A review on the modeling and simulations of solid-state diffusional phase transformations in metals and alloys

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Abstract. Solid-state diffusional phase transformations are vital approaches for controlling of the material microstructure and thus tailoring the properties of metals and alloys. To exploit this mean to a full extent, much effort is paid on the reliable and efficient modeling and simulation of the phase transformations. This work gives an overview of the developments in theoretical research of solid-state diffusional phase transformations and the current status of various numerical simulation techniques such as empirical and analytical models, phase field, cellular automaton methods, Monte Carlo models and molecular dynamics methods. In terms of underlying assumptions, physical relevance, implementation and computational efficiency for the simulation of phase transformations, the advantages and disadvantages of each numerical technique are discussed. Finally, trends or future directions of the quantitative simulation of solid-state diffusional phase transformation are provided.

Keywords: Solid-state diffusional phase transformation / numerical simulation / empirical and analytical models / phase-field models / cellular automata / Monte Carlo models / molecular dynamics methods

1 Introduction

Mechanical and functional properties of materials such as metals and alloys are largely dependent on their microstructure characteristics which include specific volume fraction of spatially distributed phases with different compositions and/or crystal structures, the size and morphology of grains with different orientations and their spatial distribution [1,2]. Due to solid-state diffusional phase transformation, which involves nucleation, growth and impingement, directly results in the arrangements of constituent phases with different grains size and morphology, it plays an important role in the production of materials with various microstructures [3]. For better control over the material microstructures and thus tailor the properties of metals and alloys, comprehensively understanding and manipulating the process of solid-state diffusional phase transformations are vital and necessary. However, during the phase transformations process, the microstructure evolution is extremely complex and nonlinear in nature because it is affected by heterogeneous grains size of parent phase, asynchronous transformation in different grains at different times, crystallographic anisotropy, thermodynamics, kinetics, and other factors [4]. Therefore, the numerical simulation techniques that can

compensate for restrictions of experimental conditions and dynamically reconstruct microstructure evolution are increasingly attractive.

At present, the most advanced numerical simulation methods include empirical and analytical models [5–7], phase field models [8,9], cellular automaton models [10–12], Monte Carlo models [13] and molecular dynamics methods [14]. Empirically-based model, which is developed on the basis of the classical Johnson-Mehl-Avrami-Kolmogorov (JMAK) theory, plays a key role in simulation and prediction of transformations including recrystallization and phase transformation where nucleation, growth and impingement mechanisms operate [15]. Different from empirically-based model, analytical model is developed on the classical physics and phenomenological theory. In general, empirical and analytical models focus more on providing average information such as the average grain size and phase volume fraction of microstructure evolution in macroscale. By contrast, mesoscopic models including phase field models, cellular automaton and Monte Carlo models can reconstruct the evolution of grain morphology and spatial distribution, solute concentration field in addition to giving macroscopic average information [16]. The phase-field method has become an important and extremely versatile technique for simulating solidification, precipitate growth, coarsening, grain growth, martensitic transformations, dislocation dynamics, crack propagation and so on. However, the large

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Fig. 2. Planar interface migration and solution partitioning of a binary A–B alloy with initial concentration for component B [26].

interface migration. If the concentration of component B in parent phase and new phase are $X^{\beta,eq}$ and $X^{\alpha,eq}$ near the interface, respectively, the kinetics of the transformation is controlled by diffusion. Actually, the phase transformation is of the mixed-mode character, the concentration of component B in β -phase at the interface is greater than $X^{\beta,eq}$ and less than X_0 (Fig. 2).

Following Hillert [32], the driving force for the phase transformation is equal to the change of Gibbs energy in the system before and after transformation. The change of Gibbs energy for forming per mole of α phase (Fig. 3) is

$$F_{chem} = (1 - X^{\alpha,eq}) + X^{\alpha,eq}(\mu_B^\beta - \mu_B^\alpha). \quad (1)$$

The Gibbs energy is available for (a) the trans-interface diffusion (F_{chem}^m) which means the diffusion of solute in interface, (b) the diffusion of solute in parent phase near the interface and the change in lattice (F_{chem}^t). The driving force for trans-interface diffusion is proportional to $\mu_B^\beta - \mu_B^\alpha$ [33].

Svoboda [21] et al. assumed that the interface was negligibly thin relative to the grain size, and the diffusion coefficients of solute in interface were slightly larger than those in parent phase. Therefore, the diffusive fluxes in interface were supposed as practically same as in parent phase near the interface. There is no reason to expect any discontinuity of chemical potential of the solute across the interface. Thus, in the approximation of the sharp interface,

$$\mu_A^\alpha \neq \mu_A^\beta, \mu_B^\alpha = \mu_B^\beta.$$

As a consequence,

$$F_{chem}^t = 0, F_{chem} = F_{chem}^m = (1 - X^{\alpha,eq})(\mu_A^\beta - \mu_A^\alpha) \quad (3)$$

In Figure 3, it can be found that the driving force F_{chem} (F_{chem}^m) reaches the maximum as the concentration X_{int} of solute B is equal to X_0 while the driving force decreases to 0 as X_{int} approaches $X^{\beta,eq}$. Hence, it is reasonable to write F_{chem} as a function of $(X_{int} - X^{\beta,eq})$. Eriksson [34] evaluated the $f(X_{int} - X^{\beta,eq})$ by thermodynamics software e.g., CHEMSAGE, and the function f is linear for a sufficiently

Fig. 3. Schematic representation of molar Gibbs energy for the $\beta \rightarrow \alpha$ transformation in an A–B alloy in order to derive the driving force acting on interface [32,36].

large interval of X_{int} and $X^{\beta,eq}$. Therefore, a factor $\tilde{\beta}$ was introduced in the function,

$$F_{chem} = \tilde{\beta}(X_{int} - X^{\beta,eq}) \quad (4)$$

2.2 Nucleation of new phase

It is extremely short in time for nucleation process of the new phase, and the nucleus in nanoscale is tiny. Therefore, to directly observe and analyze the nucleation process is particularly difficult by experiments. Aiming at this problem, in the first half of the 20th century, Gibbs [35], Becker [36], Cahn and Hilliard [37,38] conducted systematic theoretical analysis for nucleation and then developed a series of nucleation theoretical models to derive the nucleation rate, activation energy barrier, size and equilibrium shape of the critical nucleus.

2.2.1 Classical nucleation theory

The classical nucleation theory is based on the assumption that the thermodynamic properties of a nucleus are uniform and the same as the equilibrium bulk counterparts within the nucleus, and that the interface between the nucleus and the parent phase is sharp [39]. In the classical nucleation theory [22], the nucleation rate is dependent on the number of critical nucleus determined by the activation energy barrier of heterogeneous nucleation and the jump frequency of solute atoms across interface which follows Arrhenius equation. Thus, the nucleation rate is [40]

$$\dot{N}(T(t)) = C\omega \exp\left(-\frac{\Delta G_{het}^*(T(t)) + Q_N}{RT(t)}\right), \quad (5)$$

where C is the density of nucleation sites of new phase, ω is the frequency factor, $\Delta G_{het}^*(T(t))$ is the activation energy barrier of heterogeneous nucleation and Q_N is the activation energy of atomic migration across interface. The classical nucleation models include the continuous nucleation models, pre-existing nuclei models, Avrami nucleation models and mixed nucleation models.

2.2.1.1 Continuous nucleation

When the undercooling or the overheating is very large, $\Delta G_{het}^*(T(t))$ can be neglected and the nucleation rate per unit volume is only determined by the atomic mobility for transport through the interface. The nucleation rate is [41]

$$\dot{N}(T(t)) = N_0 \exp\left(-\frac{Q_N}{RT(t)}\right), \quad (6)$$

where N_0 is the temperature-independent nucleation rate, Q_N is the activation energy for the jumping of atoms through the interface between the particle of critical size and the matrix. In this mode of nucleation, it is assumed that the nucleation rate is constant at constant temperature and the number of nuclei is zero at the beginning of transformation. The continuous nucleation often operates in the crystallisation of amorphous alloys.

2.2.1.2 Saturation by pre-existing nuclei

In contrary to the assumptions of continuous nucleation, Cahn supposed that preferential nucleation at grain boundaries, edges or corners caused saturation of the nucleation sites at the beginning of transformation and the further nucleation rate is zero. The saturation of the nucleation sites is depended predominantly on the degree of undercooling or superheating. In this case, the nucleation rate is [42]

$$\dot{N}(T(t)) = N^* \delta\left(\frac{T(t) - T_0}{\varphi}\right), \quad (7)$$

where N^* is the number of (pre-existing) nuclei per unit volume, $\delta\left(\frac{T(t) - T_0}{\varphi}\right)$ denotes Dirac functions and φ is the constant heating/cooling rate.

2.2.1.3 Avrami nucleation

According to this nucleation mechanism, the particles of supercritical size (nuclei) are formed from the particles of subcritical size, so the total number of particles of subcritical and supercritical size is constant [43,44]. In this case, the nucleation rate is

$$\dot{N}(T(t)) = -\dot{N}_{sub} = \lambda N' \exp\left(-\int_0^t \lambda d\tau\right), \quad (8)$$

where λ is the frequency of becoming the particles of supercritical size (nuclei) from the particles of subcritical size, which follows Arrhenius equation. N' is the number of subcritical particles at $t = 0$.

2.2.1.4 Mixed nucleation

In practice, the nucleation process may involve a variety of different nucleation mechanisms, which is so-called mixed nucleation phenomenon. It often represents a combination of the pre-existing nuclei and continuous nucleation modes. The nucleation rate is equal to some weighted sum of the nucleation rates according to continuous nucleation and pre-existing nuclei [41].

2.2.2 Non-classical nucleation theory of Cahn and Hilliard

In contrast to the classical theory, the non-classical nucleation theory, which is developed by Cahn and Hilliard [37] firstly, is based on the diffuse-interface description of the interfaces (or gradient thermodynamics). Poduri and Chen [39] extended the non-classical theory of Cahn and Hilliard to describe the phase transformations involving both compositional and structural changes associated with ordering. Heo and Chen [45] gave a briefly review on the recent advances in modeling and predicting nucleation during solid-phase transformations based on the diffuse-interface or non-classical description of critical nucleus profiles.

2.3 Growth of new phase

The growth of new phase in solid-state diffusional phase transformations is the migration of the phase interface in essence. According to the description from section 2.1, there exist three control modes including the diffusion-controlled mode, the interface-controlled mode and the mixed-mode for the migration of interface. Here, the boundary conditions for non-equilibrium interface [46] and the diffusion-controlled and mixed-mode kinetics of the growth for new phase are given as follows.

2.3.1 Interface boundary conditions

At the interface, the flux $J_{\alpha/\beta}$ of solute B atoms into the parent phase by the migration of interface is

$$J_{\alpha/\beta} = \frac{1}{V_m} (X^{\alpha,eq} - X_{int}) V(t), \quad (9)$$

where $V(t)$ is the velocity of the moving interface, V_m is the molar volume of element A in parent phase.

In the parent phase near the interface, the diffusive flux J_{diff} of solute B atoms along its gradient is

$$J_{diff} = -\frac{1}{V_m} D \frac{\partial X}{\partial x} \Big|_{x=L}. \quad (10)$$

Here, D is the diffusivity of solute B atoms in parent phase, L is the position of interface and $\frac{\partial X}{\partial x} \Big|_{x=L}$ is the solute concentration gradient in parent phase near the interface.

Since the solute B atoms cannot accumulate at the interface, $J_{\alpha/\beta} = J_{diff}$. The velocity of moving interface is acquired by

$$V(t) = \frac{D}{(X_{int} - X^{\alpha,eq})} \frac{\partial X}{\partial x} \Big|_{x=L}. \quad (11)$$

2.3.2 Diffusion-controlled growth kinetics

For the diffusion-controlled phase transformation, in equation (10), X_{int} is equal to $X^{\beta,eq}$. In order to solve the velocity of moving interface, the solute concentration gradient $\frac{\partial X}{\partial x} \Big|_{x=L}$ is prerequisite. Since the interface is moving, $\frac{\partial X}{\partial x} \Big|_{x=L}$ is extremely difficult to solve. However, the distance $L(t)$ of interface migration is proportional to $\sqrt{Dt}$, the so-called ‘‘constant-radius’’ approximate solution [47,48] and the exact solution of Carslaw and Jaeger [49] were proposed, which was subsequently examined by

Aaron [50] et al. In a strict sense, the so-called “constant-radius” approximate solution is valid only for very small supersaturation Ω ($\Omega < 0.1$). For larger values of Ω , the exact solution of Carslaw and Jaeger is available [51].

In case of the “constant-radius” approximate solution, the distance of interface migration is

$$L(t) = \sqrt{2\Omega Dt}, \quad (12)$$

and the supersaturation can be write

$$\Omega = (X_\beta - X_{int}) / (X^{\alpha,eq} - X_{int}). \quad (13)$$

In general, X_β is assumed as equal to X_0 without taking the soft impingement into account.

In a similar way, the exact solution of Carslaw and Jaeger, in which the supersaturation Ω is replaced by a parameter λ , is expressed as

$$L(t) = 2\lambda\sqrt{Dt}. \quad (14)$$

The parameter λ has a relation with the supersaturation Ω as

$$\{\lambda^2, \exp(\lambda^2)\} \cdot [\exp(-\lambda^2) - \lambda\pi^{\frac{1}{2}}\text{erfc}(\lambda)] = \frac{\Omega}{2}. \quad (15)$$

Thus, the velocity of moving interface can be written as

$$V(t) = dL/dt. \quad (16)$$

2.3.3 Mixed-mode growth kinetics

For the mixed-mode phase transformation, in equation (10), $X^{\beta,eq} < X_{int} < X_\beta$. In general, X_β is equal to X_0 without taking into account the soft impingement. In order to solve the velocity of moving interface, not only the solute concentration gradient $\frac{\partial X}{\partial x}|_{x=L}$, but also the concentration X_{int} as a function of time t should be acquired. To tackle the evolution problem of solute concentration field in parent phase near the interface, Sietsma [26] et al. introduced a Zener-like approach and Svoboda [21] proposed an analytical technique by developing a finite difference numerical method.

In the Zener-like approach, Sietsma et al. assumed the concentration gradient $\frac{\partial X}{\partial x}|_{x=L}$ was constant and concentration gradient field extended over a distance l into the parent phase. Thus,

$$\frac{\partial X}{\partial x}|_{x=L} = \frac{X_{int} - X_\beta}{l}. \quad (17)$$

When the interface migrates to the position L , the new phase forms with a volume V^α and an interfacial area A^α . On account of conservation of B-atoms at the interface,

$$l = \left(\frac{2V^\alpha}{A^\alpha}\right) \left(\frac{X^{\alpha,eq} - X_\beta}{X_\beta - X_{int}}\right). \quad (18)$$

According to Christian [52], the interface is proportional to the driving force

$$V(t) = MF_{chem}. \quad (19)$$

Here, M is the effective interface mobility with taking the effects of solute drag or transformation strain into account.

By substituting (4) into (18), plugging (16) and (17) into (10), and then combining (18) with (10), the concentration X_{int} will be acquired that

with $\Delta X_\beta = X^{\alpha,eq} - X_\beta$, the parameter Z is given by

$$Z = \frac{D}{M\tilde{\beta}} \frac{A^\alpha}{V^\alpha}. \quad (21)$$

According to Svoboda [21], the evolution of the interface is governed by the following system of equations: the bulk diffusion equation

$$\frac{\partial X}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial X}{\partial x} \right), \quad (22)$$

and the initial condition is

$$X(x, t = 0) = X_0. \quad (23)$$

By combining (4),(10) with (18), the boundary conditions at the phase interface are obtained as

$$\begin{cases} \frac{\partial X}{\partial x} = -\frac{1}{V_m D} M X \tilde{\beta} (X - X^{\beta,eq}), \\ \text{with } X = X_{int} \quad x = L(t) \quad x \rightarrow \infty, X = X_0 \end{cases} \quad (24)$$

For the differential equation (21), by considering the boundary initial conditions (Eq. (23)), a nonlinear Volterra integral equation is derived for the mole fraction X_{int} , which is simplified as

$$X_{int} = X_0 - \sqrt{\frac{D}{\pi}} \int_0^t \frac{1}{V_m D} M X_{int} \tilde{\beta} (X_{int} - X^{\beta,eq}) \frac{d\tau}{\sqrt{t - \tau}}. \quad (25)$$

By plugging (24) and (4) into (8), the velocity of moving interface is

$$V(t) = \frac{1}{V_m} M \tilde{\beta} (X_0 - X^{\beta,eq}) \left(\frac{1 - 2M \tilde{\beta} X_0}{V_m \sqrt{D\pi}} \sqrt{t} \right). \quad (26)$$

2.3.4 Impingement of grains in new phase

For the phase transformations that proceed by the formation of nuclei and the growth of these nuclei, it is impossible that a new phase grows into its parent phase without any limit. In other words, the collision process between two growing neighboring grains is inevitable, which results in obstructing growth of the neighboring grains. It is so-called impingement phenomenon. In

$$X_{int} = \frac{ZX_\beta + X_\beta(X^{\alpha,eq} + X^{\beta,eq}) + \sqrt{(ZX_\beta + X_\beta(X^{\alpha,eq} + X^{\beta,eq}))^2 (Z + 2X_\beta) (ZX_\beta^2 + 2X_\beta X^{\alpha,eq} X^{\beta,eq})}}{Z + 2X_\beta}, \quad (20)$$

general, two impingement modes may occur. One is the hard impingement considering only the geometric factor, and the other is the soft impingement involving a compositional change. In the case of soft impingement, when the diffusion fields start to overlap, the phase transformation will slow down [53,54]. However, for the solid-state diffusional phase transformations, soft impingement has been found to prevail, and there usually are wide diffusion layers around the growing nuclei impinging on each other [55,56]. Initially a mean field approximation [27,57] was used to take into account the soft impingement effect in the diffusion-controlled growth models. However, it is available for mean field approximation in an assumption that a nucleus grows in isolation, which doesn't consider any effect of the neighboring nuclei on the diffusion field. Subsequently, to deal with the overlap of diffusion fields for the neighbouring grains in more strict ways, many diffusion-controlled models [58,59] and mixed-modes models [60,61] have been developed to describe the soft impingement effect more accurately.

3 Numerical simulation techniques for solid-state phase transformation

3.1 Empirical and analytical models

In studies of solid-state diffusional phase transformations involving nucleation, growth and impingement, the classical empirical and semi-empirical models, such as Johnson-Mehl-Avrami-Kolmogorov (JMAK) approach [52,62] or modified JMAK approach (JMAK-like equations) [63,64] and physical analytical models (for example, Zener-Hillert equation, the thermal activation principle of interface of Christian), always play important roles. The years 1937 through 1941 mark an important period in the history of metallurgy. In these years, Johnson and Mehl, Avrami, and Kolmogorov derived expressions for the transformed fraction f as a function of time t in the isothermal transformations [43,65]. The famous Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation is

$$f = 1 - \exp\left\{-\left[k_0 \exp\left(-\frac{Q}{RT}\right)\right] t^n\right\}, \quad (27)$$

but the JMAK formula can only be validated when the auxiliary conditions imposed in the original equation are not violated, such as: either pure site saturation at time $t=0$ or pure continuous nucleation, large undercooling or overheating for forming high driving force, and randomly dispersed nuclei which grow isotropically [65,66]. In other words, the growth exponent n , the effective activation energy Q and the pre-exponential factor k_0 are constant relative to time and temperature. By introducing additivity rule into the original JMAK equation, the application the JMAK-like equation was extended to the non-isothermal transformation. However, the kinetic parameters remain constant [67], which follows so called "iso-kinetics". In practice, due to nonrandom distribution of nuclei [68], anisotropic growth [69] and the temperature dependence of the diffusion coefficient and the solute concentration at

interface [7], these models which follow so called "iso-kinetics" are invalid for solid-state diffusional isothermal or non-isothermal phase transformations. Recently, since Cahn [70] first proposed the modified JMAK model with considering nucleation in grain boundary, edge and corner, lots of modified JMAK models by introducing the transient nucleation [71], the spatially correlated nucleation [72], the mixture of nucleation modes, the necessarily associated size-dependent growth [73] or the non-parallel anisotropic growth [74], and the hard or soft impingement, were derived. Shneidman et al. [75] developed a modified JMAK model by considering the effects of transient nucleation, size-dependent growth rate and their correlativity. Tomellini [76] introduced the impingement factor into the JMAK equation to tackle two processes: spatially correlated nucleation with constant nucleation rate and instantaneous cluster growth where cluster overgrowth prevails. By considering variable kinetic parameters (i.e., $n(t)$, $Q(t)$, $k_0(t)$ for isothermal case; $n(T)$, $Q(T)$, $k_0(T)$ for non-isothermal case) and the mixture of site saturation, continuous nucleation and Avrami nucleation, Liu et al. [77] proposed a general, flexible and modular analytical model, which expounded the influence of the different nucleation and growth modes on the time and temperature dependencies of the transformation rate and the kinetic parameters. For the treatment of the anisotropic effect, up to now, there exist two approaches: one is the phenomenological extension of JMAK-like formulation by adding (one or more) new variables which provide freedom to improve the agreement where anisotropic growth occurs [15], the other is devoting more attention to the derivation of analytical description with physically realistic variables (e.g. the growth rate anisotropy and the orientation) according to the physical essence of anisotropic effect [78]. In order to describe the mutual blocking of growing particles determined by all relevant orders due to the anisotropic effect, Kooi [74,79] developed an analytical model based on Monte Carlo (MC) simulations by incorporating anisotropic growth into the Johnson-Mehl-Avrami-Kolmogorov models. With respect to the effect of the thermal history, Song [80] proposed a generalized iso-kinetics conditions and additivity rule involving the thermal history-dependent instantaneous reaction rate by introducing a thermal history-related function. So far, a proper analytical approach in the spirit of JMAK-like theory, which can comprehensively consider the different modes of nucleation, growth and impingement, the interactions between non-randomly dispersed nucleation and anisotropic growth (involving single grain or multiple grains) in solid-state phase transformation, has not yet been developed. In physical analytical models, Zener-Hillert [81] equation established the theoretical foundation for the diffusion-controlled growth kinetic of lamellar phase. Subsequently, Ivantsov [82], Horvay and Cahn [83] derived a more generally applicable equation with taking into account the elliptic-parabolic or spherical surface for the tip of new phase. Trivedi [84] introduced the capillary phenomenon and interface dynamics into the equation of Ivantsov. Since the anisotropic effect of strain energy, diffusion and crystallography were not considered, these models were still incompetent to predict solid-state diffusional phase

Fig. 4. (A) Sharp interface: properties are discontinuous at the interface; (B) Diffuse interface: properties evolve continuously between their equilibrium values in the neighboring grains [17,36].

transformations accurately. Over all, much effort still should be paid to study the kinetic models of solid-state diffusional phase transformations with integration of different factors and involving structure evolution.

3.2 Phase-field models

The phase-field approach has emerged as an important and extremely versatile technique for simulating microstructure evolution at the mesoscale level. Initially, the phase-field models were used to simulate dendrite formation in solidification process. Subsequently, with the increasing computer power, the applicability of phase-field models was extended to solid-state transformations, grain growth, dislocation dynamics, crack propagation, electromigration and solid-state sintering and so forth [17].

In the conventional modeling techniques for phase transformation, the regions separating the compositional or structure domains are treated as mathematically sharp interfaces and the multi-domain structure is described by the position of the interfacial boundaries (Fig.4(A)). These models are also called sharp-interface models. The local interfacial velocity is determined by part of boundary conditions or the driving force on the interface. Due to these approaches involve explicit tracking of the interface position [17,85], it becomes difficult to simulate complex microstructure in two-dimension or three-dimension. Therefore, the phase-field modeling, which is able to predict the evolution of arbitrary complex grain morphologies without any presumption on their shape or mutual distribution and explicitly tracking the of the interface position, is very popular. The principal characteristic of phase-field model is the diffuseness of the interface between two phases, so it is sometimes also called diffuse interface models. The view of diffuse interface dates back to van der Waals [86] and Cahn & Hilliard [37]. Chen, Wang, and Khachaturyan [87,88] is first to introduce the diffuse-interface (Fig.4(B)(B)) into solid-state phase transformation

modeling. About the historical evolution of diffuse-interface models and the basic concepts of phase-field models, Moelans [17] gave a comprehensive introduction. In phase-field models, the transformation is described by the temporal and spatial evolution of a set of conserved (for concentration field) and non-conserved (involving information on local structure and orientation) field variables which are continuous across the interfacial regions separating the neighboring phases or structures. The evolution of these field variables are governed by the Cahn-Hilliard nonlinear diffusion equation [37,38] and the time dependent Ginzburg-Landau relaxation equation [89,90].

In solid-state diffusional phase transformation, microstructures have the thermodynamically unstable features. The driving force of the temporal and spatial evolution of the microstructure usually consists of a reduction in the bulk-chemical free energy (F_{bulk}), a decrease of the total interfacial energy (F_{int}) between different phases or between the neighboring grains with different orientation in the same phase, the relaxation of the elastic-strain energy (F_{elast}) generated by the lattice mismatch and external energies (F_{appl}) due to applied stress, temperature, electrical, and magnetic fields and so on [91]. Thus, the total free energy of a system is

$$F_{tot} = F_{bulk} + F_{int} + F_{elast} + F_{appl}. \quad (28)$$

In phase-field models, the total free energy [92] described by a set of conserved ($c_1, c_2, \dots$) and non-conserved ($\eta_1, \eta_2, \dots$) field variables can be written as

$$F_{tot} = \int \left[f(c_1, c_2, \dots, c_n, \eta_1, \eta_2, \dots, \eta_p) + \sum_{i=1}^n \alpha_i (\nabla c_i)^2 \right. \\ \left. + \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^p \beta_{ij} \nabla_{ijk} \nabla_{j\eta k} \right] d^3r + \iint G(r-r') d^3r d^3r', \quad (29)$$

where f is the local free-energy density, α_i and β_{ij} are the gradient energy coefficients. The evolution of conserved and non-conserved field variables can be obtained by solving the following the Cahn-Hilliard nonlinear diffusion equation [37] and the Ginzburg-Landau relaxation equation [90],

$$\frac{\partial c_i(r, t)}{\partial t} = \nabla M_{ij} \nabla \frac{\delta F_{tot}}{\delta c_j(r, t)}. \quad (30)$$

$$\frac{\partial \eta_p(r, t)}{\partial t} = -L_{pq} \nabla \frac{\delta F_{tot}}{\delta \eta_q(r, t)}, \quad (31)$$

here, M_{ij} is related to the mobility of atom or interface and L_{pq} is the symmetrical matrix of dynamic structural operator related to the non-conserved field variables. Therefore, in phase-field models, to accurately describe the microstructure evolution in solid-state diffusional phase transformation including nucleation, anisotropy growth, hard or soft impingement needs to establish the appropriate correlation functions of the field variables and the phenomenological parameters for reflecting aforementioned effects.

In recently, many phase-field models, incorporated with nucleation phenomena [93–95], anisotropy effects [96–99] and elasticity/plasticity [100–104] and macroscopic behaviours [105], have been proposed for better quantitatively predicting the microstructure evolution in solid-state diffusional phase transformations. Zhang, Chen and Heo [96] developed a phase-field model combined with the minimax technique to predict the morphology of critical nuclei during solid-state diffusional phase transformation in both two and three dimensions, which took into account the anisotropic interfacial energy as well as the anisotropic long-range elastic interactions. Then, by incorporating with diffuse-interface critical nuclei in phase-field simulations through the explicit nucleation algorithm, the temporal growth kinetics of the introduced nuclei were obtained [95]. Mecozzi et al. [106] have successfully performed two- and three-dimensional simulations of a grain growth during austenite-to-ferrite transformation by the multi-phase-field (MPF) method, where the interfacial energy and mobility of all interfaces were assumed to be constant. Because the nucleation typically takes place on a much smaller length scale than the further growth of new phase, as above, lots of phase-field models can only be used to study the one of nucleation or growth. To sample frequently enough to observe nucleation would require an impractically large number of integration cycles to be performed in order to observe growth kinetics in real alloys, Simmons et al. [107] introduced a Poisson seeding algorithm into the Phase Field equations instead of the Gaussian-distributed Langevin noise terms for simulating nucleation. Wang [108] used the quantitative phase field method to study the concurrent nucleation and growth in a diffusion-controlled phase transformation. However, in their works the growth behavior and morphology of simulated grains are isotropic, which is unrealistic in actual phase transformation. Therefore, a series of phase-field models,

integrated with the anisotropy growth, have been developed. Yamanaka [109] used a multi-phase-field model with considering the dependence of the interfacial energy and mobility on phase and crystal orientation to simulate growth of the ferrite. Wei [97] used the Loginova phase-field model with introducing a highly anisotropic function related to the anisotropy strength of the interfacial energy and interface thickness, and the Kim-Kim-Suzuki (KKS) phase-field models [S.G. Kim, W.T. Kim, T. Suzuki Phys. Rev. E, 60 (1999), pp.7186–7197] with a thin interface thickness which could enlarge the simulation domain to a large dimension, to simulate the growth of widmanstatten ferrite from grain boundary allotriomorphic ferrite with perturbed interface during isothermal austenite-ferrite transformation. In addition, the effect of elasticity/plasticity resulted from elastic or even plastic deformations should not be neglected. Recently the phase field models, containing the description of elastoviscoplastic material behaviour of the phases combined with diffusion and phase transformation, can be classified into two main groups of theories [110–112]. One is the interpolation models relying on a single set of constitutive equations and interpolation of material parameters, the other is the homogenization models based on the mixture of free energy and dissipation potentials associated with distinct behaviors of the phases. These models have been applied to study the mechanical effect on the diffusion-controlled growth of the precipitates.

Furthermore, for complex multicomponent systems, the phase-field models coupled with thermodynamic and kinetic databases were developed to put more physics into the expansion of the free energy function in the Ginzburg-Landau equation. Steinbach [113] discussed details of a direct coupling between the Multiphase-Field method and the CALPHAD method and used the CALPHAD –coupled Phase-Field model to simulate solidification microstructure formation in Ni-base superalloys. Wang et al. [114] presented a Multiphase-Field model with inputs from CALPHAD thermodynamic and DICTRA kinetic databases and simulated the growth and dissolution of a precipitates in Ti–Al–V on experimentally relevant length and time scales.

In addition, a number of the phase-field simulations for solid-state phase transformations have been conducted in three-dimensions (3D). In the complex phase transformations, due to that the two-dimensional (2D) models cannot simulate the basic microstructural features, the three-dimensional (3D) simulations which show a realistic representation of the actual microstructure become more attractive. M.Militzer [115] used the phase field method to simulate the austenite-to-ferrite phase transformation in steel in three-dimensional (3D) space. It was found that the effect of the exact morphology of the initial 3D austenitic microstructure on the kinetics was shown to be small and three-dimensional (3D) simulations predict slower transformation rates compared with two-dimensional (2D) simulations. Cui [116] developed a three-dimensional, non-isothermal phase-field model to systematically investigate the interactions between the temperature, stress, and microstructure fields in shape memory alloys.

As previously mentioned, the phase-field model exhibits the tremendous capability of quantitatively predicting the complex microstructure evolution in solid-state phase transformation. However, for phase-field models [17], there are two major difficulties in achieving more precise quantitative description of the real phase transformation with the coexistence of different nucleation modes, mixed growth mode, anisotropy growth, impingement effect and elasticity/plasticity effect. First, phase-field models contain a great many of phenomenological parameters related to the thermodynamic properties, phase composition, the interfacial structure, the diffusion of solute elements, and the elastic/plastic properties of the coexisting phases. Most of these parameters are difficult to measure. Second, in actual, the width of the interface is several orders smaller than the microstructure features such as grains and precipitates, so massive computer resources will be consumed by resolving the evolution of phase-field variables at the interface and also covering the system with realistic dimensions. Aiming at the problem of excessive computation times and insufficient computer memory, using interface field [117] especially adaptive grids providing a local remeshing at the interface have turned out to be beneficial [118]. For solid-state phase transformation, the Fourier-spectral method with semi-implicit time stepping is usually more appropriate than the technique based on adaptive meshing on account of a large number of grains or precipitates involved [119]. However, these computing techniques are either limited by the number of CPU cores or are too intractable to implement in three-dimensional simulations. Thus, the GPU-based parallel computing technology is extremely attractive in scientific computation owing to the GPU's massive computation capacity and high memory bandwidth. In the past few years, many researchers have successfully applied the GPU parallel computing algorithm into two-dimensional or three-dimensional phase-field simulations of dendrite growth [120,121]. To increase the system size towards relevant dimensions, the width of the diffuse interface must be taken artificially large. Much effort has been made in developing phase-field models that allow changing the interface width without affecting interfacial properties or introducing spurious effects [17]. However, a general solution has not yet been found. Therefore, there will still be increasing efforts to develop the more powerful and feasible large-scale three-dimensional (3D) phase-field model.

3.3 Cellular automaton models

Cellular automata are synchronous algorithms, first introduced by von Neumann in 1963, and later on in 1986 by Wolfram to a broader scientific public, which describes the discrete spatial and temporal evolution of complex system by applying local (or sometimes mid-range) deterministic or probabilistic transformation rules to the cells of a regular (or non-regular, random) grid with local connectivity [122,123]. Since Hesselbarth [123] et al. used the cellular automaton approach for the simulation of recrystallization, in the past several decades, it gradually becomes very promising and popular for

Fig. 5. Neighboring type in cellular automata: (A) von Neumann configuration; (B) Moor configuration.

simulating the microstructure evolution due to its computation efficiency, flexibility in multi-scale bridging, and physical consistency. Cellular automaton method has been successfully performed in two- or three-dimensional modeling and simulations of dynamic and static recrystallization [124,125], grain coarsening [126], solidification [126], solid-state phase transformation [127], micro-shear band and shear band propagation [128], cracks propagation [129], etc. It provides a deeper insight into the mechanism and morphological complexity of them without time-consuming solution of complicated partial differential equations. So far, all these models can be classified into several main groups that referred as the classical cellular automaton, frontal cellular automaton [130], irregular and shapeless cellular automaton [131], and virtual front tracking model based on cellular automaton [132].

In the classical cellular automata, take the two-dimensional model as an example, the entities of the automaton are the types of the neighboring cells (Fig. 5), the state variables of cells in space evolving with time and cell status update rules without any restrictions [133]. A cellular automata simulation for complex microstructure evolution proceeds by discrete simulation steps (namely discrete time steps) consisting of the computation of the new states ($t_0 + \Delta t$) of the all cells based on their current states (t_0), which can be presented as the following function with Moor configuration in two-dimension,

$$\xi_{i,j}^{t_0+\Delta t} = f\left(\xi_{i-1,j-1}^{t_0}, \xi_{i-1,j}^{t_0}, \xi_{i-1,j+1}^{t_0}, \xi_{i,j-1}^{t_0}, \xi_{i,j+1}^{t_0}, \xi_{i+1,j-1}^{t_0}, \xi_{i+1,j}^{t_0}, \xi_{i+1,j+1}^{t_0}\right). \quad (32)$$

where $\xi_{i,j}^{t_0}$ is the value of the state variable of the cell (i, j) at the time t_0 , and the function f specifies the set of transformation rules which determine the updated state of a cell based on the cell's previous state and the states of all cells in the local neighborhood of that cell. Besides, some conditions at the outer boundaries of the grid such as periodic, reflexive or fixed grid are applied in order to study the infinite target domain by simulating a finite representative region.

The most of cellular automata models, which can be found in literature, are two-dimensional(2D). 2D cellular automata models are simpler and faster in calculation in account of having less elements, connections and complicated algorithms. However, microstructure evolution is

pointedly three-dimensional phenomena, the results obtained by 2D cellular automata models cannot always be directly transferred to a real 3D process [130]. Therefore, 3D cellular automata models attracted a growing number of researches [134,135]. Due to more cells in simulated domain and more neighbours for each cell relative to 2D models, the 3D models require significantly more memory and time for the calculation, which increases the difficulty in accurately predicting real microstructure evolution.

During the implementation of the classical automaton models, some problems and aspects needing to be improved have been encountered. One of the most significant is the inherent and artificial anisotropy introduced in the computations by the mesh of squared cells, which causes that the preferential growth directions of all the simulated grains are aligned with the mesh axis or at 45 degree and thus leads to the growth kinetics without physical significance. For the problem, Stefanescu et al. [127] developed a cellular automaton model coupled with virtual interface tracking scheme (Fig. 6). In this model, the procedure of constructing virtual sharp interface for capturing new interface cells in a time step is as follows. First, for all interface cells, the length L_ϕ dependent on the local growth angle ϕ is assumed equal to $f_s = 1$ (new phase fraction f_s) and measured from the interface cell center along the normal direction of the local interface, which can be written as (Fig. 6(A))

$$L_\phi = \frac{\Delta x}{\max(|\cos(\phi)|, |\sin(\phi)|)}, \quad (33)$$

here cells size is Δx . The position of the new interface at time $t + \Delta t$ can be gauged from the interface cell center along the normal direction of the local interface at a distance proportional to the f_s in one cell. And the entire virtual sharp interface at time $t + \Delta t$ will be described by connecting the position of new interfaces in all interface cells. Second, the parent phase cells, found inside the area surrounded by the entire virtual sharp interface, are considered captured and will become new interface cells (Fig. 6(B)). Subsequently, after capturing the new interface cells and then updating the state variables, the procedure is repeated again in the next time step.

Another problem is that interface energy and mobility relies on its curvature which is dependent on the orientation of the interface surface, meanwhile, the method of using the symmetrical grid to discretize the surface in such a way that only a very limited number of orientations are represented cannot resolve curvature [131]. For this problem, Janssens et al. [136] first presented the random grid or irregular cellular automaton based on Voronoi cells to solve this problem by local variation of the cell lattice geometry (Fig. 7(A)). Afterwards the shapeless or point cellular automata were developed from the random grid or irregular cellular automaton by Janssens. In this model, shapeless cell shapes are not computed explicitly and only a point position is used, which makes much more flexible in definition of neighborhood (Fig. 7(B)).

In addition, no cell state is actually changed until the end of the solution step when the states of all cells are updated simultaneously in the classical cellular automata,

Fig. 6. Illustration of (A) determining the position of sharp virtual interface, and (B) capturing rules for new interface cells [127,134].

which directly influences the calculation time. Much effort has been focused on developing modified cellular automaton models allowing for significant acceleration of the calculation especially in the three-dimensional tasks. In order to only consider the small area near the front of moving interface for growing grains from the calculations in the current step, Svyetlichnyy [137,138] presented the FCA (frontal cellular automata) algorithm. FCA consists of a complex of the millions of cells with the same multi-states automaton (Fig. 8). The series of automaton states includes the initial matrix state q_0 , the frontal cell q_1 , the boundary cell q_2 , the cell inside the grain q_3 , the transient state q_4 accompanied with calculation of the time delay, nucleation state q_5 , the cell in the edge of the grain q_6 , and the cell in the corner of the grain q_7 . Besides, some conditions used by transition rules respectively are the nucleation condition I_0 , the time delay condition I_1 which controls grain growth or mobility of interface, the conditions I_2 and I_3 which determine nucleus location (on grain boundary, inside the grain, in the edge or corner of the grain), and state change condition I_4 which refers as that neighboring cells transits from the states q_2, q_3, q_6, q_7 into the transient state q_4 for all neighbors of all frontal cells. For the phase transformation, in FCA, the initial states of the cell before transformation can be arbitrary ($q_1 - q_7$), and then the conditions ($I_1 - I_7$) are responsible for the transformation. The boundary conditions such as periodic displacement conditions and full open conditions are usually used. Relative to the classical cellular automata, the most advantage of FCA is found out allowing for recognition of the changes in cells state without studying their neighborhood.

In the formulation of cellular automaton models for solid-state diffusional phase transformation, each cell represents a volume of real material characterized by certain attributes with a distinct phase or grain, solute concentration and an orientation indicator. There are several state variables with describing certain attributes used on each cell in phase transformation such as the phase state variables, the solute atom concentration variables, the orientation variables, the velocity and displacement variables of the moving interface, and volume fraction variables. The cellular automaton will be in progress by

Fig. 7. Illustration of (A) cells distribution in a two-dimensional irregular cellular automata based on the Voronoi cells, and (B) a shapeless cell on a curved interface and its spherical neighborhood [121].

Fig. 8. Illustration of FCA (frontal cellular automata).

synchronously updating these state variables for all lattice cells in each time step, and thus spatial and temporal microstructure evolution is described. In recently, many cellular automaton models for solid-state diffusional phase transformation have been developed to focus on simulating the austenite-ferrite phase transformations in Fe-C alloy in which interstitial solute carbon atoms have high diffusion coefficient [139–141]. However, as regard to substitution solid solution like Fe-Mn or Ti-Al-Mo alloy, the attractive force occurs from the solute atoms on the moving interface, which is so-called solute drag without existing in interstitial solid solution. According to Cahn [138], the solute atoms have different drag effects in three regimes of the interface velocity. Therefore, the effects of solute drag for solid-state phase transformation in substitution solid solution cannot be neglected. Furthermore, in most of these models, the growth behavior and morphology of simulated grains were assumed to be isotropic [141,142], which was not correspondent with practice. Besides, because the nucleation typically takes place on a much smaller length scale than the further growth of new phase, as with the phase-field models, the cellular automata is not able to simulate the process of different nucleation modes and mixed growth mode occurring in sequence. And last but definitely not least, above mentioned models, the phase transformation is supposed to happen with only the diffusion-controlled or the interface-controlled kinetics in the isothermal condition without considering the effect of the thermal history. A cellular automaton model [143] coupled with Svoboda's analytic solution of diffusional phase transformation was established to divide the diffusion-, mixed- or interface-controlled transformation in isothermal and non-isothermal processes. However, due

to the critical conditions could not be obtained as a result of the difficult-to-measure constant factor in the driving force model, and due to only taking into account the cooling rate-dependent transformation temperature, the cellular automaton model was not enough to simulate the actual non-isothermal transformation. All in all, much effort should be focused on improving the cellular automata models for better modeling and simulation of the solid-state phase transformation in the future.

3.4 Monte Carlo models

MC models were developed from Ising and Potts models of ferromagnetic systems used in statistical physics [144]. Initially they were used to simulate grain growth by Anderson et al. [145], after that they have been widely used to model the microstructure evolution in materials such as the recrystallization and the phase transformation. In Monte Carlo models [146], space is discretized into a set of lattice points onto which a continuum microstructure is mapped at a length scale above that of atoms and below that of grains, similarly to the probabilistic cellular automaton models. The grain boundaries are defined as existing between lattice sites of neighbouring grains. The energy of the system is represented by a Hamiltonian which sums the interfacial energy of the system. The Monte Carlo models simulate curvature-driven grain boundary motion by the random movement of kinks (2D) or ledges (3D) along the grain boundaries controlled by the transition rules. Due to the calculations of grain boundary curvature and energy are ambiguous and the transition rules governing the change of voxel state are often not physically justified, the physical meaning of units of length, time and energy in Monte Carlo models is often unspecified [147]. Nonetheless, the numerical implementation is straightforward and decent computational efficiency can be achieved in the Monte Carlo models, especially since the algorithm is very suitable for parallelization, the Monte Carlo models are still frequently used to model the complex microstructure evolution in materials.

3.5 Molecular dynamics methods

Molecular dynamics simulation serves as an essential technique for the investigation of fundamental atomic behaviors in metals and alloys, which was developed by Alder and Wainwright in the late 1950s [148]. It has

facilitated scientific discovery of interactions among particles or atoms since molecular dynamics method allows us to examine the varying atomic configurations at finite temperatures by incorporating statistical mechanics [149]. The molecular dynamics methods simulate microstructure evolutions from the atomistic point of view by solving the particle trajectories derived from the interatomic forces. Numerical integration of atomic motion is carried out on the interatomic forces, which results in the particle velocity. The velocity of the particles follows the Maxwell–Boltzmann distribution, which is temperature dependent. Then, the particle position is obtained by further integrating the velocity. Molecular dynamics methods have evolved as the powerful tool to investigate the mechanisms of physical phenomena such as nucleation, and nucleus growth which are difficult to observe experimentally [14], [150].

4 The comparison of different numerical simulation techniques

As above, the theoretical researches of solid-state diffusional phase transformations and the primary numerical modeling techniques are discussed. All these phase transformation models characterized by complex mathematical formulations present various predictive capabilities. In the following, the advantages and disadvantages of each modeling technique will be discussed in terms of the underlying assumptions, physical relevance, implementation and computational efficiency for the simulation of the solid-state diffusional phase transformations.

Historically, the classical empirical and semi-empirical models represented by Johnson-Mehl-Avrami-Kolmogorov (JMAK) approach were commonly used for simulations of phase transformations. The JMAK formula are valid only in conditions of either pure site saturation at initial moment or pure continuous nucleation, large undercooling or overheating for forming high driving force, and randomly dispersed nuclei which grow isotropically. In these models, all attention is focused on the kinetics while the microstructural aspects are essentially ignored, and thus its only provide average information such as the average grain size and phase volume fraction of microstructure evolution on macroscale. Afterwards, several upgrades of the model with integration of the mixed nucleation modes, anisotropic growth, and the hard or soft impingement effects were proposed. Much effort has been paid on developing the models involving structure evolution, and the approach is still commonly used. Compared with the JMAK approach, the phase field models and the cellular automaton models can reconstruct the evolution of grain morphology and spatial distribution, solute concentration field in addition to giving macroscopic average information.

The phase-field modeling is a mechanistic-based microstructure modeling method, in which phenomenological character and the equations for the evolution of the phase field variables are derived based on general thermodynamics and kinetics principles. It can predict the evolution of arbitrary complex microstructure without

any presumption on their shape or mutual distribution and explicitly tracking the of the interface position, meanwhile, provide an insight into controlling mechanisms in solid-state diffusional phase transformations [151,152]. Because a large number of grains or precipitates are involved in solid-state diffusional phase transformation, the Fourier-spectral method with semi-implicit time stepping and uniform mesh is usually more appropriate than the technique based on adaptive meshing in phase-field models [17]. However, the phase-field models contain a large number of phenomenological parameters related to the thermodynamic properties, the phase composition, the interfacial structure, the diffusion of solute elements, and the elastic/plastic properties of the coexisting phases, meanwhile, most of these parameters are difficult to measure. Besides, the phase field simulations are more computationally intensive than the JMAK approach and the cellular automata.

Relative to the classical empirical models and the phase-field models, the cellular automata models are more easily implemented without solving complex partial differential equations and its can be used to capture many aspects of the microstructure physics in solid-state diffusional phase transformation. Since the discrete nature of the algorithms is well suited for parallelization, the cellular automaton methods possess the high computational efficiency. However, a precise calculation of the mean curvature which is necessary for grain boundary migration by capillarity remains difficult [98]. Moreover, due to the sharp interface in the cellular automaton models, compared with the phase-field models with the diffuse-interface, the cellular automaton approach is less than accurate to predict solid-state diffusional phase transformation. Besides, limitations of the cellular automata also lie in the dependence on the underlying solution grid and the types of the neighboring cells. In addition, for solid-state diffusional phase transformations, the time step in the cellular automata simulation is virtual or defined as e.g., the ratio between the cell size and maximum interface velocity, or a scaled ratio between the average cell size and the average interface velocity, which is deficient in physical meanings [153].

The Monte Carlo model as usually is very similar to the probabilistic cellular automata model in terms of implementing. Both models describe the discrete spatial and temporal evolution of complex system by applying local transformation rules to the grids with local connectivity. The differences between them lie in the transition rule and the method of updating the state of each cell [154]. In the Monte Carlo models the transition rule is determined by the reduction in local free energy, whereas the cellular automata model is more flexibility to adjust the transition rule for matching kinetics of a particular experimental system. Therefore, the Monte Carlo simulations lack physical length and time scales, and the results are difficult to match to experiment. In the Monte Carlo models sites are chosen at random for updating, whereas in the cellular automata models all sites update simultaneously. Thus, the cellular automata models are generally more efficient than the Monte Carlo models.

The phase-field models, the cellular automata models and the Monte Carlo models in mesoscale allow the simulation of a relatively large representative volume element that can be composed of thousand to million grains. However, the effects and physical mechanisms are predefined and pre-implemented in these models, it is impossible for them to resolve the mechanisms of phenomena acting at the atomic scale. In this case, the molecular dynamics simulations are utilized to describe atomic interactions to make up for the disadvantage of mesoscopic models. Compared to these mesoscopic models, the representative volume element that can be simulated by the molecular dynamics models in a reasonable time is very limited, which occasionally results in insufficient statistical representativeness and undesired effects of the size of the simulated volume [155]. With increasing computational power, large scale atomistic simulations can be conducted with several million or even billion atom systems, e.g. into studying phase transformation kinetics [156], deformation and fracture in metallic systems [157].

5 The future prospects

Although various numerical simulation techniques as above have been successfully used to describe the solid-state diffusional phase transformations, there will also be increasing efforts in the accuracy and efficiency of models. The new trends or future directions for the simulation of solid-state diffusional phase transformation will be expected.

5.1 Integrating the nucleation phenomena (mixed-modes, nuclear morphology)

Nucleation of the new phase typically takes place on the much smaller length scale than the subsequent growth of nucleus and it is generally extremely short in time for nucleation process. Moreover, in practice, the distribution of nucleus is not random and there are various nucleation phenomena. It has been found that the nucleation was either related to time like transient nucleation and continuous nucleation, or correlated with space like nucleation in grain boundary, edge and corner at parent phase. In addition, the morphology of the critical nucleus is very complicated by additional contact angle conditions for nucleation occurring at the planar defects. The existing models on mesoscopic scale can only describe a single nucleation mode with ignoring the morphology of nucleus, and thus it is not feasible to consider both the nucleation and the growth at the same time for these models. However, many models represented by the molecular dynamics on microscopic scale and nanoscopic scale are benefited to accurately capture the grain boundary energy and interfacial energy and predict the geometry of the nucleus by tracking motion of atoms. Therefore, future efforts are expected to be focused on coupling between mesoscopic simulation and microscopic or nanoscopic calculations for complex nucleation phenomena in solid-state diffusional phase transformation.

5.2 Incorporating with the anisotropic effect

In general, the fundamental process underlying the microstructure evolution in solid-state diffusional phase transformations is the migration of interface or growth of new phase in a broader sense. The kinetics and morphology of grains growth in new phase are determined by the properties of interfaces such as the anisotropic interfacial energy and mobility. Anisotropy of the interfacial energy and mobility reflects the atomistic crystallographic structure of interfaces, meanwhile, the low-energy interfaces structures leads to the faceted interface as well. At present, many findings allow to make a rough estimate successfully for the anisotropic grain boundary energy in case of the same lattice structure and composition. However, with respect to the interfacial energy, the effects of lattices structure and chemical composition also remain largely unexplored and the anisotropy of interfacial mobility is difficult to measure, which make it impossible to accurately predict anisotropic growth of grains in new phase.

5.3 Introducing the hard or soft impingement effect

In general, for the phase transformation consisting of nucleation and growth, the collision process between neighboring grains is inevitable. When the impingement occurs, with decreasing of the distance between the edges of neighboring grains, the diffusion fields start to overlap, at the same time, the concentration gradient becomes more flat, the growth rate is predicted to decrease locally and thus the phase transformation slows down. In that case, the growth law cannot be considered as given a priori before collision process since it is a function of the local environment of each grain. However, at present, due to the lack of knowledge on the exact nature of diffusion layers for the hard and soft impingement, the collision process between grains described in the existing models is now less effective than the genuine impingement process.

5.4 Considering the thermal history

In the past few decades, various analytical models have been successfully developed to predict the non-isothermal transformations process with the use of the additivity concept in the isokinetic condition. The conventional additivity rule is only valid in the assumption that non-isothermal transformations process is described as the summation of a series of short period isothermal transformation process, which implies that the instantaneous reaction rate only depends on the current state of every short period isothermal transformation process. However, in practice, the diffusion field around new phase during non-isothermal transformation has an intrinsic memory of the thermal history as a result of the temperature dependence of the diffusion coefficient and the local equalized solute concentration at the interphase boundary, which leads to a temperature path-dependent instantaneous growth rate. Therefore, most of analytical models introduced the conventional additivity rule usually overestimate or underestimate the measured extent of

precipitation reactions. At present, for more accurately predicting solid-state diffusional phase transformations, there has been increasing efforts to be spent on creating the thermal history-related function, and developing a generalized additivity rule which involves the thermal history-determined instantaneous reaction rate.

5.5 Coupling with macroscopic deformation

Solid-state diffusional phase transformations are always not immune to the effect of the elastic deformation and plastic deformation such as the stored energy, the dynamic and static recrystallization, the globularization and the deformation heating and so on during the metal forming process. When the solid-state phase transformation takes place after the elastic-plastic deformation, in other words, the deformation is applied in single-phase region at high temperature or in two-phase region with isothermal conditions and then the cooling treatment is performed at given rate. The stored energy is the main factor for contributing to the driving force of the phase transformation. However, if the solid-state phase transformation process operates simultaneously with deformation, not only the stored energy, the dynamic and static recrystallization, the globularization and the deformation heating have significant influences on the kinetics and crystallography (orientation relationship, morphology) of phase transformation, but also in turn the changes of the volume fractions of constituent phases and grains morphology on the mesoscale affect the deformation resistance on the macroscale. Up till now, due to lack of knowledge on the exact mechanism of the interaction of phase transformation and deformation, few investigations are performed on modeling the phase transformation coupled with macroscopic deformation.

5.6 Improving computational efficiency and accuracy for quantitative simulation

Numerical simulation can provide the important insights into the role of special material or process parameters on the volume, shape and spatial distribution of new phase, orientation relationships between new phase and parent phase, or kinetics in solid-state diffusional phase transformation. However, the more versatile and feasible technique for quantitative predicting the microstructure evolution is required both the high computational efficiency and the accuracy for the numerical solution. As is known to all, the more accurate solution of details of the microstructure evolution requires the finer mesh. In contrast, the coarser mesh is more benefit to the high efficient calculation. For the phase-field models, a finite volume or finite element discretization based on adaptive meshing which provides a local re-meshing at the interfaces, or artificially enlarging the width of the diffuse interface is often applied to improving the accuracy of simulation quantitatively and the computational efficiency. However, the problem of excessive computation times and insufficient computer memory is still not solved with the use of these methods. For the cellular automaton models, it is more easily implemented without the excessive computation times and

solving complex partial differential equations. However, once coupled with the finite element simulation on macroscale which provides the macroscopic information for the cellular automaton models, huge amounts of computational resources will be consumed by the numerical solution of the coupled system. Although a series of powerful parallel algorithms are developed to improving the computational efficiency, it is still difficult for the cellular automaton methods to simulate the microstructure evolution with a more fine mesh for accurate solution of details as a result of unreasonable computation time and inadequate computer memory.

6 Conclusions

The modeling and simulation of the solid-state diffusional transformations in metals are reviewed and the results may be summarized as follows:

- The traditional diffusion-controlled and interface-controlled modes fail to correctly describe the growth kinetics of new phase over the entire course of the transformation. The mixed-mode model which can consider both the effects and the varying relative importance of two extreme kinetics modes provides an appropriate approach to describe the character of actual phase transformation accurately.
- The nucleation, the growth of new phase with diffusion- and mixed-mode character, and the impingement effects of the growing neighboring grains are described briefly.
- Aiming at the precision prediction of the nucleation, the growth and the impingement in the transformation, the developments of the empirical and analytical models, the phase-field models, the cellular automaton models, the Monte Carlo models and the molecular dynamics methods are summarized in detailed. Five numerical techniques provide good tools for the simulation of complex microstructure evolution.
- By comparing with these models, it is found that: the empirical and analytical models only provide average information on macroscale; the mechanistic-based phase field simulation can predict the evolution of arbitrary complex microstructure without any presumption on their shape or mutual distribution and explicitly tracking the of the interface position while it is more computationally intensive; the cellular automata models are more easily implemented and possess the high computational efficiency while its lack physical meanings on the time scale and the growth kinetics of grains; the Monte Carlo model as usually is very similar to the cellular automata model; the molecular dynamics simulations are utilized to describe atomic interactions to make up for the disadvantage of mesoscopic models while the representative volume element that can be simulated is very limited.
- Increasing efforts will be expected, to focus on exploring more advanced numerical simulation techniques coupled with atomistic calculations and macroscopic simulation, for predicting many important or non-negligible phenomena such as the mixture of different nucleation modes, the anisotropic growth caused by the anisotropic

interfacial energy or mobility, the hard and soft impingement, and the effect of the thermal history and the elastic or plastic deformation.

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