

Numerical modelling of moving interfaces under local equilibrium conditions



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ABSTRACT

A new method is presented to simulate moving interfaces during diffusion-controlled growth under local equilibrium conditions. The position and compositions of the interface are obtained directly from the equilibrium state of the subsystem around the moving interface, without iterative calculation between diffusion fluxes and solute balance conditions. The method is applicable to general multi-component systems, and it ensures the consistency in compositions and solute balance at the interfaces; Those are ascribed to the presented consideration of subsystem around the interface region in a discretized form. Explicit equations of interface compositions and position in discretized variables are also presented for the simplified ternary systems of two-solution and compound/solution. The validity and usefulness of the method is demonstrated by simulations of the two important ternary systems; The simulation results illustrate the features of diffusion-controlled growth with different alloy compositions and diffusivities of solutes in both systems.

1. Introduction

During diffusional phase transformations of alloys, the evolution of concentration field governs growth kinetics. In moving interface problems where solute partitioning occurs at the interphase boundary, certain thermodynamic conditions (e.g., local equilibrium or para-equilibrium) are usually assumed at the interface, and there also exist solute balance conditions. Denoting two phases across the interface as S and L, and interface position as $z = R$, diffusion equations in each phase and interphase boundary conditions for n -component systems are written as

$$\frac{\partial c_j^S}{\partial t} = -\frac{\partial J_j}{\partial z} \text{ for } z < R, \quad \frac{\partial c_j^L}{\partial t} = -\frac{\partial J_j}{\partial z} \text{ for } z > R, \quad (1a)$$

$$c_j^S(R, t) = c_j^{S,e}, \quad c_j^L(R, t) = c_j^{L,e}, \quad (1b)$$

$$(c_j^{S,e} - c_j^{L,e}) \frac{dR}{dt} = J_j^{S/L} - J_j^{L/S}, \quad (1c)$$

where subscripts $j = 1, 2, \dots, n-1$ are for solute elements and n for solvent element; $c_j^{S,e}$ and $c_j^{L,e}$ are compositions at the interface. Solute fluxes J_j can be expressed in gradients of either concentration or diffusion potential, i.e.,

$$J_j = -\sum_{l=1}^{n-1} D_{jl} \frac{\partial c_l}{\partial z} \quad \text{or} \quad J_j = -\sum_{l=1}^{n-1} L_{jl} \frac{\partial \bar{\mu}_l}{\partial z}. \quad (2)$$

For the moving interface problems, the interface position (or velocity) and interface compositions should be found as a part of the solution besides the concentration fields in each phase. In general multi-component systems, the interface compositions (so called operating tie-line) are coupled with the solute balance conditions (Eq. (1c)) and cannot be determined by thermodynamic conditions alone. In conventional simulations (such as in a commercial software DICTRA), iterative calculations are performed by using trial values of interface velocity and interface compositions to find the operating tie-line at each time step [1–4]. Binary systems are exceptional because *a priori* interface compositions are uniquely determined by the local equilibrium condition without the kinetics of diffusion. The consistency of interface compositions and solute balance conditions is one of main concerns in numerical simulations of the problems. Some analytic solutions of idealized situations in (semi)infinite domains are available [5]. However, practical investigations of actual situations (e.g., variable diffusivities, finite system size, more than three components) usually need computational simulations.

In this study, a new method is presented to simulate moving interfaces with equilibrium partitioning of solutes, i.e., local equilibrium conditions at the interfaces. In the method, the position and

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compositions of the interface are obtained directly from the equilibrium state of the subsystem around the moving interface without iterative calculation between diffusion fluxes and solute balance conditions. The method is simple and applicable to general multi-component systems. Because it is based on the conservative nature of diffusion equation and the thermodynamic equilibrium nature of interface compositions in a discretized system, the consistency in compositions and solute balance at the interfaces is evident. Firstly, the discretization scheme for the interface position is described for binary systems in the next section. Although *a priori* values of interface compositions are given in binary problems, a basic idea for solving general multi-component problems can be drawn from the physical meaning of the discretized equations. Then the general case of finding the interface compositions and position in multi-component systems will be explained. Some useful formulations of simplified ternary systems are also presented to express analytically the equations of interface compositions and position in discretized variables. To illustrate the validity and usefulness of the method, simulations of two important ternary systems are described in the section of examples, which is followed by some discussion. A uniform cell size, constant diffusivities in each phase, and concentration-gradient-driven fluxes without cross effect are assumed in the following sections. However, these are adopted just for brief expression of discretization. Applying non-uniform grid spacing, spherical or cylindrical geometry, variable diffusivities, and diffusion-potential-gradients-driven solute fluxes to the present method is straightforward.

2. Moving interface in a binary system

Consider N grid points placed in the center of each control volume (cell) in a discretized space of system (Fig. 1). A cell that contains the interface will be denoted by “S/L-cell”. Concentrations of both phases c^S , c^L and an additional variable r are assigned to the S/L-cell to represent interface compositions and relative interface position (or volume fraction of S phase) within the cell. $r = 0.5$ when the interface is located at the center of the S/L cell. Overall concentration of the S/L-cell is then given by $c = rc^S + (1-r)c^L$. Let the k -th cell (denoted by “ k -cell”) be the S/L-cell at time t , then the global position of the interface is tracked by $R = z_k + (r - 0.5)dz$. The task of numerical computation here is, with the values of previous time step $R(t)$, $c^S(t)$, $c^L(t)$, to find the values of current time step $R(t + \Delta t)$, $c^S(t + \Delta t)$, $c^L(t + \Delta t)$ that satisfy the diffusion equations and solute balance conditions. For $c_{1-k-2}^S(t + \Delta t)$ and $c_{k+2-N}^L(t + \Delta t)$ (S- and L-cells not in contact with the S/L-cell), a standard discretization scheme of diffusion equation can be used. The discretization of diffusion equation is based on the control-volume (or finite volume) formulation [6,7], which will not be repeated here. However, for the S/L-cell (k -cell) and its two neighbors ($k-1$ - and (k

+ 1)-cells, a different scheme is applied as explained below.

The discretization of diffusion equation is described in an explicit time scheme. *A priori* values of interface compositions (which can be varied with time in non-isotherm conditions) $c^{S,e}(t + \Delta t)$ and $c^{L,e}(t + \Delta t)$ are given in binary alloys by local equilibrium condition alone. In the first step, “temporary” values of $c_{k-1,imp}^S$, $c_{k,imp}$, $c_{k+1,imp}^L$ and r_{imp} in the k -cell are evaluated using the interface compositions and the discretized diffusion equations as follows.

$$c_{k-1,imp}^S = c_{k-1}^{S,0} + \frac{J_1 - J_2}{\Delta z} \Delta t, \quad c_{k,imp} = c_k^0 + \frac{J_2 - J_3}{\Delta z} \Delta t, \quad c_{k+1,imp}^L = c_{k+1}^{L,0} + \frac{J_3 - J_4}{\Delta z} \Delta t, \quad (3a)$$

$$r_{imp} = \frac{c_{k,imp} - c^{L,e}}{c^{S,e} - c^{L,e}} \quad (3b)$$

with

$$J_1 = -D^S \frac{c_{k-1}^{S,0} - c_{k-2}^{S,0}}{\Delta z}, \quad J_2 = -D^S \frac{c_k^{S,0} - c_{k-1}^{S,0}}{0.5(1+r^0)\Delta z}, \quad J_3 = -D^L \frac{c_{k+1}^{L,0} - c_k^{L,0}}{0.5(2-r^0)\Delta z}, \quad J_4 = -D^L \frac{c_{k+2}^{L,0} - c_{k+1}^{L,0}}{\Delta z}, \quad (3c)$$

where superscript ‘0’ denotes the value in the previous time step. $c_{k,imp}$ in Eqs. (3a) and (3b) represent overall concentration of the k -cell that is a temporary S/L-cell at the moment. In the second step, depending on the evaluated value of r_{imp} , three situations are considered as follows.

(Case I) $0 \leq r_{imp} < 1$: the interface is still located within the k -cell at $t + \Delta t$.

When the interface stays within the k -cell during $t \sim (t + \Delta t)$, Eq. (3a)–(3c) ensure the solute balance condition with the updated values of overall concentration $c_{k,imp}$ and relative interface position r_{imp} in the S/L-cell. Hence, the values of current time step are simply given by

$$c_{k-1}^S(t + \Delta t) = c_{k-1,imp}^S, \quad c_k(t + \Delta t) = c_{k,imp}, \quad c_{k+1}^L(t + \Delta t) = c_{k+1,imp}^L, \quad (4a)$$

$$r(t + \Delta t) = r_{imp} \quad (4b)$$

(Case II) $r_{imp} \geq 1$: the interface moved into ($k + 1$)-cell.

Considering the status change of k -cell (S-cell at $t + \Delta t$) and ($k + 1$)-cell (S/L-cell at $t + \Delta t$), concentrations at $t + \Delta t$ are given as

$$c_{k-1}^S = c_{k-1,imp}^S, \quad c_k^S = c^{S,e}, \quad c_{k+1} = rc^{S,e} + (1-r)c^{L,e}. \quad (5a)$$

The relative interface position r in Eq. (5a) is for the new S/L-cell, i.e., ($k + 1$)-cell, and can be found from the following relation of solute conservation within the subsystem of “ k - and ($k + 1$)-cells”.

$$c_k^S + c_{k+1} = c_{k,imp} + c_{k+1,imp}^L$$

Substituting Eqs. (3a) and (5a) into the above equation and rearranging yields the relative interface position r in ($k + 1$)-cell at $t + \Delta t$ as

$$r(t + \Delta t) = \left(\frac{J_2 - J_4}{\Delta z} \Delta t - (c^{S,e} - c_k^0) + (c_{k+1}^{L,0} - c^{L,e}) \right) \frac{1}{(c^{S,e} - c^{L,e})}. \quad (5b)$$

(Case III) $r_{imp} < 0$: the interface moved into ($k-1$)-cell.

In this case, ($k-1$)-cell becomes the new S/L-cell at $t + \Delta t$. Following the same way as in case II, concentrations of the cells and the relative interface position r within ($k-1$)-cell can be obtained as

$$c_{k-1} = rc^{S,e} + (1-r)c^{L,e}, \quad c_k^L = c^{L,e}, \quad c_{k+1}^L = c_{k+1,imp}^L, \quad (6a)$$

$$r(t + \Delta t) = \left(\frac{J_1 - J_3}{\Delta z} \Delta t + (c_k^0 - c^{L,e}) + (c_{k-1}^{S,0} - c^{L,e}) \right) \frac{1}{(c^{S,e} - c^{L,e})}. \quad (6b)$$

The physical meaning of the above discretized equations can be explained. For example, while deriving Eq. (5b) in case II, we have an equation,

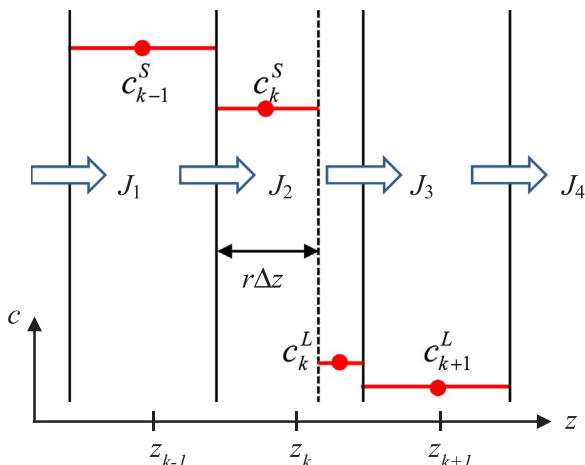


Fig. 1. Schematic illustration of discretized system around the moving interface (dashed line). Fluxes of Eq. (3c) are indicated in the S/L-cell and its two neighbor cells.

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