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LATTICE BOLTZMANN SIMULATIONS FOR ANISOTROPIC CRYSTAL GROWTH OF A BINARY MIXTURE

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ABSTRACT

Phase field models are powerful tools to simulate the interfaces evolution in glass melt solidification mechanism, including crystallization phenomena. The purpose of this work is the numerical implementation of a phase field model for solidification of a dilute binary mixture by using the Lattice Boltzmann equations. The proposed Boltzmann method is based on the BGK approximation for kinetic equations relative to the phase field, supersaturation and temperature. In order to simulate the anisotropic term in the phase field equation, the equilibrium distribution function is a modification of the one used in the standard method for the advection-diffusion equation. Simulations are carried out for anisotropic crystal growth for various thermal conditions, i.e., for several values of undercooling and different values of Lewis number.

KEY WORDS: Lattice Boltzmann method, Phase field model, anisotropic crystal growth, dilute binary mixture, computational methods, Thermodynamics.

1. INTRODUCTION

In the vitrification process of radioactive waste with the cold crucible technique, the high gradient of temperature imposed to the glass leads to the formation of a skull melter. In this area, the melted glass is frozen (high viscosity) and crystals of different compositions and different shapes appear. To understand this process dynamics we propose in this work a numerical method, based on the Lattice Boltzmann (LB) equation, for simulating a phase-field model of crystal growth. The phase-field theory is an approach for modeling the processes of solidification and crystallization by considering the interface between the solid phase and the liquid phase as a diffuse one. In a phase-field model, the interfacial conditions such as the Gibbs-Thomson condition and the equation of mass balance are replaced by one equation defined over the whole domain of computation. This equation describes the evolution of an order parameter which varies smoothly in the diffuse interface.

Although Lattice Boltzmann methods have been used to simulate crystal growth, they are primarily applied to hydrodynamic equations [8]. The solidification model implemented in [1] is based on an enthalpy-porosity approach [11] for a pure substance, and it is simulated by a LB method in [4]. Finally, in [9] the phase-field model of binary mixture is inspired from [7] and the LB equation is still applied for simulating the Navier-Stokes equations. In this work, we focus on a phase-field model applied to a dilute binary mixture [10]. For this model, the connections with its equivalent “sharp interface” model is well established [3]. For simplicity, a “symmetrical” model is considered, i.e., the thermal diffusivities and the diffusion coefficients are equal in

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solid and liquid. This assumption cancels the anti-trapping current [5] in the supersaturation equation. The anti-trapping current is needed for non-symmetrical models to avoid unphysical effects of the diffuse interface (e.g. anomalous trapping of solute). In section 2, the mathematical model will be presented and the physical meaning of each term will be reminded. Section 3 will detail the LB schemes for each equation. Simulations will be presented in section 4, and section 5 will conclude this paper.

2. MATHEMATICAL MODEL FOR A DILUTE MIXTURE

In this paper, based on the assumption that Péclet numbers for mass and heat transports are small, we consider only diffusion mechanisms.

The phase-field model is based on three coupled PDEs, the first one for modeling the phase-field ϕ , the second one for modeling the supersaturation U and the third one for modeling the dimensionless temperature θ . The equations are written as in [10]:

$$\tau(\mathbf{n})\frac{\partial\phi}{\partial t} = W_0^2\nabla\cdot(a_s^2(\mathbf{n})\nabla\phi) + W_0^2\nabla\cdot\mathcal{N} + (\phi - \phi^3) - \lambda(Mc_\infty U + \theta)(1 - \phi^2)^2, \quad (1)$$

$$\left(\frac{1+k}{2} - \frac{1-k}{2}\phi\right)\frac{\partial U}{\partial t} = D\nabla^2 U + [1 + (1-k)U]\frac{1}{2}\frac{\partial\phi}{\partial t}, \quad (2)$$

$$\frac{\partial\theta}{\partial t} = \kappa\nabla^2\theta + \frac{1}{2}\frac{\partial\phi}{\partial t}. \quad (3)$$

The interface position is calculated by equation (1) in which W_0 is the diffuse interface width, λ is the strength of coupling with U and θ , k is the partition coefficient, \mathbf{n} is the unit normal vector pointing from solid to liquid and defined by:

$$\mathbf{n} = -\frac{\nabla\phi}{|\nabla\phi|} \quad (4)$$

Anisotropy in the kinetics is incorporated as in [6] via the dependence of $\tau(\mathbf{n})$. This dependence is taken into account by a unique anisotropy function $a_s(\mathbf{n})$ with $\tau(\mathbf{n}) = \tau_0 a_s^2(\mathbf{n})$ where τ_0 is a characteristic time of the system and $a_s(\mathbf{n}) = 1 - 3\varepsilon_s + 4\varepsilon_s \sum_{\alpha=x,y} n_\alpha^4$, where ε_s is the anisotropy strength. The second term on the right-hand side in Eq. (1) is responsible for the anisotropic crystal growth of dendrite, where \mathcal{N} is defined by:

$$\mathcal{N}(\mathbf{x}, t) = |\nabla\phi|^2 a_s(\mathbf{n}) \left(\frac{\partial a_s(\mathbf{n})}{\partial(\partial_x\phi)}, \frac{\partial a_s(\mathbf{n})}{\partial(\partial_y\phi)} \right)^T. \quad (5)$$

In Eq. (1), M is a material-dependent coefficient involving the latent heat, specific heat, liquidus slope and partition coefficient, c_∞ is the concentration far from the interface and corresponds to the initial mixture concentration. The term $\phi - \phi^3$ is the derivative of the double-well potential with respect to ϕ . For this model, $\phi = +1$, $\phi = -1$ and $-1 < \phi < +1$ represent the solid phase, liquid phase and diffuse interface respectively.

In Eq. (2), supersaturation U represents a dimensionless normalized concentration defined by $U = 2 \times (c - c_0(\phi)) / (1 + k - (1 - k)\phi)\Delta c$ with $\Delta c = c_l^0(1 - k)$ and $c_0(\phi) = c_l^0 - \Delta c(1 + \phi)/2$ where c_l^0 is the equilibrium concentration in the liquid. D is the diffusion coefficient that is taken identical in the liquid and solid phases. Note that the term $(1 + k - (1 - k)\phi)$ before the time derivative of U can be interpreted as a linear interpolation of the concentration c in the diffuse zone by taking $\phi = +1$ in the solid, $\phi = -1$ in the

liquid and using the partition relation $c_s = kc_l$. The term $0.5 \times [1 + (1 - k)U] \partial\phi/\partial t$ is responsible for the rejection of excess solute that is not solidified at the interface.

In Eq. (3), κ is the thermal diffusivity. The dimensionless temperature θ is defined as: $\theta = C_p(T - T_M)/L$, where C_p is the specific heat, T_M is the melting temperature, and L is the latent heat. The physical meaning of the term $(1/2)\partial_t\phi$ is the release of latent heat at the interface.

We recall that the form of the phase field model comes from a variational calculation of the free energy functional $\mathcal{F} = \int dV \left[(W^2(\mathbf{n})/2) |\nabla\phi|^2 + f_{AB}(\phi, c, T) \right]$ where $W(\mathbf{n})$ is the width depending on the normal vector of the interface. This functional is defined by the sum of two terms. The first one is a gradient energy term and the second one is the bulk energy density of the binary mixture of A and B. The density energy $f_{AB}(\phi, c, T)$ is defined by:

$$f_{AB}(\phi, c, T) = f(\phi, T_M) + s(\phi)(T - T_M) + \frac{1}{\nu_0} RT_M (c \ln(c) - c) + e(\phi)c \quad (6)$$

The first term on the right-hand side of Eq. (6), is a double-well potential function $f(\phi, T_M) = -\phi^2/2 + \phi^4/4$ and, for this function, the positions of the two minima are $\phi = \pm 1$, i.e., if $\phi = +1$ the phase is solid and if $\phi = -1$ the phase is liquid. In the second term, $s(\phi)$ is an interpolation function of the entropy, the third term is the binary mixture entropy where R is the gas constant and ν_0 is the molar volume. Finally, in the last term, $e(\phi)$ is an interpolation function of the internal energy.

3. LATTICE BOLTZMANN METHOD

In this section, we present the Lattice Boltzmann (LB) method for solving the phase field model introduced in section 2. In order to establish the equilibrium distribution function relative to the phase field equation, the presentation is based on an analogy with the classical LB scheme for solving the following Advection-Diffusion Equation (ADE):

$$\frac{\partial u}{\partial t} = \nabla \cdot (D\nabla u) - \nabla \cdot (\mathbf{v}u) + Q. \quad (7)$$

In Eq. (7), $u(\mathbf{x}, t) \equiv u$, D is the diffusion coefficient, \mathbf{v} is the velocity and Q is the source term. We apply the following Lattice Boltzmann scheme ([12] for example) :

$$f_i^{Tr}(\mathbf{x} + \mathbf{e}_i\delta x, t + \delta t) = f_i^{Tr}(\mathbf{x}, t) + w_i Q(\mathbf{x}, t)\delta t - \frac{1}{\zeta_u} \left[f_i^{Tr}(\mathbf{x}, t) - f_i^{(0)Tr}(\mathbf{x}, t) \right] \quad (8)$$

where $f_i^{Tr}(\mathbf{x}, t)$ is the distribution function (the index Tr indicates the algorithm for solving the ADE), index i identifies the displacement directions: $i = 0, \dots, N$ where N is the total number of directions which depends on the lattice, \mathbf{e}_i is the displacement vector also depending on the lattice (see table 1), δx is the space-step, δt is the time-step and w_i are the lattice-dependent weights. The equilibrium distribution function $f_i^{(0)Tr}(\mathbf{x}, t)$ is defined by:

$$f_i^{(0)Tr}(\mathbf{x}, t) = w_i u(\mathbf{x}, t) \left(1 + \frac{1}{e^2} \mathbf{e}_i \cdot \mathbf{v}(\mathbf{x}, t) \frac{\delta t}{\delta x} \right). \quad (9)$$

Moments of zeroth-, first- and second-order of $f_i^{(0)Tr}$ are respectively $\sum_{i=0}^N f_i^{(0)Tr} = u$, $\sum_{i=0}^N f_i^{(0)Tr} \mathbf{e}_i = \mathbf{v}u\delta t/\delta x$ and $\sum_{i=0}^N f_i^{(0)Tr} \mathbf{e}_i \mathbf{e}_i = e^2 u \mathbf{I}$ where \mathbf{I} is the identity tensor of rank 2 and e^2 is a lattice-dependent coefficient which arises from the calculation of second-order moment. Values of e^2 and weights w_i are indicated

Table 1 Values of weights and value of e^2 for each lattice.

Lattices	N	w_0	$w_{1,\dots,4}$	$w_{5,\dots,8}$	e^2
$D2Q5$	4	$1/3$	$1/6$	—	$1/3$
$D2Q9$	8	$4/9$	$1/9$	$1/36$	$1/3$

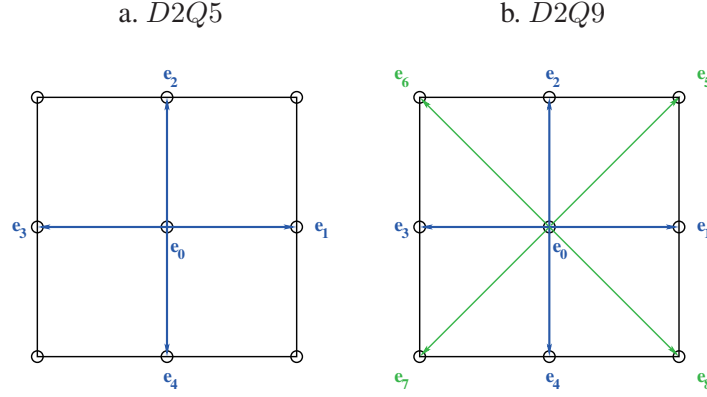


Fig. 1 Lattices of LB scheme.

in Table 1 for two lattices. The diffusion coefficient D is linked to the relaxation time ζ_u defined by:

$$\zeta_u = \frac{\delta t}{e^2 \delta x^2} D + \frac{1}{2}. \quad (10)$$

In this scheme, the ADE diffusive term, $\nabla \cdot (D \nabla u)$, is taken into consideration by the first term in brackets on the right-hand side of Eq. (9) while the advective term, $-\nabla \cdot (\mathbf{v}u)$ is taken into consideration by the second term. The presence of the function u in the diffusive terms and advective terms explains its presence in factor of Eq. (9).

3.1 Lattice Boltzmann scheme for phase field model

3.1.1 Phase field equation The phase field equation Eq. (1), presents some similarities with the ADE Eq. (7). In Eq. (1), the first term on the right-hand side is a diffusive term, the second one can be compared to an advective term without the explicit presence of ϕ in the divergence, and the last one is responsible for the coupling between ϕ , U and θ , and can be compared to a source term.

By following this analogy, the Lattice Boltzmann scheme applied to simulate the phase-field equation is based on the BGK collision as

$$\tau^*(\mathbf{n})g_i(\mathbf{x}+\mathbf{e}_i\delta x, t+\delta t) = g_i(\mathbf{x}, t) - (1-\tau^*(\mathbf{n}))g_i(\mathbf{x}+\mathbf{e}_i\delta x, t) - \frac{1}{\zeta_\phi(\mathbf{x}, t)} \left[g_i(\mathbf{x}, t) - g_i^{(0)}(\mathbf{x}, t) \right] + w_i Q_\phi(\mathbf{x}, t) \delta t, \quad (11)$$

with the equilibrium distribution function $g_i^{(0)}(\mathbf{x}, t)$ defined by:

$$g_i^{(0)}(\mathbf{x}, t) = w_i \left(\phi(\mathbf{x}, t) - \frac{1}{e^2} \mathbf{e}_i \cdot \mathcal{N}(\mathbf{x}, t) \frac{\delta t}{\delta x} \right). \quad (12)$$

where $\tau^*(\mathbf{n})$ is defined by $\tau^*(\mathbf{n}) = \tau(\mathbf{n})/W_0^2$. The function $Q_\phi(\mathbf{x}, t)$ that appears in Eq. (11) is assimilated to

the source term and is defined as follows:

$$Q_\phi(\mathbf{x}, t) = [(\phi - \lambda(Mc_\infty U + \theta)(1 - \phi^2))(1 - \phi^2)] / W_0^2. \quad (13)$$

The phase-field ϕ is calculated after the displacement stage and the update of boundary conditions by $\phi(\mathbf{x}, t) = \sum_{i=0}^N g_i(\mathbf{x}, t)$. The Lattice Boltzmann scheme for the phase-field equation differs from the standard LB method for Advection-Diffusion equation (ADE) on two points. The first difference is the presence in Eq. (11) of: (i) a factor $\tau^*(\mathbf{n})$ in front of $g_i(\mathbf{x} + \mathbf{e}_i \delta x, t + \delta t)$ in the left-hand side and, (ii) an additional term $(1 - \tau^*(\mathbf{n}))g_i(\mathbf{x} + \mathbf{e}_i \delta x, t)$ in the right-hand side. The latter term is non-local in space, i.e., it is involved in the collision step at time t and needs the knowledge of g_i at neighboring nodes $\mathbf{x} + \mathbf{e}_i \delta x$. Those two terms are involved to take into account the factor $\tau(\mathbf{n})$ in front of the time derivative $\partial\phi/\partial t$ in Eq. (1). We can see it by carrying out the stage of Taylor expansions for $g_i(\mathbf{x} + \mathbf{e}_i \delta x, t + \delta t)$ and $(1 - \tau^*(\mathbf{n}))g_i(\mathbf{x} + \mathbf{e}_i \delta x, t)$ in the Chapman-Enskog expansions. The method is inspired from [12].

The second difference with the LB algorithm for classical ADE, is the definition of the equilibrium distribution function $g_i^{(0)}$ Eq. (12). The absence of phase-field $\phi(\mathbf{x}, t)$ in the divergence term (1), explains its presence in the first term into brackets in Eq. (12) and not in front of the brackets. Moreover, note the sign change in front of the scalar product, corresponding to the sign change of the advective term for ADE to $+\nabla \cdot \mathcal{N}$ for the phase-field equation. Finally, the coefficient $a_s^2(\mathbf{n})$ plays a similar role as a «diffusion» coefficient in Eq. (1). This coefficient is a function of position and time (through \mathbf{n} depending on ϕ). The relaxation time $\zeta_\phi(\mathbf{x}, t)$ is a function of position and time and must be updated for each time step by the following relationship:

$$\zeta_\phi(\mathbf{x}, t) = \frac{\delta t}{e^2 \delta x^2} a_s^2(\mathbf{n}) + \frac{1}{2}. \quad (14)$$

Note that the scheme is fully explicit: all terms on the right-hand side of (11) as well as the factor $\tau^*(\mathbf{n})$ are defined at t .

3.1.2 Temperature equation Once the phase field ϕ is known at $t + \delta t$, it is used for the calculation of the temperature θ and supersaturation U . The LB algorithm for solving the heat equation Eq. (3) is the standard one for solving the diffusion equation. The LB scheme is written [2] as:

$$h_i(\mathbf{x} + \mathbf{e}_i \delta x, t + \delta t) = h_i(\mathbf{x}, t) - \frac{1}{\zeta_\theta} \left[h_i(\mathbf{x}, t) - h_i^{(0)}(\mathbf{x}, t) \right] + w_i S(\mathbf{x}, t) \delta t \quad (15)$$

with the equilibrium distribution function $h_i^{(0)}(\mathbf{x}, t) = w_i \theta(\mathbf{x}, t)$. By analogy with the ADE, note that because of the absence of the advective term in the heat equation Eq. (3), the equilibrium distribution function $h_i^{(0)}$ does not involve the second term (the one with the scalar product) contained in brackets in Eq. (9).

This remark can be demonstrated formally by carrying out the Chapman-Enskog expansions. Moments of zeroth-, first- and second-order of $h_i^{(0)}$ are respectively $\sum_{i=0}^N h_i^{(0)} = \theta$, $\sum_{i=0}^N h_i^{(0)} \mathbf{e}_i = \mathbf{0}$ and $\sum_{i=0}^N h_i^{(0)} \mathbf{e}_i \mathbf{e}_i = e^2 \overline{\theta \mathbf{I}}$. The coupling term with a phase field is given by :

$$S(\mathbf{x}, t) = \frac{1}{2} \frac{\partial \phi}{\partial t}(\mathbf{x}, t). \quad (16)$$

In this work, the time derivative is approximated by a central finite difference: $\frac{\partial \phi}{\partial t} \simeq \frac{\phi(t+\delta t) - \phi(t-\delta t)}{2\delta t}$. At the first time step, an explicit Euler scheme is used. As for the phase field, the temperature is calculated after the step of displacement (and update of boundary conditions) by $\theta(\mathbf{x}, t) = \sum_{i=0}^N h_i(\mathbf{x}, t)$. The thermal diffusivity

is considered as constant and identical for each phase. The relaxation time ζ_θ is constant during the time iterations. It is initialized before the time loop by the relationship $\zeta_\theta = \frac{\delta t}{e^2 \delta x^2} \kappa + \frac{1}{2}$.

3.1.3 Supersaturation equation In Eq. (2), the first term on the right-hand side is of diffusive type and the second one is responsible of coupling between ϕ and U . The latter one is comparable to the source term that will be noted $E(\mathbf{x}, t)$. We recall that the diffusion coefficient is the same in the liquid and solid phase. The Lattice Boltzmann scheme applied to simulate Eq. (2) is the following:

$$\eta f_i(\mathbf{x} + \mathbf{e}_i \delta \mathbf{x}, t + \delta t) = f_i(\mathbf{x}, t) - (1 - \eta) f_i(\mathbf{x} + \mathbf{e}_i \delta \mathbf{x}, t) - \frac{1}{\zeta_U} \left(f_i(\mathbf{x}, t) - f_i^{(0)}(\mathbf{x}, t) \right) + w_i E(\mathbf{x}, t) \delta t \quad (17)$$

where $f_i(\mathbf{x}, t)$ is the distribution function, $\eta = ((1 + k) - (1 - k)\phi) / 2$. The equilibrium distribution function is defined by $f_i^{(0)}(\mathbf{x}, t) = w_i U(\mathbf{x}, t)$. The supersaturation is calculated after the moving step and update boundary conditions by $U = \sum_{i=0}^N f_i(\mathbf{x}, t)$. The relaxation time ζ_U is given by the following relationship $\zeta_U = \frac{\delta t}{e^2 \delta x^2} D + \frac{1}{2}$.

4. VALIDATIONS AND SIMULATIONS

4.1 Validations with a finite difference code

In this section, we present the validation of the Lattice Boltzmann method by comparison with the results from a Finite Difference (FD) code in 2D. These validations are performed for a model of pure substances, i.e., a case for which the crystal and the surrounding glass matrix have the same composition. We solve both equations (1) and (3) respectively with the LBE and the FD method. For the latter, a centered scheme with the closest neighbors is used for the discretization of all differential operators. An explicit scheme of first order is also used for the time evolution. For the LBE method the D2Q9 lattice was used for the phase-field Eq. while the D2Q5 lattice was used for the temperature equation.

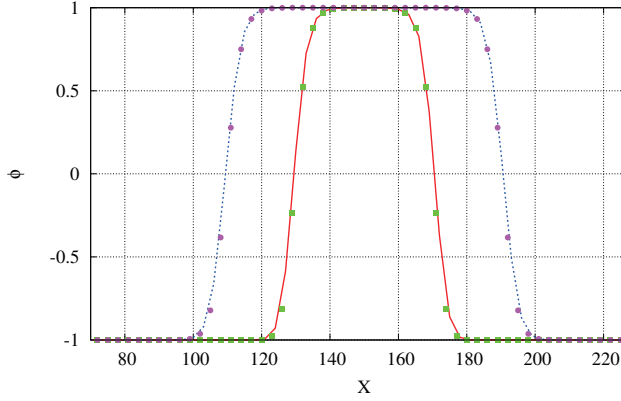
In the following validations, the computational domain is square and the boundary conditions are zero flux on each side of the domain. The mesh is composed of 301×301 nodes, the discretization step in space is $\delta x = \delta y = 0.01$. The interface width is chosen such as $W_0 = 2.5\delta x$, the coupling coefficient $\lambda = 12.5$ and the characteristic time is $\tau_0 = 4.89 \times 10^{-3}$ [10]. The time-step is chosen such as the relaxation parameter η_θ is not so close to 0.5. The initial condition for the phase-field equation is a diffuse sphere set in the center of the computational domain. For temperature, the initial value is $\theta_0 = -0.3$. Values of other parameters are indicated in Tab. 2. The results of comparisons are presented in Figure 2 at time $t = 10^3 \delta t$ and $t = 2 \times 10^4 \delta t$ for phase-field (Fig. 2a) and temperature (Fig. 2b).

In comparison to the standard numerical methods, the main advantages of the LBE are well-known: easy implementation of algorithm (collision and streaming steps) and easy implementation of boundary conditions (bounce back). The method can also be extended for the fluid flows simulations by modifying the equilibrium distribution function. The main drawback of this method is the lost of local character of collision to take into account the parameter $\tau(\mathbf{n})$ and the function η . Moreover this collision is unstable for several values of the partition coefficient k . The development of a more stable method is currently in progress.

4.2 Sensitivity to undercooling

In the following simulations, the D2Q9 lattice was used for the supersaturation equation. The computational domain and the boundary are the same as those used in the previous subsection 4.1. The time-step is chosen such as the relaxation parameter η_U is not close to 0.5. The initial condition for supersaturation is a constant

a. Profiles of phase-field at $t = 10^3\delta t$ and $t = 2 \times 10^4\delta t$



b. Temperature isovalues

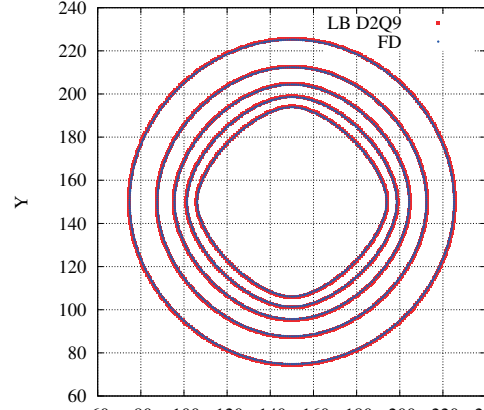


Fig. 2 Validations of the LB method with the finite difference method. (a) x -profiles at $t = 10^3\delta t$ and $t = 2 \times 10^4\delta t$. (b) Temperature isovalues at $2 \times 10^4\delta t$.

Table 2 Parameters of simulations

Physical parameters				Numerical parameters			
Symbol	Parameter	Dim	Data	Symbol	Parameter	Dim	Data
D	diffusion coefficient	$[L]^2/[T]$	0.4	N_x	total number of nodes x	$[-]$	301
κ	thermal diffusivity	$[L]^2/[T]$	0.4	N_y	total number of nodes y	$[-]$	301
k	partition coefficient	$[-]$	0.8	$\delta x = \delta y$	space step	$[L]$	0.01
Mc_∞	slope of liquidus	$[-]$	0.1	N_t	total number of time steps	$[-]$	10^5
ε_s	strength of anisotropy	$[-]$	0.05	δt	time step	$[T]$	10^{-5}
λ	strength of coupling	$[-]$	12.5				
τ_0	relaxation time	$[T]$	4.89×10^{-3}				
W_0	diffuse interface width	$[L]$	0.025				

value: $U_0 = 0$. Values of other parameters are indicated in Tab. 2. For these parameters, the phase-field evolution is presented in Fig. 3a. In this first simulation, the initial value of temperature is $\theta_0 = -0.35$, the values of diffusion coefficient D and thermal diffusivity κ are equal to 0.4, corresponding to a Lewis number equal to 1, with the Lewis number defined as the ratio between the thermal diffusivity and the diffusion coefficient: $Le = \kappa/D$.

We keep the same value of the Lewis number and we now test the sensitivity of the results with the undercooling. The undercooling is defined by $C_p(T_m - T_0)/L$ which is equivalent to a negative dimensionless temperature θ_0 . In Fig. 3b, we can see the effect of three initial values of θ_0 (-0.27 , -0.30 and -0.35) on the shape of phase-field at $t = 0.5$. When the initial temperature is far from the melting temperature, the crystal grows faster. Indeed, in that situation, the latent heat released at the interface during the solidification process can be evacuated more quickly inside the liquid phase, involving a faster growth of the crystal.

4.3 Lewis number effect

In order to test the sensitivity to the Lewis number, the diffusion coefficient D was kept constant ($D = 0.4$) and two values of the thermal diffusivity κ were chosen: $\kappa = 0.4$ and 2, corresponding to a Lewis number equal to 1 and 5 respectively. The initial temperature is $\theta_0 = -0.30$. For both values of the Lewis number, the fields of concentration (C), dimensionless temperature (T), phase-field (P) and supersaturation (U) are presented in Fig. 4 at $t = 0.3$. The model is adapted to a solidification process of a binary mixture with a solid concentration that is lower than the liquid one. As expected, we remark that the concentration is higher near the interface

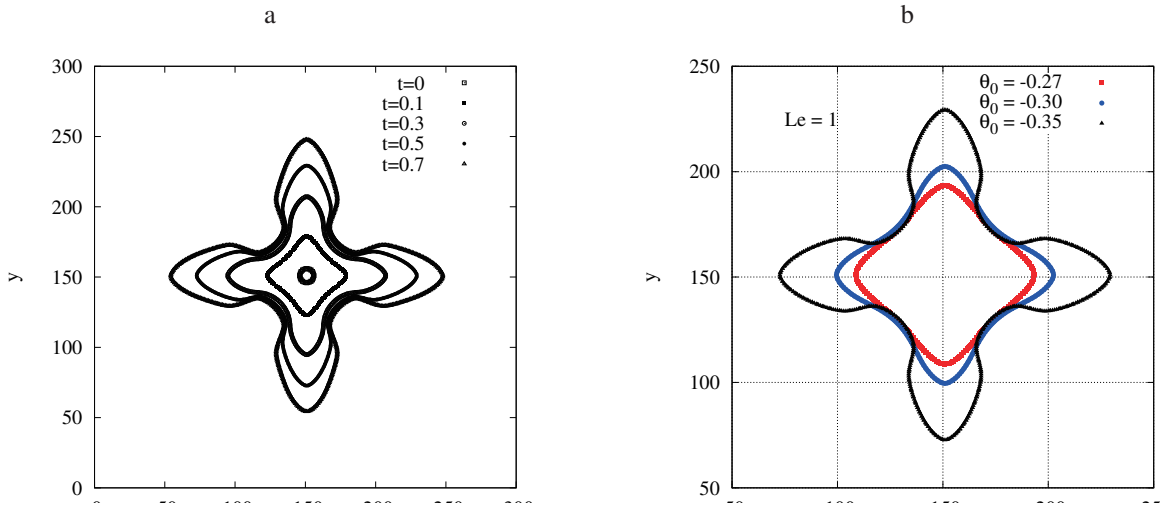


Fig. 3 Iso-values $\phi = 0$ of phase-field for $Le = 1$. (a) Evolution for $\theta_0 = -0.35$; (b) undercooling effect for $\theta_0 = -0.27$ (red), $\theta_0 = -0.30$ (blue) and $\theta_0 = -0.35$ (black) at $t = 0.5$.

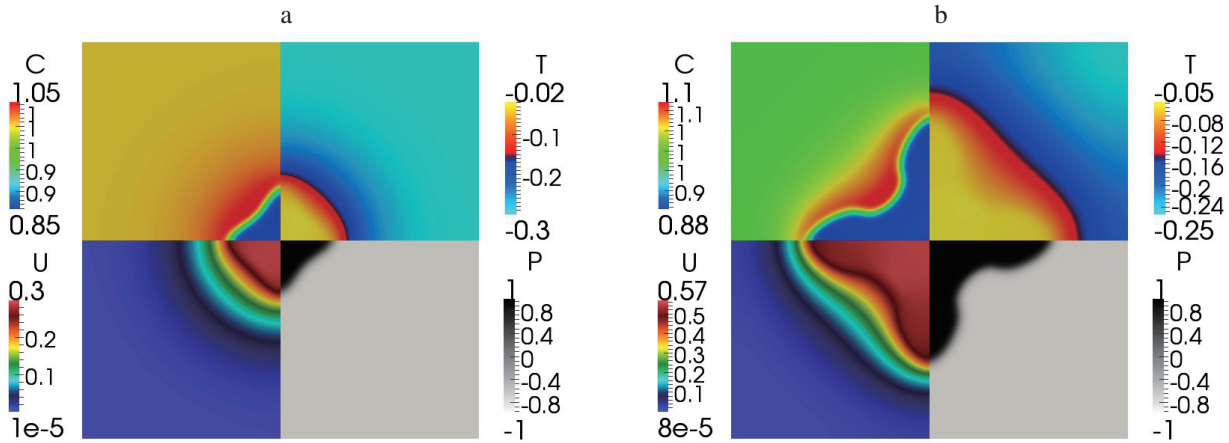


Fig. 4 Fields of concentration (C), temperature (T), supersaturation (U) and phase-field (P) at $t = 0.3$ for $\theta_0 = -0.30$, (a) $Le = 1$ and (b) $Le = 5$.

because here the concentration in excess is rejected outside the solid phase. Finally, the comparison of results for both values of Lewis number $Le = 1$ and $Le = 5$ (Figs. 4a and 4b respectively) shows that a higher Lewis number involves a faster crystal growth. The physical mechanism is the same as the one involved in the previous simulations. The higher thermal diffusivity allows for the latent heat released at the interface to diffuse more quickly inside the liquid phase.

5. CONCLUSION AND PERSPECTIVES

In this study, a Lattice Boltzmann method has been developed for the simulation of a phase field model with thin interface limit. This model is well adapted to simulate the crystal growth of a dilute binary mixture with coupled heat and solute diffusion. For this purpose, a new equilibrium distribution function is established for solving the phase field equation compared to the standard method for advection-diffusion equation. It was also necessary to modify the collision steps in the equations of phase field and supersaturation to take into account the terms in front of the time derivative.

Several sensitivity simulations to model parameters were performed which showed their impact on the crystal

structure obtained. We chose to show the effects of the initial temperature and the Lewis number. It was observed that a lower initial temperature involves a faster growth of the crystal structure. Comparing two simulations performed by increasing the Lewis number value from $Le = 1$ to $Le = 5$, we observed that increasing the Lewis number has the effect of increasing the growth velocity of the crystal structure.

Two main perspectives are expected to pursue this work. The first one is to study the case where the partition coefficient k is less than 0.6 because, for these values, the algorithm presented instabilities and the second one is to add the antitrapping term in the solute conservation equation.

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REFERENCES

- [1] Chatterjee, D. and Chakraborty, S., "A hybrid lattice boltzmann model for solid-liquid phase transition in presence of fluid flow," *Physics Letters A*, 351, pp. 359–367, (2006).
- [2] Dawson, S. P., Chen, S., and Doolen, G., "Lattice boltzmann computations for reaction-diffusion equations," *Journal of Chemical Physics*, 98(2), pp. 1514–1523, (1993).
- [3] Echebarria, B., Folch, R., Karma, A., and Plapp, M., "Quantitative phase-field model of alloy solidification," *Physical Review E*, 70(061604), pp. 1–22, (2004).
- [4] Jiaung, W.-S., Ho, J.-R., and Kuo, C.-P., "Lattice boltzmann method for the heat conduction problem with phase change," *Numerical Heat Transfer*, 39, pp. 167–187, (2001).
- [5] Karma, A., "Phase-field formulation for quantitative modeling of alloy solidification," *Physical Review Letters*, 87(11), pp. 1–4, (2001).
- [6] Karma, A. and Rappel, W.-J., "Quantitative phase-field modeling of dendritic growth in two and three dimensions," *Physical Review E*, 57(4), pp. 4323–4349, (1998).
- [7] Kim, S. G., Kim, W. T., and Suzuki, T., "Phase-field model for binary alloys," *Physical Review E*, 60(6), pp. 7186–7197, (1999).
- [8] Medvedev, D. and Kassner, K., "Lattice boltzmann scheme for crystal growth in external flows," *Physical Review E*, 72(056703), pp. 1–10, (2005).
- [9] Miller, W., Rasin, I., and Succi, S., "Lattice boltzmann phase-field modelling of binary-alloy solidification," *Physica A*, 362, pp. 78–83, (2006).
- [10] Ramirez, J. C., Beckermann, C., Karma, A., and Diepers, H.-J., "Phase-field modeling of binary alloy solidification with coupled heat and solute diffusion," *Physical Review E*, 69(051607), pp. 1–16, (2004).
- [11] Voller, V., Cross, M., and Markatos, N., "An enthalpy method for convection/diffusion phase change," *International Journal for Numerical Methods in Engineering*, 24, pp. 271–284, (1987).
- [12] Walsh, S. and Saar, M., "Macroscale lattice-boltzmann methods for low peclet number solute and heat transport in heterogeneous porous media," *Water Resources Research*, 46(W07517), pp. 1–15, (2010).