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Computationally Efficient Phase-field Simulation Studies Using RVE Sampling and Statistical Analysis

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ABSTRACT

For large-scale phase-field simulations, the trade-off between accuracy and computational cost as a function of the size and number of simulations was studied. For this purpose, a large reference representative volume element (RVE) was incrementally subdivided into smaller solitary samples. We have considered diffusion-controlled growth and early ripening of δ' (Al_3Li) precipitate in a model Al-Li system. The results of the simulations show that decomposition of reference RVE can be a valuable computational technique to accelerate simulations without a substantial loss of accuracy. In the current case study, the precipitate number density was found to be the key controlling parameter. For a pre-set accuracy, it turned out that large-scale simulations of the reference RVE can be replaced by simulating a combination of smaller solitary samples. This shortens the required simulation time and improves the memory usage of the simulation considerably, and thus substantially increases the efficiency of massive parallel computation for phase-field applications.

1. Introduction

The structural and many functional properties of materials are determined by their microstructure. Modern alloy design encompasses a detailed understanding of the microstructure and the processes of microstructure modification to tailor materials to specific applications. In these complex tasks, modelling and simulation are widely utilized to predict microstructure and property evolution of materials during their synthesis, processing and performance. Many computer models utilized in materials science describe the microstructure by using a spatially resolved representative volume element (RVE). An RVE is the smallest statistical representation of a microstructure [1,2] that samples all it's relevant features. Determining the size of the RVE is not trivial [3–6] because in most materials the microstructural features are heterogeneously distributed and occur at different length scales. Hence, establishing the optimal size of the RVE is a difficult task. In fact, it has been pointed out by many investigations [7–10] that the more heterogeneous a microstructure is the finer it has to be resolved. An example is the problem of grain growth where despite the possibility for studying large-scale simulations [11–13] it was demonstrated that the size of the RVEs utilized in several grain growth simulations may not be enough to observe self-similar behaviour depending on the initial grain size distribution [14]. Evidently, the computational cost of representing a microstructure as a continuous and contiguous space is immense. This has rendered most of the algorithms memory intensive and even memory bound. To remedy this situation, it was recently proposed [15] to take advantage of supercomputers and make use of numerous solitary units to represent a microstructure. A solitary unit is a small subdivision of the volume to study that by itself is not statistically representative but once numerous units are considered they approach reality. This idea was tested for the simulation of recrystallization with excellent results [15].

The question posed in the present contribution is whether the same concept can be applied to more complex physical models e.g. phase transformations, where diffusion can impose long-range effects and a sub-division of a large RVE into solitary units may not be possible owing to these effects. This problem can be studied by means of the phase-field model where diffusion can be efficiently combined with interface kinetics [16–19]. The multi-phase-field approach [20–24] has proven its capability for

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studying many phenomena in materials science such as grain growth [11,12,25,26], recrystallization and texture evolution [27–29] and, particle pinning [30]. Besides diffusion, multiple features of elasticity [31], fluid flow [32], effect of external fields [33,34] as well as mutual coupling between different physical phenomena [35] can be conveniently integrated into the phase-field framework that enables it as a powerful technique for studying microstructure evolution.

In the present contribution, we performed phase-field simulations of diffusion-controlled precipitation combined with statistical sampling to study the trade-off between computational costs and accuracy when a reference RVE is incrementally subdivided into solitary units. The growth and early ripening of δ' (Al_3Li) in Al-Li system are studied. The results of the simulations are investigated in terms of precipitate size and spacing over the course of evolution. A systematic sampling and statistical averaging was applied to investigate the efficiency of the smaller simulations in terms of computational costs as well as accuracy of the results compared to the reference RVE simulation results.

2. Model description and simulation procedure

2.1. Multi-phase-field model

A multiphase-field method is considered in the current study. We start with the description of the total free energy by integrating the interface free energy density f^{IN} and the chemical free energy density f^{CH} over a domain Ω:

$$F = \int_\Omega \left(f^{IN} + f^{CH}\right) dV. \tag{1}$$

The interface energy density is given as

$$f^{IN} = \sum_{\alpha=1}^{N_\phi}\sum_{\beta\neq\alpha}^{N_\phi}\frac{4\sigma_{\alpha\beta}}{\eta}\{-\frac{\eta^2}{\pi^2}\nabla\phi_\alpha\cdot\nabla\phi_\beta + \phi_\alpha\phi_\beta\} \tag{2}$$

in which $\sigma_{\alpha\beta}$ is the interface energy between phases α and β, η, is the interface width and, N_ϕ is the number of existing phases. In each point of the space, the phase-field variables are constrained with $\sum_{\alpha=1}^{N_\phi}\phi_\alpha = 1$. The chemical free energy density is

$$f^{CH} = \sum_{\alpha=1}^{N_\phi}\phi_\alpha f_\alpha(c_\alpha) + \bar{\mu}\left[c - \sum_{\alpha=1}^{N_\phi}(\phi_\alpha c_\alpha)\right] \tag{3}$$

where $f_\alpha(c_\alpha)$ is chemical free energy of phase α, $\bar{\mu}$ is the Lagrange multiplier and equal to the chemical potential of solute atoms, c_α the phase concentration of phase α and c is the total concentration fulfilling $c = \sum_{\alpha=1}^{N_\phi}\phi_\alpha c_\alpha$. The interested reader can see Refs. [20,21] for detailed description of multi-phase field approach.

The evolution of the phase-fields using Eqs. (1)–(3) follows

$$\begin{aligned}\dot{\phi}_\alpha &= -\frac{\mu}{N_\phi}\sum_{\beta=1}^{N_\phi}\left(\frac{\delta}{\delta\phi_\alpha} - \frac{\delta}{\delta\phi_\beta}\right)F \\ &= \frac{\mu}{N_\phi}\sum_{\beta=1}^{N_\phi}\left[\sum_{\gamma=1\neq\beta}^{N_\phi}[\sigma_{\beta\gamma} - \sigma_{\alpha\gamma}]\left[\nabla^2\phi_\gamma + \frac{\pi^2}{\eta^2}\phi_\gamma\right] + \frac{\pi^2}{8\eta}\Delta g_{\alpha\beta}\right].\end{aligned} \tag{4}$$

Here δ indicates functional derivative, μ is the interface mobility and $\Delta g_{\alpha\beta}$ is the chemical driving force [36]. The diffusion flux $\vec{J}$ follows Fick's equation as

$$\vec{J} = -D\nabla c \tag{5}$$

where D is the diffusion coefficient. Using the continuity equation, $\dot{c} + \nabla\cdot\vec{J} = 0$, one obtains the temporal evolution of the concentration field. The chemical driving force $\Delta g_{\alpha\beta}$ is

$$\Delta g_{\alpha\beta} = m_0\Delta S_0(c - c_{eq}) \tag{6}$$

with m_0 as the slope of the line separating single matrix phase and two-phase region in the linearized T–c phase diagram, ΔS_0 as the entropy of precipitate formation and, c_{eq} as the equilibrium concentration at a flat interface. A list of variables is given in Appendix B.

2.2. Simulation procedure

In the current study, growth and early stages of ripening of stoichiometric δ' (Al_3Li) precipitates in an Al-9 at.% Li alloy was considered. A linearised phase-diagram was considered as presented in previous studies of this system [35,37]. The chemical driving force for the precipitation, $\Delta g_{\alpha\beta}$, is proportional to the undercooling towards the line separating the fcc-aluminium from the two-phase region in the linearized T–c phase diagram [38].

A large-scale simulation with 512^3 grid points was conducted as the reference RVE. This RVE domain was incrementally subdivided to samples of different size as shown in Fig. 1. An overview of the performed simulations can be seen in Table 1. The samples were defined in different 'classes' v (in the following: *64*, *128*, *256* and *512*, shown in left subscript of the variables) with corresponding cubic volumes ${}_vV$ (*64^3*, *128^3*, *256^3* and *512^3* nm^3). The number of simulations for each class was defined as the quantity n_s (see Table 1). Periodic boundary conditions were applied.

In total, 1924 precipitates were inserted on random sites in the reference system in a stepwise manner during the first 250 s. This corresponds to a classical scenario were a high number of nucleation events occurs at the beginning, and then nucleation fades out. Nucleation sites and times were kept identical for all the solitary samples. While all precipitates had the same thermodynamic and mechanical properties, each of them was indexed with a unique phase-field number which allows convenient tracking of individual precipitates. Elastic energy contributions due to the transformation were neglected for simplicity. Therefore, the precipitates grow with a generic spherical shape. Isotropic interface energy and interface mobility were $0.014\,J\,m^{-2}$ [39] and $3\times10^{-18}\,m^4\,J^{-1}\,s^{-1}$, respectively. The diffusion coefficient of Li in Al at the simulation temperature (473.15 K) was taken as $1.2\times10^{-18}\,m^2\,s^{-1}$ [40], the entropy of formation was

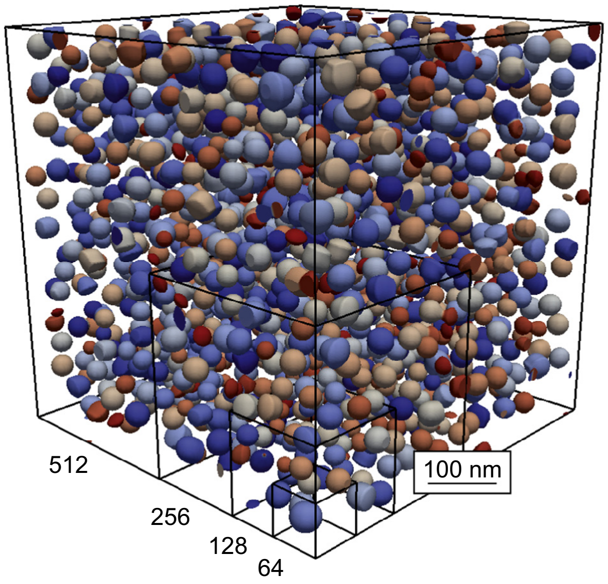

Fig. 1. A snapshot of the microstructure in the reference RVE ($512^3\,nm^3$) with exemplary insets of the subdivisions $256^3\,nm^3$, $128^3\,nm^3$, and $64^3\,nm^3$ is shown.