



# A phase field model coupled with pressure-effect-embedded thermodynamic modeling for describing microstructure and microsegregation in pressurized solidification of a ternary magnesium alloy



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## ABSTRACT

This paper presents a phase field model for describing microstructure and microsegregation in pressurized solidification of a ternary magnesium alloy, which captured essential physics associated with pressurized solidification of multi-component system, including pressure-effect-embedded thermodynamic modeling (PEE thermodynamic modeling) and interactive diffusion. This model was applied to squeeze casting of a Mg–Al–Sn alloy and revealed that the applied pressure increased solute trapping and solute accumulation in front of solid/liquid interface, which are two opposite factors contributing to microsegregation. Governed by the mechanism, the microsegregation of solute Al aggravates with applied pressure considerably, while that of Sn is rarely influenced by the pressure.

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## 1. Introduction

Magnesium alloys are attractive to automotive industry due to their low density, excellent castability and machinability [1–3], among which a new ternary system, Mg–Al–Sn alloy, is promising with better combinations of strength and ductility compared with conventional AZ91 or AM50 alloy [2,3]. Squeeze casting is an advanced near-net-shape materials processing technology, in which molten metal solidifies under applied pressure, making high-integrity castings with excellent mechanical properties [2,4–6].

Pressure is an essential factor in determining the microstructure and thus mechanical properties of squeeze castings. A change in pressure will alter phase diagrams of alloy systems dramatically [7–10] due to the change in thermodynamic driving force. This will subsequently change dendrite growth thermodynamics (such as solid solubility [10,11] and phase fractions [11,12]) and kinetics

(such as nucleation [13], tip growth velocity [14], grain size [5], secondary dendrite arm space [5] and solute diffusion coefficients [11,14]).

Microsegregation is a common phenomenon during non-equilibrium solidification especially in rapid solidification and pressurized solidification due to the solute redistribution, resulting in reduced ductility and corrosion resistance. Consequently, microsegregation in metallic alloys is highly important for applications such as process optimization and alloy development [15,16]. It was reported that parameters such as interface kinetic coefficient, surface energy, anisotropy parameter and noise amplitude have a significant influence on the microsegregation in front of solid/liquid (S/L) interface [17]. Therefore, it is important to quantify the effect of applied pressure on microsegregation of squeeze castings.

Phase field modeling [18–23] is based on solute diffusion, thermodynamic driving force and ordering potential, so it is feasible to include the effects of pressure on the thermodynamics and kinetics of dendritic growth in the models [14,24,25]. Börzsönyi et al. [24] and Shang et al. [25] introduced a melting-point-related term, caused by pressure according to the Clausius–Clapeyron relationship, into the phase field equation to investigate the effects of

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periodically-applied pressure on dendritic growth. The model they adopted was relatively simple but neglected the thermodynamic data of the studied system. Recently, our previous work [14] established a binary phase field model with pressure effect, which is thermodynamically consistent with Mg–Al alloy system. Since commercial magnesium alloys are generally based on multi-component systems, a multi-component phase field model coupled with corresponding thermodynamics is an important and imperative task in quantitative simulation of pressurized solidification. However, research so far [26] has achieved this coupling only at ambient pressure, not under applied pressure due to the lack of a systematic thermodynamic model with pressure effects in commercial CALPHAD (CALCulation of PHase Diagrams) codes, such as Thermo-Calc<sup>®</sup> [27] and PANDAT<sup>®</sup> [28]. Fortunately, Brosh et al. [8,29,30] constructed a thermodynamic model with pressure effect based on the integration of available CALPHAD descriptions at ambient pressure [31] with a composition-dependent EOS (equation of state). Nevertheless, a phase field model coupled with pressure-effect-embedded thermodynamic modeling has not been established for multi-component systems yet.

In this work, an attempt was made to establish a comprehensive phase field model coupled with PEE thermodynamic modeling to describe microstructure and microsegregation in pressurized solidification of a ternary magnesium alloy. Based on this model, the influence of pressure on microsegregation pattern in front of S/L interface and the microsegregation in microstructure of a Mg–Al–Sn alloy was investigated, and the different responses of the microsegregation of solute Al and Sn to the applied pressure were quantified.

## 2. Model description

### 2.1. Phase field model at ambient pressure

The free energy density of a phase in a multicomponent system consisting of  $(n + 1)$  components with  $n$  solutes in solid and liquid phases is illustrated as follows [19],

$$f^m = (c_{1m}, c_{2m}, \dots, c_{im}, \dots, c_{nm}) \quad (1)$$

where  $m = S$  for the solid phase or  $m = L$  for the liquid phase. The governing equations for phase field and concentration field of a multicomponent system at ambient pressure are given as follows:

$$\frac{1}{M_\phi} \frac{\partial \phi}{\partial t} = \varepsilon^2 \nabla^2 \phi - w g'(\phi) - h'_p(\phi) \left( f^S - f^L - \sum_{i=1}^n (c_{iS} - c_{iL}) \tilde{\mu}_i \right) \quad (2)$$

$$\frac{\partial c_i}{\partial t} = \nabla \cdot [1 - h_d(\phi)] \sum_{j=1}^n D_{ij}^+ \nabla c_{jL} + \nabla \cdot \left( \frac{\varepsilon}{\sqrt{2w}} (c_{iL} - c_{iS}) \right) \frac{\partial \phi}{\partial t} \frac{\nabla \phi}{|\nabla \phi|} \quad (3)$$

where  $\phi$  is the phase field, defined as  $\phi = 0$  in the bulk liquid,  $\phi = 1$  in bulk solid and  $0 < \phi < 1$  in the interfacial region between them.  $h_p(\phi)$  is a monotonous interpolation function, with  $h_p(0) = 0$  and  $h_p(1) = 1$  and  $g(\phi)$  is the double-well potential, which can be found in Ref. [14] and  $D_{ij}$  is the diffusivity in solid or liquid phase. The second term in the right hand side of the concentration equation is 'anti-trapping' current term. In this work, there are two types of 'trapping', one is 'false' trapping that is induced by phase field model with thin and finite interface width, i.e. numerical algorithm, and the other one is 'physical' trapping that results from S/L interface movement. The anti-trapping term in the diffusion equation is used to eliminate the effect of 'false' trapping [19,32].

The compositions  $c_{iS}$  and  $c_{iL}$  at a particular position in the computational domain are different but not independent of each other,

which are restricted by the equal chemical potential condition [33–35] in Eq. (4) where  $\tilde{\mu}_i$  is the chemical potential.

$$\frac{\partial f^S}{\partial c_{iS}} = \frac{\partial f^L}{\partial c_{iL}} \equiv \tilde{\mu}_i \quad (4)$$

Parameters in the phase field equations are the phase field mobility  $M_\phi$ , the gradient energy coefficient  $\varepsilon$  and the height of the parabolic potential  $w$ . The gradient energy coefficient and the height of the parabolic potential are determined by the interface energy  $\sigma$  and interface width  $2\lambda$ , and given as follows [33]:

$$\varepsilon = \sqrt{\frac{6\lambda\sigma}{\alpha}} \quad (5)$$

$$w = \frac{3\alpha\sigma}{\lambda} \quad (6)$$

In this work, we define that in the interface region,  $\phi$  changes from 0.05 to 0.95 at  $-\lambda < x < +\lambda$ , then  $\alpha \approx 2.94$ . The phase field mobility  $M_\phi$  is defined by the following equation [36],

$$M_\phi^{-1} = \frac{\varepsilon^3}{\sigma\sqrt{2w}} \left( \frac{1}{D_{1i}} \xi_1 (c_{1L}^e, c_{1S}^e) + \frac{1}{D_{2i}} \xi_2 (c_{2L}^e, c_{2S}^e) \right) \quad (7)$$

The anisotropy is introduced into the interface energy and then into the gradient energy coefficient, which is shown below [14]:

$$\sigma(\theta) = \sigma_0 [1 + \gamma \cos(\eta\theta)] \quad (8)$$

$$\varepsilon(\theta) = \varepsilon_0 [1 + \gamma \cos(\eta\theta)] \quad (9)$$

where  $\sigma_0$  and  $\varepsilon_0$  are the isotropic interface energy and gradient energy coefficient, respectively and  $\gamma$  is the anisotropy strength. For Mg based alloys with sixfold anisotropy,  $\eta = 6$ .  $\theta$  is the angle between the normal to the interface pointing to the liquid and the horizontal direction. The detailed definitions of parameters in the governing equations can be found in Refs. [14,19,33–35].

A ternary magnesium system, Mg–Al–Sn, especially AT72 (Mg–7Al–2Sn) alloy with good combination of strength and ductility [3,37] was selected for model validation. Some simulation parameters of squeeze casting AT72 alloy are given in Table 1, where 1 and 2 represent the solute Al and Sn, respectively. To reflect the solute interactions in multi-component system, the interactive diffusion coefficient was calculated using DICTRA<sup>®</sup> software and included in the simulation.

### 2.2. Phase field model coupled with PEE thermodynamic modeling

To include the pressure effect in phase field simulation, the governing equations were modified by adjusting some pressure-related parameters as follows:

**Table 1**

Parameters used in the simulation of squeeze casting AT72 alloy.

Parameters	Value	
Simulation temperature	863 K	
Initial composition, $c_1^0$	6.37 at.%	
Initial composition, $c_2^0$	0.41 at.%	
Grid size, $\Delta x$	$6.0 \times 10^{-7}$ m	
Time step, $\Delta t$	$5.76 \times 10^{-6}$ s	
Interface energy, $\sigma_0$	0.093 J/m <sup>2</sup>	Ref. [14]
Interface width, $2\lambda$	$4\Delta x$	Ref. [14]
Anisotropy strength, $\gamma$	0.1	
Molar volume, $V_m$	$1.36 \times 10^{-5}$ m <sup>3</sup> /mol	Ref. [14]
$D_{11}^L(P_0, 863 \text{ K})$	$1.21 \times 10^{-9}$ m <sup>2</sup> /s	DICTRA <sup>®</sup>
$D_{12}^L(P_0, 863 \text{ K})$	$+6.53 \times 10^{-10}$ m <sup>2</sup> /s	
$D_{21}^L(P_0, 863 \text{ K})$	$+1.07 \times 10^{-11}$ m <sup>2</sup> /s	
$D_{22}^L(P_0, 863 \text{ K})$	$5.50 \times 10^{-10}$ m <sup>2</sup> /s	

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