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Solidification and Precipitation Microstructure Simulation of a Hypereutectic Al–Mn–Fe–Si Alloy in Semi-Quantitative Phase-Field Modeling with Experimental Aid

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Abstract: In this study, microstructural evolution during solidification of a hypereutectic Al–Mn–Fe–Si alloy was investigated using semi-quantitative two-/three-dimensional phase-field modeling. The formation of faceted Al_6Mn precipitates and the temperature evolution during solidification were simulated and experimentally validated. The temperature evolution obtained from the phase-field simulation, which was balanced between extracted heat and latent heat release, was compared to the thermal profile of the specimen measured during casting to validate the semi-quantitative phase-field simulation. The casting microstructure, grain morphology, and solute distribution of the specimen were analyzed using electron backscatter diffraction and energy-dispersive spectroscopy and compared with the simulated microstructure. The simulation results identified the different Fe to Mn ratios in $\text{Al}_6(\text{Mn}_x\text{Fe}_{1-x})$ precipitates that formed during different solidification stages and were confirmed by energy-dispersive spectroscopy. The precipitates formed in the late solidification stage were more enriched with Fe than the primary precipitate due to solute segregation in the interdendritic channel. The semi-quantitative model facilitated a direct comparison between the simulation and experimental observations.

Keywords: Al_6Mn ; precipitation; phase-field modeling; microstructural analysis

1. Introduction

Precipitation behavior in Al alloys is of great interest due to its strong influence on the mechanical properties through a hardening effect [1–3]. Small changes in the concentrations of alloying elements or heat treatment conditions can readily alter the mechanical properties and product quality by modifying the microstructure. For example, Mn is alloyed in Al to enhance strength, formability, and corrosion resistance [4–6]. However, undesired formation of large, faceted Mn-containing precipitates in high-Mn content alloys can diminish the desired properties. In the context of materials tailored under a process–structure–property relationship, it is important to elucidate the microstructural evolution that results from the processing conditions. Recent advances in process–structure relationship modeling techniques [7] have made it possible to illustrate the underlying physical nature in an interpretable form.

The phase-field approach is now one of the most widely adopted methods in microstructural evolution and phase transformation modeling [8–16]. Combined with computational thermodynamic databases, it can quantitatively simulate the solidification microstructure of alloys with consideration of latent heat release during phase transformation, anisotropy of interfacial energy and mobility. Wang et al. [14] simulated the three-dimensional (3D) growth morphology of the primary Si precipitate phase in hypereutectic Al–Si alloys using the phase-field approach. The proposed interface anisotropy

model successfully illustrated the formation of faceted Si grains, which was validated by comparison with scanning electron microscopic (SEM) images. Köhnen et al. [17] conducted two-dimensional (2D) phase-field simulation to examine the elemental distribution and epitaxial growth of solidification in additively manufactured X30Mn21 powder. Although phase-field modeling proved its functionality in solidification simulations, the literatures focuses on examining a few features of the method such as a precipitate morphology evolution without an interaction with matrix phase [14], 2D growth under rapid solidification conditions [17], 3D simulation in a binary alloy [15], or without considering solute redistribution [16].

In addition, most studies on the precipitation of Al alloys were carried out in the hypoeutectic region, where the precipitate forms as a secondary phase in the Al matrix [4–6,18]. In this study, microstructural evolution during solidification of a hypereutectic Al–Mn–Fe–Si alloy was studied with regard to the morphology and chemistry of the precipitates using the phase-field approach with experimental aid. To effectively capture the microstructural evolution, the thermal history during solidification was used as a primary process condition for the simulations. This approach utilized direct comparisons between the measured and the simulated temperature evolution, and resulting microstructures in semi-quantitative manner. The simulation results elucidated the phase evolution of multi-component/multi-phase alloy during solidification in each time/temperature step.

2. Materials and Methods

The phase-field model utilizes the phase-field parameter $\phi = \phi(\vec{x}, t)$ to represent the temporal/spatial evolution of phases and the corresponding microstructural changes. The multiphase-field approach proposed by Steinbach et al. [9,19] was implemented in MICRESS [20], a phase-field solver, to simulate the microstructural evolution in multi-component, multi-phase alloys which was used in this work. When coupled with CALPHAD (CALculation of PHase Diagrams)-type thermodynamic and kinetic databases, it has effectively facilitated kinetic simulations in various systems [8,11,13,14]. In this model, the evolution of multiphase-field parameter can be described using the following equation:

$$\frac{\partial \phi_\alpha}{\partial t} = \sum_{\beta \neq \alpha}^v M_{\alpha\beta}^\phi [b \Delta G_{\alpha\beta} - \sigma_{\alpha\beta} (K_{\alpha\beta} + A_{\alpha\beta}) + \sum_{\gamma \neq \alpha \neq \beta}^v j_{\alpha\beta\gamma}], \quad (1)$$

where, $M_{\alpha\beta}^\phi$ is the phase-field mobility, $\Delta G_{\alpha\beta}$ is the thermodynamic driving force, $K_{\alpha\beta}$ is the curvature term, $A_{\alpha\beta}$ is the interface anisotropy where $0 \leq \phi_i \leq 1$ and $\sum_\alpha \phi_\alpha = 1$ are always satisfied, b is the numerical weight constant, and $j_{\alpha\beta\gamma}$ is the triple-junction term. In this study, two types of interface anisotropy were applied to depict the different growth natures of dendritic Al grains and Al_6Mn precipitates. Interfacial stiffness (σ^*) and mobility (μ) anisotropy functions for Al grains are defined as follows [21]:

$$a_{\sigma^*}^{\text{Al}} = 1 - \delta_{\sigma^*} \cdot 4 \cdot (n_x^4 + n_y^4 + n_z^4 - 0.75), \quad (2)$$

$$a_{\mu}^{\text{Al}} = 1 + \delta_{\mu} \cdot 4 \cdot (n_x^4 + n_y^4 + n_z^4 - 0.75), \quad (3)$$

where $\vec{n} = (n_x, n_y, n_z)$ is the interface normal vector, and the coefficients δ_{σ^*} and δ_{μ} were set to 0.05 for both. Similarly, anisotropy functions for faceted Al_6Mn were defined as follows [21]:

$$a_{\sigma^*}^{\text{Al}_6\text{Mn}}(\theta) = [\delta_{\sigma^*} + (1 - \delta_{\sigma^*}) \cdot \tan|\theta|/\kappa \cdot \tanh(\kappa/\tan|\theta|)]^{-1}, \quad (4)$$

$$a_{\mu}^{\text{Al}_6\text{Mn}}(\theta) = \delta_{\mu} + (1 - \delta_{\mu}) \cdot \tan|\theta|/\kappa \cdot \tanh(\kappa/\tan|\theta|), \quad (5)$$

where θ is the angle between $\vec{n}$ and the pre-defined facet vector, and the coefficients δ_{σ^*} , δ_{μ} , and κ were set to 0.7, 0.5, and 0.75, respectively. Pre-defined {101} facet planes of octahedral Al_6Mn were adopted in accordance with Kang et al. [22] and Yang et al. [23]. The nucleation of the precipitates followed

a model proposed by Greer et al. [24] which is widely used in phase-field simulations involving the nucleation of phases [10,25,26]. The onset of the nucleation and growth of the precipitate occurred when a seed of precipitate achieved the desired undercooling which is inversely proportional to the seed radius. The size distribution of the precipitate seeds was taken from the positive tail of a normal distribution as shown in Figure 1. The given distribution was determined to depict reasonable primary precipitate distribution and to be compatible with the experimental observations.

Figure 1. Size distribution of the precipitate seed.

During solidification, the overall heat flux is a balance between the heat extraction upon cooling and the latent heat released upon phase transformation when the geometrical interferences are neglected. Therefore, the temperature change (dT) can be calculated as [27].

$$dT = \frac{1}{\bar{c}_p} (\dot{q} dt - dL) \quad (6)$$

where $\dot{q}$ is the heat extracted per unit volume, $\bar{c}_p$ is the average heat capacity, and dL is the latent heat contribution which is given by the transformation kinetics. Consequently, a semi-quantitative kinetic simulation can be achieved by comparing experimental and simulated domain temperature evolution. The TCAL6 [28] and MOBAL5 [29] databases from Thermo-Calc software [30] were coupled with phase-field simulations through the TQ-Interface to perform the thermodynamic and diffusion calculations, respectively.

A hypereutectic Al–Mn alloy was melted at 1003 K in an electric furnace, degassed using an Ar gas bubbling filtration, and poured into a steel mold preheated to 473 K. The chemical composition of the specimen is listed in Table 1 that was analyzed by Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) using an Agilent 5100/5110 VDV ICP-OES (Agilent, Santa Clara, CA, USA). The temperature evolution of the cast was measured by Type-K thermocouples directly inserted into the melt (see Supplementary Material for the detailed design). The measured temperature profile was used as a primary process parameter in the phase-field simulations. The initial cooling rate near the pouring temperature was 13.5 K/s. The microstructure of the as-cast specimen was analyzed by scanning electron microscopy (SEM), electron backscatter diffraction (EBSD), and energy-dispersive spectroscopy (EDS) using a JSM-7900F microscope (JEOL Ltd., Tokyo, Japan) equipped with Symmetry EBSD (Oxford Instruments NanoAnalysis, High Wycombe, UK) and an X-Max 150mm² EDS module (Oxford Instruments NanoAnalysis, High Wycombe, UK). The accelerating voltage was 15 kV for the EBSD and EDS analyses. The obtained EBSD–EDS micrographs were analyzed using Aztec (4.3, Oxford Instruments NanoAnalysis, High Wycombe, UK and OIM Analysis (8.1, EDAX LLC, Mahwah NJ, USA) software to determine the orientation characteristics and grain size statistics.

Table 1. Chemical composition of the as-cast alloy specimen analyzed by Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES).

Element	Al	Mn	Fe	Si	Zn	Ti
Composition (wt%)	Bal.	2.7	0.2	0.07	0.01	0.02

3. Results and Discussion

During the solidification of the hypereutectic Al–2.7Mn–0.2Fe–0.07Si alloy, four major phases were expected to appear in the following sequence from the equilibrium phase fraction and Scheil–Gulliver calculations as shown in Figure 2: liquid $\rightarrow$ liquid + Al₆Mn $\rightarrow$ liquid + Al₆Mn + α -Al $\rightarrow$ liquid + Al₆Mn + α -Al + α -Al(Mn,Fe)Si. After solidification is complete, Al₁₂Mn forms from solid state phase transformation out of α -Al at temperatures below 547 K; however, this is beyond the scope of this work. In the stoichiometric Al₆Mn precipitate phase, the Mn sublattice site is partially occupied by Fe to form Al₆(Mn_{*x*},Fe_{1–*x*}). The Fe-to-Mn ratio in the precipitate increases as solidification proceeds due to the limited solubility of Fe in the α -Al phase and subsequent Fe-enrichment in the interdendritic melt channel.

Figure 2. (a) Equilibrium phase fraction change with temperature (b) Scheil–Gulliver solidification calculation.

The microstructure of the as-cast specimen was analyzed by backscattered electron (BSE) imaging and EBSD, as shown in Figure 3. The low and high magnification BSE micrographs presented in Figure 3a,b reveal three distinctive types of precipitate: large, faceted Al₆Mn primarily formed during solidification; fragmented Al₆Mn in the interdendritic channel; and fine-dispersed Al₁₂Mn in the matrix. Two Al₆Mn precipitates formed in different solidification stages and exhibited different Fe-to-Mn ratios in the EDS analysis (Table 2). The average site fraction determined from the Mn-to-Fe ratio was Al₆(Mn_{0.80},Fe_{0.20}) for precipitates in the interdendritic channel, which is due to the enrichment of Fe rejected from the α -Al solidification front in the residual melt. On the other hand, the primary precipitate exhibited Al₆(Mn_{0.91},Fe_{0.09}) which is close to the Mn-to-Fe ratio in the nominal composition. The Al content measured in the smaller precipitates was higher than the stoichiometric content, which was caused by the interaction of the electron beam with the matrix beneath the precipitates. Figure 4 shows the precipitate distribution and the grain shapes analyzed with EBSD. The average α -Al grain size measured with EBSD was 357 ± 140 μ m, where small precipitates occupying less than 15 pixels were excluded from the grain size calculation. This value was used to determine the 2D and 3D simulation domain sizes in the phase-field simulations.

Table 2. EDS point and linescan data from Figure 3b. *x* denotes the site fraction of Mn in Al₆(Mn_{*x*},Fe_{1–*x*}) precipitate.

Element (wt%)	1	2	3	4	Point ID 5	6	7	8	9	Averaged Profile in Figure 3b
Al	81.67	82.65	79.05	80.24	77.66	82.19	83.17	81.99	83.72	69.46
Mn	15.13	14.15	14.28	15.55	17.59	13.93	14.23	13.89	14.80	2.64
Fe	3.20	3.20	6.67	4.21	4.75	3.87	2.60	4.12	1.48	27.90
<i>x</i>	0.83	0.82	0.69	0.79	0.79	0.79	0.85	0.77	0.91	0.91

Figure 3. Backscattered electron (BSE) micrographs (a) low-magnification image (b) high-magnification image with energy-dispersive spectroscopy (EDS) linescan profiles along the yellow line.

Figure 4. Orientation map analyzed with EBSD where black line indicates grain tolerance angle over 5 degrees.

Microstructural evolution during solidification is closely related to the thermal history of the system. The temperature change can be roughly estimated by Equation (6) with reasonable assumptions of the nucleation and transformation kinetics. Since the expected total phase fraction of the precipitates was determined to be less than 8 mol% in the Scheil–Gulliver simulation, the latent heat contribution mainly came from the phase transition between liquid and α -Al. Based on the thermal history estimated from the measured temperature profile, 2D and 3D phase-field simulations were conducted. In the simulations, two major solid phases were considered to be formed from the liquid phase: Al_6Mn precipitate and α -Al matrix. The formation of α -Al(Mn,Fe)Si was neglected since the expected phase fraction was less than 0.1 mol% and the phase was not observed in the microscopic analysis. Primary and interdendritic Al_6Mn precipitates were assigned to have identical phase-field indexes and were distinguished by their Fe contents.

Figure 5a compares the simulated and experimentally measured temperature profiles. The related simulation parameters are listed in Table 3. Due to the limitation of the available study on the phase interactions in hypereutectic Al–Mn system, interface energies were set to be similar to the Al–Si system [14] which exhibits faceted precipitates. Interface mobilities were set to be fast enough to maintain a diffusion-controlled solidification regime. The nucleation kinetics of the primary precipitate were not discernable in both the simulated and measured temperature profiles, while recalescence and

the extended temperature arrest near the eutectic temperature were evident, which can be attributed to the formation of the solid α -Al phase. As shown in Figure 5b, during microstructural evolution, over time, nucleation and growth of the primary precipitate do not pose significant effects on the temperature evolution. Meanwhile, the formation of α -Al (colored in red in the phase map) was found to have significant delay on cooling. The primary precipitates continued to grow with faceted shapes until they were captured in the solid α -Al phase as the solubility and the diffusion of Mn and Fe in solid Al are limited. When the fully solidified microstructure was compared with the EBSD phase map, as shown in Figure 5c, the simulated results effectively depicted the morphological characteristics of the grain and phase distributions. The elongated precipitates seen in Figures 4 and 5c were not considered in the simulations since these precipitates exhibit similar chemical constitution to the faceted primary precipitate. Due to the limited solubility of Fe and Si in the solid α -Al phase, most of them were segregated in the interdendritic channels as shown in Figure 6.

Figure 5. (a) Simulated and measured temperature profiles (b) 2D simulated microstructural evolution (c) observed using EBSD and simulated phase maps in scale-matched form.

Table 3. Phase-field simulation parameters.

Parameter	Value	Unit
Simulation grid size	1	μm
2D simulation domain size	1000×1000	μm^2
3D simulation domain size	$125 \times 125 \times 125$	μm^3
Interface thickness	3.0	cells
Heat extraction rate	8.8×10^7	$\text{J/s} \cdot \text{m}^3$
$\sigma_{\text{liq-Al}}$	0.09	J/m^2
$\mu_{\text{liq-Al}}$	10^{-10}	$\text{m}^4/\text{J} \cdot \text{s}$
$\sigma_{\text{liq-ppt}}$	0.5	J/m^2
$\mu_{\text{liq-ppt}}$	10^{-12}	$\text{m}^4/\text{J} \cdot \text{s}$
$\sigma_{\text{Al-ppt}}$	0.2	J/m^2
$\mu_{\text{Al-ppt}}$	10^{-9}	$\text{m}^4/\text{J} \cdot \text{s}$

To resolve the difference between the primary and interdendritic precipitates, a 3D simulation was conducted with a domain size of $125 \times 125 \times 125 \mu\text{m}^3$. An α -Al nucleus was placed in the corner of the domain, and the symmetric boundary conditions for the x, y, and z directions were applied based on the cubic symmetry of the face-centered cubic α -Al phase. This configuration gave a diagonal α -Al grain size of $433 \mu\text{m}$, which sufficiently covers the average grain size estimated in the EBSD analysis. The simulation results presented in Figure 7 show well-defined facet planes of the primary precipitates, supporting the current model used in the simulations. After the primary precipitates randomly

nucleated and grew, an α -Al nucleus appeared in the bottom-left corner. Finally, small precipitates appeared in the interdendritic channel. The largest precipitate size was 55.2 μm , which is a reasonable value compared with the experimental observations. Figure 8 shows the Mn and Fe distribution of the region where the corresponding phase is indexed as Al_6Mn . An increase in the Fe concentration is evident moving from the bottom-left corner to top-right according to the shift of the α -Al solidification front. The stoichiometry of the primary precipitate was found to be $\text{Al}_6(\text{Mn}_{0.94}, \text{Fe}_{0.06})$, which is similar to the initial liquid concentration ratio. The interdendritic precipitate, $\text{Al}_6(\text{Mn}_{0.82}, \text{Fe}_{0.18})$, showed a higher Fe content, similar to the value measured with EDS. The limited solubility of Fe in the solid α -Al phase induced severe segregation of Fe in the interdendritic liquid channel, which led to the formation of Fe-concentrated precipitate in the last stage of solidification.

Figure 6. Simulated elemental distributions.

Figure 7. 3D simulated microstructural evolution.

Figure 8. Mn and Fe distributions in the precipitates when the solidification was completed.

4. Conclusion

In summary, 2D and 3D phase-field simulations were conducted to investigate the microstructural evolution during solidification in a hypereutectic Al–Mn–Fe–Si alloy. The applied model successfully demonstrated the formation of the faceted precipitate morphology and the different Mn-to-Fe ratios of the precipitates formed in the different solidification stages. Due to the strong segregation of the alloying elements in the liquid phase, the precipitate that formed in the interdendritic channel exhibited a higher Fe content than the primary precipitate. The semi-quantitative simulations, which adopted the thermal history of the specimen as the simulation condition, allowed for a direct comparison between the measured and the simulated temperature evolution reflecting latent heat release and recalescence during the solidification process. The simulated results containing information about the spatial distribution of the phases and compositions obtained with proper consideration of the process conditions can be transferred to future methods for further integrated process–structure–property simulations.

Supplementary Materials: The following are available online at <http://www.mdpi.com/2075-4701/10/10/1325/s1>, Figure S1: Construction design details of the casting mold, Figure S2: Simulation scheme, Figure S3: Precipitate size distribution at the end of simulation ($t = 11.2$ s, $T = 920$ K).

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