Application of multi-phase-field lattice Boltzmann method to semi-solid deformation

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Abstract. Mechanisms of semi-solid deformation are crucial for reducing solidification defects. In this study, a multi-phase-field lattice Boltzmann (MPF-LB) model, which can simulate growth of multiple dendrites with liquid flow, solid motion and collision, is applied to semi-solid deformation. An elastic contact is introduced to the MPF-LB model to consider collision of two grains. The semi-solid deformation with globular morphology is simulated in the two-dimension by the MPF-LB method. Through the simulations, high potential of the MPF-LB model as the evaluation method of semi-solid deformation is confirmed.

1. Introduction
In the casting process, semi-solid deformation causes serious solidification defects, such as porosity, cracking and macrosegregation [1]. To reduce these defects, it is crucial to elucidate the mechanisms of semi-solid deformation. However, it is very difficult because semi-solid deformation, aside from being a high-temperature and opaque phenomena, is a very complicated multi physics problem including solid-liquid phase transformation, liquid flow, solid motion, solid-solid interaction, solid deformation, and so on.

Owing to recent in-situ observations using synchrotron X-ray radiography, detailed phenomena and mechanisms in semi-solid deformations are gradually being unveiled. It was reported that, for globular materials, rearrangement by translation and rotation of solid grains is a dominant deformation in a wide range of solid fractions, fS (fS < 0.8) [2-5]. Meanwhile, for globular materials with a high fS (fS > 0.9) and for equiaxed dendritic morphology [2, 6], deformations of the solid have been observed in addition to the rearrangement of grains. In both solid morphologies, the grain rearrangement causes a dilation which has the greatest effect on producing defects. Indentation experiments of semi-solid materials have also shown transgranular liquation cracking [7] and plastic deformation [8] which results in grain refinement.

Modeling and simulation studies are indispensable for a better understanding of semi-solid deformation under various conditions [9]. The finite element method is a powerful tool to simulate the macroscopic mechanical behavior of a semi-solid material [10, 11], where information on the microstructure is not considered nor introduced through constitutive equations [12]. Finite element simulations have also been conducted for dendritic solid [13] and equiaxed globular grain structures [14]. Moreover, deformation simulations during dendrite growth with an external force have been performed using the phase-field method [15]. However, the liquid flow is not computed in the above simulations. Flow of intergranular liquid has been simulated by a granular model [16, 17]. For globular
materials in a range where solids can be considered as a rigid body, a discrete element method was used and could successfully capture some phenomena observed during in-situ observations [18].

As mentioned above, some models succeeded in expressing specific phenomena in semi-solid deformation. However, there is currently no model which can express all phenomena occurred in semi-solid deformation: solid-liquid phase transformation, liquid flow, solid motion, solid-solid interaction, solid deformation, fragmentation of solid and so on. In our previous study [19], we have developed a multi-phase-field lattice Boltzmann (MPF-LB) model which can simulate the growth of multiple dendrites with motion, liquid flow, collision, and coalescence and subsequent grain growth by extending a single-dendrite growth model with motion [20-22]. The model would have great potential to simulate semi-solid deformation. In this study, as a first step of our phase-field study on semi-solid deformation, the MPF-LB model [19] is applied to the semi-solid deformation of a globular material, and the suitability of the MPF-LB model as an evaluation method of semi-solid deformation is investigated.

2. Model

In the MPF-LB model developed in [19], dendrite growth and grain growth after coalescence of multiple grains are expressed by MPF method, liquid flow is computed by LB method, and motion of solids is expressed by solving equations of motion of solids assumed to be a rigid body. Also, a perfectly inelastic collision is assumed for simplicity, when two solids collide with each other. In this study, an elastic collision is introduced in a contact problem of two grains. In addition, the coalescence of grains is not considered, because usually the solid-solid interface energy is larger than twice that of the solid-liquid interface energy [23] and an isothermal condition maintaining a semi-solid condition is assumed in the following simulations.

Multiple grains are expressed by multiple phase-field variables, where phase-field variable \( \phi \) is defined as \( \phi = +1 \) in the \( i \)-th grain and \( \phi = -1 \) in the others. The time evolution of \( \phi \) is expressed by [24]

\[
\tau(\theta) \left( \frac{\partial \phi}{\partial t} + U_s \nabla \phi \right) = \nabla \left( W(\theta) \nabla \phi \right) - \frac{\partial}{\partial x} \left( W(\theta) \frac{dW(\theta)}{d\theta} \frac{\partial \phi_i}{\partial x} \right)
+ \frac{\partial}{\partial y} \left( W(\theta) \frac{dW(\theta)}{d\theta} \frac{\partial \phi_i}{\partial y} \right) - \left( \frac{\phi_i}{+\phi_i} \right)^3 - \lambda^* (1-\phi_i^3)^2 u
\]

where \( \tau(\theta) \) and \( W(\theta) \) are the phase-field relaxation time and interface thickness, respectively, having anisotropy as \( \tau(\theta) = \tau_{\text{an}}(\theta)^2 \) and \( W(\theta) = W_{\text{an}}(\theta) \), where \( \theta \) is the crystal orientation, \( \tau_{\text{an}}(\theta) \) is the anisotropy function with a form of \( \tau_{\text{an}}(\theta) = 1 + \epsilon \cos(4\theta) \), and \( \epsilon \) is the anisotropy strength. \( \lambda^* \) is a coefficient regarding thermodynamic driving force, and \( U_s \) is the velocity vector of the grain.

The advection-diffusion equation of solute can be expressed as

\[
\frac{1}{2} \left[ 1 + k - (1-k)h(\phi) \right] \left( \frac{\partial u}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = \nabla \left[ D_s q(\phi) \nabla u - \mathbf{J}_{\text{sr}} \right] + \frac{1}{2} \left[ 1 + (1-k)u \right] \frac{\partial h(\phi)}{\partial t} - \nabla \cdot \mathbf{J}
\]

where \( \phi \) is the sum total of phase-field variables expressing the solid, \( C_l \) is the solute concentration in the liquid, \( u = (C_l - C^s)/(C_l^s - C^s) \) is the dimensionless supersaturation, \( C_l \) is the solute concentration in the solid, \( C_l^s \) is the equilibrium concentration in the liquid, \( C_s^s \) is the equilibrium concentration in the solid, \( k = C_s/C_l = C_s^s/C_l^s \) is the partition coefficient, \( q(\phi) = [kD_s + D_l + (kD_s - D_l)\phi]/(2D_l) \), \( D_l \) is the diffusivity of the solute in the liquid, \( D_s \) is the diffusivity of the solute in the solid, \( \nabla \mathbf{J} \) is the noise term [25], and \( \mathbf{J}_{\text{sr}} \) is the anti-trapping current term [24].
The LB equations can be expressed by [20]

\[
f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) - \frac{1}{\tau_{\text{LBM}}} \left[ f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t) \right] + \rho \omega_i \left[ \frac{3(c_i - \mathbf{U})}{c_i^2} + \frac{9(c_i \cdot \mathbf{U})c_i}{c_i^4} \right] \cdot \mathbf{G} \Delta t \tag{3}
\]

where \( f_i \) is the particle velocity distribution in the \( k \)-th direction, \( f_i^{eq} \) is the equilibrium distribution function, \( c_i \) is the discrete particle velocity vector, \( \Delta t \) is the time increment, \( \tau_{\text{LBM}} \) is the LB relaxation time, \( \rho = \sum q f_i \) is the liquid density, \( \mathbf{U} \) is the liquid velocity vector computed by \( \rho \mathbf{U} = \sum q \mathbf{c}_i f_i \). \( Q \) is the number of discrete velocities, \( w_i \) is the weight function, \( \mathbf{G} = -2 \rho \mathbf{h}/W_0 ((1 + \phi)/2)^2 (\mathbf{U} - \mathbf{U}_i) \) is the dissipative drag force vector, \( \nu = (\eta_{\text{LBM}} - 0.5) \Delta x^2/(3 \Delta t) \) is the dynamic viscosity, and \( h = 2.757 \) [26].

The velocity of \( i \)-th rigid body grain, \( \mathbf{U}_{is} \), is computed as the sum of the translational velocity \( \mathbf{U}_i \), and the rotational velocity \( \omega_i \), as \( \mathbf{U}_{is}(\mathbf{x}, t) = \mathbf{U}_i + \omega_i \times (\mathbf{x} - \mathbf{X}_i) \), where \( \mathbf{X}_i \) is the centroid position of the \( i \)-th grain. \( \mathbf{U}_i \) and \( \omega_i \) are computed by the equations of motion:

\[
M_i \frac{d\mathbf{U}_i}{dt} = \mathbf{F}_i, \quad I_i \frac{d\omega_i}{dt} = \mathbf{T}_i \tag{4}
\]

Here, \( M_i \) is the mass and \( I_i \) is the moment of inertia. The total force, \( \mathbf{F}_i \), and the total torque, \( \mathbf{T}_i \), acting on the \( i \)-th grain are expressed by

\[
\mathbf{F}_i = -\sum_{\omega \in \xi} \{ \mathbf{G}(\mathbf{x}, t) + \mathbf{F}_{ci} \} \Delta V, \quad \mathbf{T}_i = -\sum_{\omega \in \xi} \left[ (\mathbf{x} - \mathbf{X}_i) \times (\mathbf{G}(\mathbf{x}, t) + \mathbf{F}_{ci}) \right] \Delta V \tag{5}
\]

where \( \Omega_i \) is the solid-liquid interface domain of the \( i \)-th grain and \( \Delta V = \Delta x^2 \). \( \mathbf{F}_{ci} \) is the collision force acting on the \( i \)-th grain by contact with the \( j \)-th grain. Here, an elastic contact model [27] is introduced and \( \mathbf{F}_{ci} \) is expressed by

\[
\mathbf{F}_{ci} = \sum_{j=1}^{n} k_n p_i^2 p_j^2 \mathbf{n}_y \tag{6}
\]

where \( p_i = (\phi_i + 1)/2, k_n \) is a coefficient related to normal spring constant, \( n \) is the number of non-zero phase-field variables on a grid point, and \( \mathbf{n}_y \) is the unit normal vector expressed by \( \mathbf{n}_y = \nabla(p_i - p_0)/|\nabla(p_i - p_0)| \). The overlap distance between the \( i \)-th and \( j \)-th grains is represented by the overlap of diffuse interface, \( p_i^2 p_j^2 \).

**Table 1. Material and simulation parameters.**

| Quality            | Symbol | Value                        |
|--------------------|--------|------------------------------|
| Initial concentration | \( c_0 \) | 0.01296 at.frac.            |
| Grid size          | \( \Delta x \) | 1.0 \( \mu \)m              |
| Interface thickness | \( W_0 \) | \( \Delta x/0.4 = 2.5 \) \( \mu \)m |
| Diffusion coefficient in liquid | \( D_l \) | 3.0\times\times10^{-9} m^2/s |
| Diffusion coefficient in solid | \( D_s \) | 3.0\times\times10^{-13} m^2/s |
| Partition coefficient | \( k \) | 0.14                         |
| Anisotropic strength | \( \varepsilon_4 \) | 0.02                        |
| Gibbs-Thomson constant | \( \Gamma \) | 2.4\times\times10^{7} Km     |
| Liquidus slope     | \( m \) | -620 K/at.frac.             |
| Temperature        | \( T_0 \) | 923.6 K (\( u_0 = -0.20 \)) |
|                    |        | 921.0 K (\( u_0 = -0.40 \)) |
|                    |        | 916.7 K (\( u_0 = -0.60 \)) |
| Time increment     | \( \Delta t \) | 6.667\times\times10^{-5} s |
| LB relaxation time | \( \tau_{\text{LBM}} \) | 1                           |
3. Computational conditions

The MPF-LB method shown in the previous section is applied to an isothermal shear deformation of semi-solid Al-3wt%Cu alloy with globular morphology [3, 18, 28]. Table 1 shows material and simulation parameters. Figure 1 shows the computational and initial conditions for the solidification simulations to prepare the globular morphology. The square computational domain is divided into 1024 × 1024 grid points with grid size \( \Delta x = 1 \mu m \). The wall and push plate are expressed by the 0-th phase-field variable \( \phi_0 \), where the interface between the wall and push plate and liquid phase is formed by one-dimensional equilibrium phase-field profile of \( \phi_0 = \tanh(r/(2^{0.5}W_0)) \). The diffusion coefficient \( D_s \) in the wall and push plate is set to zero. At the initial condition shown in figure 1, a nondimensional supersaturation \( u_0 \) is set to \( u_0 = -0.2 \), \( -0.4 \) and \( -0.6 \), and 120 solid seeds are placed in an equilateral triangular array. To prepare the semi-solid mixture with globular morphology, solidification simulations are performed until a quasi-equilibrium state is achieved from the initial condition shown in figure 1. Figure 2 is the computed semi-solid systems with globular morphology. The regular hexagonal array of globular solids is observed except neighboring walls. The solid fractions \( f_s \) for figure 2 are \( f_s = (a) \ 0.274 \), \( (b) \ 0.458 \) and \( (c) \ 0.634 \), respectively. These values are slightly larger than the equilibrium values for \( u_0 \), because there is the walls and push plate. From those conditions, the push plate is pushed into the semi-solid mixture with a constant velocity of \( U_{\text{plate}} = 6 \mu m/s \); then the right-hand side of equation (1) is set to zero only for \( \phi_0 \). The coefficient representing spring constant is fixed to be \( k_n = 0.0437 \text{ N/mm}^3 \).

Figure 1. Computational and initial conditions. Black, blue and light blue regions are the wall and push plate (\( \phi_0 > -1 \)), solid and liquid, respectively. Number of solid seeds is set to 120.

Figure 2. Computed semi-solid structures with globular morphology for \( u_0 = (a) \ -0.2 \ (f_s = 0.274) \), \( (b) \ -0.4 \ (f_s = 0.458) \) and \( (c) \ -0.6 \ (f_s = 0.634) \).
Figure 3. Time slices during semi-solid deformation for $u_0 = -0.2$ ($f_s \approx 0.30$).

Figure 4. Time slices during semi-solid deformation for $u_0 = -0.4$ ($f_s \approx 0.45$).

Figure 5. Time slices during semi-solid deformation for $u_0 = -0.6$ ($f_s \approx 0.65$).

4. Results
Figures 3-5 are the time slices during semi-solid deformation by push plate from the structures shown in figure 2. Solid-liquid interfaces are indicated by the black lines with $\sum p_i^2 < 0.85$, and the liquid and solid velocities are expressed by red arrows, of which the length shows the magnitude of velocity. The displacement of the top surface of the push plate are (a) 80 µm, (b) 160 µm, (c) 240 µm, and (d) 320 µm in figures 3-5. Depending on the solid fractions $f_s$, different rearrangement of solids and velocity patterns are observed.

In figure 3 ($f_s \approx 0.30$), a fan-shaped flow pattern is formed ahead of the push plate and maintained during the simulation. The flow pattern is quite similar to the one observed in in-situ observations [3, 28]. Due to the right upward flow on the push plate, bands of liquid and dense grain are alternatively formed toward the 45° direction after (b) $4 \times 10^5$th step, which result in the formation of dilatancy.

In figure 4 ($f_s \approx 0.45$), similar behavior to figure 3 can be observed in the early stage of figures 4(a)-(b). However, latter stages in figures 4(c)-(d) show different deformation patterns, where the
longitudinal force ahead of the push plate is supported by a line of solids in the left side. Due to being pushed upward, some grains located on the top side migrate to the right as shown in figures 4(d).

In figure 5 ($f_s \approx 0.65$), deformation occurred as in a metal solid, where atoms are arranged in a regular pattern. In figure 5(a), the pink dashed line indicates the firstly activated slip surface, where the slip on the surface occurred until around the $1.7 \times 10^5$th step. At the step in figure 5(a), slip occurred on the surface indicated by the yellow dashed line. The deformation in figure 5(b) is similar to that in figure 4(d). Meanwhile, due to more dense solid grains, the upward forces are applied overall in front of the push plate compared to figure 4(d). In figure 5(c), grain A was pushed out to the right from the longitudinal solid line on the left. Then, since grain A pushed the other surrounding grains, the grain array drastically changed in the deformation from figure 5(b) to figure 5(c). In figure 5(d), grain B was also pushed out from the left line to the right. The pushing out of grains A and B displaced grain C to the right, into the right solid line.

As shown in figures 3-5, it was confirmed that the semi-solid deformation in the small solid fraction (figure 3) behaves like liquid flow, where the rearrangement of grains is the dominant deformation mechanism, while that in the large solid fraction (figure 5) behaves like a solid deformation, where the solid interaction is the dominant deformation mechanism. In the intermediate condition (figure 4), both deformation behaviors could be observed. In the small solid fraction, the semi-solid deformation is very similar to that observed in the experimental observations [3, 28] and discrete element simulation [18]. In the high solid fraction, plastic deformation of a grain would occur in a real situation. The introduction of the plastic deformation in grains is future work. Also, shrinkage of grains (e.g. a grain indicated by the black arrow in figure 3(d)) and morphological changes of grains due to solidification/melting and liquid flow were observed in figures 3-5. This is another advantage of the present MPF-LB model. On the other hand, mechanical interaction between grains expressed by equation (6) is too strong; thus, liquid phase is always left between grain boundaries. This problem should be solved in next study.

5. Conclusions
The MPF-LB model, which can simulate growth of multiple dendrites with motion and liquid flow, was applied to semi-solid deformation with globular morphology. Here, the coalescence of grains was not considered and an elastic contact model was introduced to the MPF-LB model. By using the model, the simulations of semi-solid deformation by push plate were performed for three different solid fractions. It was observed that, in the small solid fraction, the rearrangement of grains due to the liquid flow was the dominant deformation mechanism, and, in the high solid fraction, solid-solid interaction was the dominant deformation mechanism and it caused the rearrangement of grains. From the results, it was confirmed that the MPF-LB model has high potential as an evaluation model of semi-solid deformation.

In future work, the contact model in a diffuse interface will be improved and the plastic deformation in grains will be considered. Three-dimensional simulations are also expected, though the computational cost is high [29-32].

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