}-2u_{k,l}^{drift}+u_{k,l+1}^{drift}}{\Delta y^2}=f_{k,l}, \quad k=2,\ldots,M; \quad l=2,\ldots,N \tag{8}$$

where M and N denote number of nodes in x and y directions, respectively.

The unknowns are located strictly in the interior of grid since u^{drift} is known at the boundaries from the boundary conditions, and hence there are $(M-1)(N-1)$ unknowns. The iterative update of the Jacobi iteration can now be written as:

$${}^{(n+1)}u_{k,l}^{drift}=\frac{\left({}^{(n)}u_{k-1,l}^{drift}+{}^{(n)}u_{k+1,l}^{drift}\right)\Delta y^2+\left({}^{(n)}u_{k,l-1}^{drift}+{}^{(n)}u_{k,l+1}^{drift}\right)\Delta x^2-\Delta x^2\Delta y^2 f_{k,l}}{2(\Delta x^2+\Delta y^2)}, \tag{9}$$

Moreover, to calculate the drift velocity the Poisson equation must be solved:

$$\mathrm{div}(\upsilon^{drift})=\mathrm{div}(\mathrm{grad}\ u^{drift}+\mathrm{rot}\ u^{drift})=-\sum_{i=1}^{r}\mathrm{div}(\Omega_i c_i \upsilon_i^d) =f(x,t) \tag{10}$$

where u^{drift} denote the unknown drift potential.

In order to solve the problem numerically we need to replace the second order partial derivatives with second-order finite difference approximations:

$$\frac{u_{k-1,l}^{drift}-2u_{k,l}^{drift}+u_{k+1,l}^{drift}}{\Delta x^2}+\frac{u_{k,l-1}^{drift}-2u_{k,l}^{drift}+u_{k,l+1}^{drift}}{\Delta y^2}=f_{k,l}, \quad k=2,\ldots,M; \quad l=2,\ldots,N \tag{11}$$

where M and N denote number of nodes in x and y directions, respectively.

The unknowns are located strictly in the interior of grid since u^{drift} is known at the boundaries from the boundary conditions, and hence there are $(M-1)(N-1)$ unknowns. The iterative update of the Jacobi iteration can now be written as:

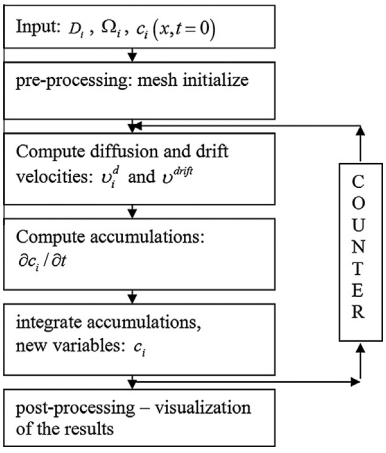

Fig. 1. The flow-chart depicting the various steps involved in the calculations.