A coupled thermomechanical, thermal transport and segregation analysis of the solidification of aluminum alloys on molds of uneven topographies

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Abstract

A coupled thermomechanical, thermal transport and segregation analysis of aluminum alloys solidifying on uneven surfaces is presented here. Uneven surfaces are modelled as sinusoids with different wavelengths and amplitudes. Effects of various coupling mechanisms between the solid-shell deformation, air-gap formation, heat transfer, fluid flow and segregation, near the mold-metal interface, are observed for different mold topographies during the early stages of solidification of an aluminum alloy. The role of inverse segregation, arising from shrinkage driven flow in the melt, melt superheat and varying mold surface topography on nucleation of air-gaps and evolution of stresses in the solidifying shell is examined. The numerical model consists of a volume-averaged solidification model coupled with a small-deformation model combining elasto-viscoplastic deformation in the solidifying shell with air-gap nucleation and imperfect contact at the metal/mold interface. Heat transfer at the mold-metal interface is either contact pressure or air-gap dependent and is modelled using the actual contact pressure or air-gap size obtained from the contact sub-problem at the metal-mold interface. Variation in heat transfer leads to variations in fluid flow, segregation and stresses developing in the solid and mushy-zone, which in turn affect the morphology of the growing solid-shell. A wavelength range that leads to a reduction in equivalent stresses, segregation and growth front morphology unevenness, in the evolving solid-shell, is obtained for varying solute concentrations. One of the main objectives of the current analysis is to seek optimal mold surface topographies that minimize surface defects leading to desired cast surface morphologies.

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1. Introduction

During the early stages of solidification of aluminum alloys, phenomena occurring at the solid-shell/mold interface have a direct influence on the formation of surface defects such as cracks, liquation and inverse segregates. This in turn has profound influence on the final macro-morphology and microstructure of the cast alloy. Removal of surface defects from castings leads to large material, monetary and energy losses. One of the main motivations of the current study is to obtain a detailed understanding of the surface-defect formation process in cast aluminum alloys and explore the role of tuned mold surface topographies to minimize or eliminate these defects.

Very often during casting of metals or alloys, air-gaps form at the metal-mold interface leading to a non-uniform heat transfer rate into the casting. This in turn affects other transport phenomena and stress-development in the solid-shell. Semi-analytical studies of air-gap nucleation during solidification of a pure metal on sinusoidal surface topographies were carried out in [1–3] using a thermo-hypoelastic perturbation theory neglecting plastic deformation. Gap nucleation times for different sinusoidal wavelengths and for different mold-shell material combinations were obtained in [1–3] and the concept of a critical wavelength was introduced to classify different surface topographies based on air-gap nucleation locations. The deformation of solidifying bodies has been studied in [4–6] using a hypoelastic rate-dependent small-deformation model. The mold surface here was however assumed to be planar and air-gap formation was not modeled. In [7], a thermo-mechanical analysis of solidification to predict the air-gap thickness at the metal-mold interface was presented, but segregation and solute transport were not modeled. In verti-

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cally solidified casts, inverse segregation is commonly observed at the bottom due to exudation and shrinkage driven flow. Exudation is the process of the interdendritic liquid being forced through the solid shell, past the original casting surface and into the air-gap [8–10]. This is usually caused either by the remelting of the evolving solid shell or due to the metallostatic pressure of the liquid column. Inverse segregation leads to a solute enriched zone at the bottom of solidified castings and the mushy zone through which exudation occurs is depleted of solute elements. This results in a heterogeneous solute distribution and leads to non-uniform mechanical properties and defects such as bleed bands, cold shuts and segregates in the cast product which increase its susceptibility to failure during further mechanical operations [11]. In [8–10], a model of surface segregation in aluminum alloys driven by exudation and solidification shrinkage was presented. Air-gap formation in their model was expressed mathematically through a variable convective heat transfer coefficient at the boundary. Effect of shrinkage driven fluid flow on segregation, arising during solidification of alloys, has also been modelled in [12–16]. The development of constitutive relations for deformation of the mushy-zone has been addressed in [17–19] using both experimental and numerical investigations. In [17], a new hot-tearing criterion for metal alloys was proposed and a critical deformation rate introduced beyond which nucleation first started. In [18], a continuum model was presented for an isotropic two-phase mushy-zone and hot-tearing criteria for metal alloys were determined from variation in parameters like casting speed, solidification interval and cooling contraction of the solid phase. Constitutive models for viscoplastic deformation and thermal strain in solidifying aluminum alloys were developed in [19] based on experimental studies and thermomechanical simulations. In [20,21], the effect of strain-rate relaxation on the stability of the solid front growth morphology, during solidification of pure metals on uneven surfaces, was studied using an experimentally determined creep law.

Heat transfer at the metal-mold interface, thermal stress development, imperfect contact, air-gap nucleation, fluid flow and segregation are typical phenomena that occur at the early stages of solidification. Mold surface unevenness plays an important role during early stages of solidification and can influence the growth morphology and microstructure of the solid-shell. Understanding the effect of mold surface topography on the heat extraction process and the solid-shell growth holds the potential promise of controlling cast surface morphologies to eliminate or minimize surface defects. Very often in the casting industry, mold surfaces are given an artificial topography to enhance heat transfer and wettability characteristics. These topographies generally range from unidirectional grooves to discrete recessions or cavities. A periodic mold surface topography on the surface of a copper mold block used for immersion studies is shown in Fig. 1 with the experimental details given in [22]. In this test, the block in Fig. 1 is lowered into and held within a bath of molten aluminum for period of time sufficient to permit the growth of thin shell, at which point the block is extracted. Although this experiment involves a moving mold surface previously modelled in [23], the surface topography depicted in Fig. 1 is a bi-directional counterpart of the unidirectional topog-

Fig. 1. A mold surface with periodic 'groove' topography to control heat extraction during directional solidification (courtesy ALCOA Corp.).

raphy modeled in the present work for stationary molds. The periodic groove topography allows multi-directional heat flow at the mold/shell interface. The pitch or wavelength must be on the millimeter scale to obtain anticipated benefits.

In our previous work [24], the effect of uneven surface topography on macrosegregation in aluminum alloys solidifying on uneven surfaces, in the form of sinusoids, was examined. Air-gap nucleation was not modelled here and perfect contact at the mold-metal interface was assumed throughout the solidification process. Effects of uneven surface topography on macrosegregation and fluid flow during horizontal and vertical solidification of an aluminum–copper (Al–Cu) alloy were studied. In [25], Tan and Zabaras presented a thermomechanical analysis to study the effects of uneven mold surface topographies on early stage solidification of aluminum alloys. Constitutive models for viscoplastic deformation and thermal strain in the mushy-zone, developed in [19], were used in their numerical model. Air-gap formation at the solid-shell/mold interface was modelled by solving the contact sub-problem and therefore the contact pressure/air-gap dependent thermal boundary conditions at the interface were dynamically determined. Segregation was not modelled in [25] and solute distribution was assumed to be uniform.

In our current work, we extend the thermomechanical analysis to examine stress development, morphology of the growing solid-shell and air-gap formation at the metal-mold interface in the presence of inverse segregation caused by shrinkage driven fluid flow in the alloy. The latter is associated with feeding of the mushy zone to compensate the volume change during solidification that arises due to different densities of the solid and liquid phases. Variation in solute concentration results in local variations in liquidus temperature of the alloy. This in turn affects the solid mass fractions and consequently affects the air-gap nucle-

ation and evolution process, and the growth front morphology. Effects of varying solute concentrations are also observed in stresses developing in the solidifying shell. Modelling solute transport along with thermal and fluid transport during early stage solidification of alloys is therefore indispensable. The mold deformation is also important in understanding defect formation in the early stages of solidification since mold distortion also mitigates air-gap nucleation and solid shell distortion. However, even though our analysis can account for deformable molds, we have selected in this work to consider only rigid molds. This simplification allows for a more direct examination of the effects of inverse segregation in the morphology of the growing solid-shell.

The organization of this paper is as follows. In Section 2, the mathematical model, describing solidification and deformation of an aluminum alloy, is presented along with important assumptions invoked. The thermal coupling involving air-gap and contact pressure, previously described in [3,7,18,25] is summarized here. In Section 3, numerical discretization techniques for the governing equations are discussed briefly along with the solution and time stepping strategies. Section 4 deals with numerical examples. Numerical simulations discussed here involve coupled deformation of a directionally solidifying Al–Cu alloy along with fluid flow, segregation and air-gap formation. Fluid flow in these examples is driven by a combination of thermosolutal buoyancy and shrinkage and is one to two orders of magnitude higher than fluid flow in the corresponding examples of [25]. The effects of mold surface topography, melt superheat, different initial solute concentrations and different mold materials are observed on stress development, interfacial air-gap formation and solid-shell morphology unevenness in the examples reported here. The results obtained are compared with corresponding cases in [25] to observe changes caused by segregation on some of the above phenomena. Important observations and conclusions from the present analysis are made in Section 5.

2. Mathematical model

2.1. Description of the solidification problem

Directional solidification of an Al–Cu alloy on sinusoidal molds of wavelength, λ , and amplitude, A as shown in Fig. 2, is considered. A single domain model based on volume-averaged governing transport equations, similar to those discussed in [26–30], is used for modelling solidification of the alloy. The single set of governing transport equations, valid throughout the domain, are listed in Box 1. The volume-averaged energy equation based on enthalpy is transformed into temperature using thermodynamic and two-phase relations in the mushy-zone. The mushy-zone permeability, K , is assumed to be isotropic and is given by the Kozeny–Carman relation as:

$$K(\epsilon_l) = \frac{K_0 \epsilon_l^3}{(1 - \epsilon_l)^2}, \quad (2.1)$$

where ϵ_l denotes the volume fraction of the liquid. The parameter K_0 is related to the secondary dendrite arm spacing, d , as

$K_0 = d^2/180$. In the two-phase mushy-zone, the total solute concentration, C , is expressed in terms of the individual phase concentrations as

$$C = f_l C_l + f_s C_s, \quad (2.2)$$

where C_l is the solute concentration in the liquid phase and C_s is the solute concentration in the solid phase. Also, f_l and f_s denote the corresponding mass fractions. The density in the mushy-zone is given by

$$\rho = \rho_l \epsilon_l + \rho_s \epsilon_s, \quad (2.3)$$

where ρ_s and ρ_l denote the densities of the solid and liquid phases, respectively, while ϵ_s denotes the solid volume fraction. We assume conservation of both mass and volume. Volume fractions are related to the respective mass fractions as $\epsilon_l = \rho f_l / \rho_l$ and $\epsilon_s = \rho f_s / \rho_s$. Closure of the numerical model is achieved through separate thermodynamic relationships describing the evolution of the liquid mass fraction. These are listed below:

$$\text{Lever rule : } f_l = 1 - \frac{1}{1 - \kappa_p} \left(\frac{T - T_{liq}}{T - T_m} \right), \quad (2.4)$$

$$\text{Scheil rule : } f_l = \left(\frac{T - T_m}{T_{liq} - T_m} \right)^{1/(k_p - 1)}, \quad (2.5)$$

where the liquidus temperature, T_{liq} , is expressed as, $T_{liq} = T_m + m_{liq} C$, with T_m being the melting temperature and m_{liq} the slope of the liquidus line. Also, κ_p denotes the partition coefficient of the alloy. In our numerical model, we use the Scheil rule (Eq. (2.5)) for calculating liquid mass fractions from temperature and solute concentration in the liquid phase. C_s is calculated as

$$C_s = \frac{1}{1 - f_l} \int_{f_l}^1 k_p C_l df_l = \frac{I}{1 - f_l}, \quad (2.6)$$

where I is the required integral updated at a particular time step using the following relation:

$$I_{n+1} = I_n + 0.5 \kappa_p (C_{l,n} + C_{l,n+1})(f_{l,n} - f_{l,n+1}). \quad (2.12)$$

In Eq. (2.8), the reference concentration, C_{l0} , is the same as the initial solute concentration, C_0 . Also in Eq. (2.9), T_e and h_f denote the eutectic temperature and latent heat, respectively. Imperfect contact between the solid-shell/mold interface significantly affects thermal conditions at that interface. This in turn affects fluid flow, segregation and solid-shell growth morphology. When air-gaps form between the solid-shell and mold surface, there is a decrease in heat flux. In our numerical model, we use two different heat flux formulations, described in [3,31], to simulate the change in thermal boundary conditions caused by air-gap formation. These have been previously used in [25] and are expressed as follows:

$$q = \begin{cases} q_g = \frac{h_0}{1 + \Delta_{gap} h_0 / k_0} (T_{cast} - T_{mold}), & \text{if } \Delta_{gap} > 0, \\ q_c = \frac{1}{(R_0 + R' p_{contact})} (T_{cast} - T_{mold}), & \text{if } \Delta_{gap} = 0, \end{cases} \quad (2.13)$$

Box 1. Governing transport equations for solidification of alloys

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (\mathbf{x}, t) \in \Omega \times [0, t_{\max}], \quad (2.7)$$

$$\begin{aligned} \frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot \left(\frac{\rho \mathbf{v} \mathbf{v}}{f_1} \right) \\ = -\nabla p + \frac{p}{\epsilon_1} \nabla \epsilon_1 - \frac{\epsilon_1 \rho \mu_1}{\rho_1 K(\epsilon_1)} \mathbf{v} + \frac{\mu_1}{\rho_1} \nabla \cdot [\nabla(\rho \mathbf{v}) + (\nabla(\rho \mathbf{v}))^t], \\ - \epsilon \rho_0 g [\beta_{l,T}(T - T_0) + \beta_{l,C}(C_1 - C_{l_0})] e_g, \quad (\mathbf{x}, t) \in \Omega \\ \times [0, t_{\max}], \end{aligned} \quad (2.8)$$

$$\begin{aligned} \rho c^* \frac{\partial T}{\partial t} + \rho c_1 \mathbf{v} \cdot \nabla T \\ = \nabla \cdot [(\epsilon_1 k_1 + \epsilon_s k_s) \nabla T] - \rho_s ((c_1 - c_s)(T - T_e) + h_f) \frac{\partial \epsilon_1}{\partial t}, \\ (\mathbf{x}, t) \in \Omega \times [0, t_{\max}], \end{aligned} \quad (2.9)$$

$$\begin{aligned} \frac{\partial(\rho C)}{\partial t} + \nabla \cdot (\rho \mathbf{v} C_1) = \nabla \cdot (\rho f_1 D_1 \nabla C_1), \\ (\mathbf{x}, t) \in \Omega \times [0, t_{\max}], \end{aligned} \quad (2.10)$$

Initial conditions:

$$\begin{aligned} \mathbf{v}(\mathbf{x}, 0) = \mathbf{0}, \quad T(\mathbf{x}, 0) = T_i, \quad C(\mathbf{x}, 0) = C_0, \\ \rho(\mathbf{x}, 0) = \rho_{l_0}, \quad \frac{\rho(\mathbf{x}, 0)}{\rho_1} = 1.0, \quad \mathbf{x} \in \Omega, \end{aligned} \quad (2.11)$$

visco-plastic porous medium saturated with liquid [19]. The primary unknown in the deformation problem is the displacement vector, $\mathbf{u}$. Using a small-deformation assumption, the strain measure, $\boldsymbol{\epsilon}$ is expressed as a sum of the elastic, plastic and thermal contributions as follows:

$$\boldsymbol{\epsilon} \equiv \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^t) = \boldsymbol{\epsilon}^e + \boldsymbol{\epsilon}^p + \boldsymbol{\epsilon}^T, \quad (2.14)$$

where $\boldsymbol{\epsilon}^e$, $\boldsymbol{\epsilon}^p$ and $\boldsymbol{\epsilon}^T$ denote the elastic, plastic and thermal contributions, respectively, and are calculated through the volume-averaged model in the solid, liquid and mushy regions [25]. A hypoelastic law is used to express the stress-rate, in the whole domain, as:

$$\dot{\boldsymbol{\sigma}} = \mathcal{L}^e(\dot{\boldsymbol{\epsilon}}^e), \quad (2.15)$$

where $\mathcal{L}^e \equiv 2\mu \mathcal{I} + (\kappa - \frac{2}{3}\mu) \mathbf{I} \otimes \mathbf{I}$, with μ and κ denoting Lamé's constants. The thermal strain rate is calculated from the rates of change in temperature, T , and solid volume fraction, ϵ_s , as follows:

$$\dot{\boldsymbol{\epsilon}}^T = \frac{w}{3} (\beta_{s,T} \dot{T} + \beta_{sh} \dot{\epsilon}_s) \mathbf{I}, \quad (2.16)$$

where $\beta_{s,T}$ is the coefficient of volumetric thermal expansion, β_{sh} is the coefficient of volumetric shrinkage calculated from phase densities and w is a function of the solid fraction. There is a critical solid fraction, ϵ_s^{crit} , below which thermal strain is zero [19]. Therefore, w is expressed as

$$w = \begin{cases} 0 & \text{for } \epsilon_s < \epsilon_s^{\text{crit}}, \\ 1 & \text{for } \epsilon_s \geq \epsilon_s^{\text{crit}}. \end{cases} \quad (2.17)$$

Non-zero thermal strain is produced in the solid-shell only when ϵ_s exceeds ϵ_s^{crit} [19]. Below ϵ_s^{crit} , the developing mushy-zone has negligible strength and Eq. (2.17) reduces to

$$\dot{\boldsymbol{\epsilon}}^T = 0. \quad (2.18)$$

As described in [25], this necessitates a constraint on the stress given by

$$\boldsymbol{\sigma}' = 0 \quad \text{if } \epsilon_s < \epsilon_s^{\text{crit}}, \quad (2.19)$$

where $\boldsymbol{\sigma}'$ is used here to denote the deviatoric part of the Cauchy stress

$$\boldsymbol{\sigma}' \equiv \boldsymbol{\sigma} - \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) \mathbf{I}. \quad (2.20)$$

In the solid region, with $\dot{\epsilon}_s = 0$ and $w = 1$, Eq. (2.16) becomes

$$\dot{\boldsymbol{\epsilon}}^T = \frac{1}{3} \beta_{s,T} \dot{T} \mathbf{I}. \quad (2.21)$$

The evolution of the plastic strain obeys the normality rule

$$\dot{\boldsymbol{\epsilon}}^p = \frac{3}{2} \frac{\dot{\boldsymbol{\epsilon}}^p}{\tilde{\sigma}} \boldsymbol{\sigma}', \quad (2.22)$$

where $\dot{\boldsymbol{\epsilon}}^p$ is the equivalent plastic strain-rate and $\tilde{\sigma}$ the equivalent stress. The equivalent plastic strain evolution $\dot{\boldsymbol{\epsilon}}^p$ is specified through experiments as

$$\dot{\boldsymbol{\epsilon}}^p = \mathcal{F}(\tilde{\sigma}, s, T) = w \mathcal{F}_0(\tilde{\sigma}, s, T), \quad (2.23)$$

where Δ_{gap} is the air-gap size, p_{contact} is the contact pressure between the mold and the solid-shell, T_{cast} and T_{mold} , are temperatures of the solid-shell and mold surfaces at the metal-mold interface, respectively. The parameters R_0 , R' , h_0 and k_0 are empirical coefficients [3,31]. The heat fluxes q_g and q_c are schematically shown in Fig. 2.

2.2. Description of the deformation problem

We use a hypoelastic, rate-dependent model to describe deformation in the solidifying alloy. The mushy-zone is treated as a

Fig. 2. Alloy solidification from a mold with sinusoidal topography. The computational domain for the solid, mushy and liquid regions is only a small portion of the total domain considered to emphasize the early stages of solidification.

Table 1
Constitutive law of aluminum–copper alloy [19]

$\dot{\epsilon}_0$	σ	Q	m	δ
$9 \times 10^{-5} \text{ s}^{-1}$	5.5 kPa	154 J/mol	0.4	6.3

where $\mathcal{F}$ and $\mathcal{F}_0$ are scalar functions and w is defined as in Eq. (2.17) to account for the critical solid volume fraction. The evolution of the state variable, s (resistance to plastic deformation), is given by

$$\dot{s} = g(\tilde{\sigma}, s, T) = wg_0(\tilde{\sigma}, s, T), \quad (2.24)$$

and is also obtained from experiments. Eqs. (2.23) and (2.24) give a general framework of the constitutive law. The constitutive relationship, obtained from [19] and described in Table 1, is used in our numerical model. Values of important constants in the constitutive law are also given in Table 1. In our current analysis, we assume the deformation process of the solidifying alloy to be quasistatic and the body to be under equilibrium at all times. The equilibrium condition of the solidifying body can then be written as

$$\nabla \cdot \sigma + \rho g e_g = 0 \quad (2.25)$$

where e_g denotes the gravity field. Eq. (2.25) is obtained after simplifying the volume-averaged momentum conservation equation and neglecting the effect of the liquid-phase pressure on the solid-phase momentum equation [18,19,25]. In the liquid and mushy-zones with $\epsilon_s < \epsilon_s^{\text{crit}}$, Eq. (2.25) leads to $\sigma = -\rho g h \mathbf{I}$, since $\sigma' = 0$. With this approach, the initial stress of a particle when it solidifies is assumed to be the hydrostatic pressure at that location [5]. This initial stress condition is important for tracking the history of deformation of solid particles once they solidify.

Modelling of contact tractions (normal t_N and tangential t_T) and air-gaps between the casting and mold surface follows the scheme described in [32]. The mold separates the space into inadmissible (the mold region itself) and admissible (other regions) regions and is parameterized such that the normal vector ν points into the admissible region. The gap size (Δ_{gap}) of any point in space is defined as the shortest distance from that point to the mold. Numerically, the contact force and air-gap size are solved using augmentations. Details of this approach are given in [25] and not repeated here.

3. Numerical algorithm and computational strategies

Stabilized finite element methodologies are used to discretize the governing transport equations of fluid flow, heat and solute. A modified form of SUPG-PSPG based stabilized finite element technique for discretizing the fluid flow problem in alloy solidification systems, previously developed in [33,34], is used in this work. Thermal and solute species governing equations are discretized by SUPG based finite element methods. Supplementary thermodynamic and two-phase relationships (Eqs. (2.2)–(2.12)) are used to update mass and volume fractions, solute concentrations in individual phases and the mixture density. The multistep predictor-corrector scheme is used for ther-

mal and solute problems, while the Newton-Raphson scheme along with a global line search method is used for the fluid flow problem.

The deformation problem is discretized using a standard Galerkin residual method. Calculation of contact tractions, t_N and t_T , is performed through Uzawa's algorithm [32], in an iterative fashion involving Lagrange multipliers. Details of this algorithm, given in [32], and of the iteration procedure, given in [25], are not repeated here. The Newton-Raphson method is used for solving, u , the main unknown in the deformation problem. The linearized deformation problem is reviewed in [25]. The radial return map, discussed in [35], for hyper-elastic solids is extended to address the deformation of a solidifying body. Here the stress is updated by calculating the radial return factor, η as

$$\sigma_n = \eta \sigma'_* + \frac{1}{3} \text{tr}(\sigma'_*) \mathbf{I}, \quad (3.1)$$

where σ_* denotes the trial stress given by

$$\sigma_* = \sigma_{n-1} + \Delta t \mathcal{L}^e(\dot{\epsilon} - \dot{\epsilon}^T). \quad (3.2)$$

The parameter η is obtained after solving iteratively coupled non-linear equations for the evolution of $\tilde{\sigma}_n$ and s_n . For liquid or mushy regions where $\epsilon_s < \epsilon_s^{\text{crit}}$, the radial return factor η is set to 0 directly, since $\sigma' = 0$. The reader is referred to [25] for details of this procedure. The linear systems arising from the finite element discretization of the governing equations are solved using parallel iterative solvers.

3.1. Coupling of the various sub-problems and time integration

The various subproblems considered in our numerical model include the thermal, flow and solute transport problems and supplementary relations in the phase diagram for the solidification problem. The deformation problem in the casting also involves contact and air-gap formation at the metal-mold interface. The error criterion is based on the relative error in the solutions obtained between iterations within a particular time step. For example, in the solute solver, the error norm is defined as $\|\Delta C^{i+1}\|/\|C_n^{i+1}\|$. The fluid flow and the deformation problem are solved only once in the overall time integration process, which is summarized below:

- (1) At time t_n , all fields such as velocity v_n , temperature T_n , concentration C_n , liquid mass and volume fractions f_n and ϵ_n , displacement u_n etc. are known at each node. Fields such as stress σ_n , plastic strain ϵ_n^p , temperature T_n (for calculating thermal strain in the deformation problem), solid fraction $\epsilon_{s,n}$ and state variable s_n are known on each element integration point. Air-gap size $\Delta_{\text{gap},n}$ and contact pressure $p_{\text{contact},n}$ are also known on each integration point of the casting surface (elements of the boundary segment).
- (2) Advance to time step $t_{n+1} = t_n + \Delta t$. Set $j=0$, $v_{n+1}^{j=0} = v_n$, $T_{n+1}^{j=0} = T_n$, $f_{n+1}^{j=0} = f_n$, $C_{n+1}^{j=0} = C_n$, $u_{n+1}^{j=0} =$

- $u_n, \sigma_{n+1}^{j=0} = \sigma_n$ etc., where j is an iteration index and the subscript denotes the time level.
- (3) Compute the temperature in the casting and mold material after solving the thermal problem. This step is also an iterative process due to the coupling between thermal and solute transport problems, and also due to the latent heat release. The thermal coupling involving air-gap and contact pressure (Eq. (2.13)) also adds to the complexity.
- (4) Compute the mixture concentration C_{n+1}^{j+1} after solving Eq. (2.10) using a predictor-corrector method. This too is an iterative process.
- (5) Update the liquid solute concentration $C_{l,n+1}^{j+1}$, liquid mass and volume fractions, f_{n+1}^{j+1} and ϵ_{n+1}^{j+1} , and mixture density, ρ_{n+1}^{j+1} .
- (6) Repeat steps 3–5 so that $\|C_{l,n+1}^{j+1} - C_{l,n+1}^j\| < \epsilon_{tol}$ and $\|f_{n+1}^{j+1} - f_{n+1}^j\| < \epsilon_{tol}$ are satisfied for a specified tolerance level ($\epsilon_{tol} = 10^{-8}$ here denotes appropriate tolerance). If convergence is satisfied, set $T_{n+1} = T_{n+1}^{j+1}$, $C_{n+1} = C_{n+1}^{j+1}$ and $f_{n+1} = f_{n+1}^{j+1}$. Update I_{n+1} using Eq. (2.12) and calculate $C_{s,n+1}$ using Eq. (2.6).
- (7) Compute the superficial velocity v_{n+1}^{j+1} and pressure p_{n+1}^{j+1} in the casting after solving Eq. (2.8) using a Newton-Raphson solution method. Upon convergence, set $v_{n+1} = v_{n+1}^{j+1}$ and $p_{n+1} = p_{n+1}^{j+1}$.
- (8) Solve the deformation problem with contact to determine the displacement u_{n+1}^{j+1} and stress σ_{n+1}^{j+1} . This is a highly nonlinear problem requiring iterations. The air-gap size, $\Delta_{gap,n}^{j+1}$ and/or contact pressure $p_{contact}$ are determined at each Gauss point of surface elements on the cast shell surface. Once convergence is obtained in the deformation problem, set $n = n + 1$ and proceed to step 2.

4. Numerical investigations

Solidification of an aluminum–copper alloy is simulated in cavities, with sinusoidal surfaces characterized by an amplitude, A and wavelength, λ . The domain and boundary conditions for the deformation and solidification problems are described in Figs. 2 and 3, respectively. q and j denote the thermal and solute fluxes, respectively. Our main emphasis in all these examples is to observe the effect of transport phenomena occurring near the metal–mold interface, on stress development, air-gap formation and growth morphology unevenness in the solid-shell. The liquid metal is assumed to perfectly wet the sinusoidal mold surface at the beginning of each simulation and surface tension effects are neglected in all examples discussed here. Important physical properties of the alloy are listed in Table 2. Thermal properties of different mold materials, used in our simulations, are summarized in Table 3. The casting is assumed to be at an initial temperature, T_i . The side walls of the casting and mold are assumed to be insulated and the temperature of the top surface is assumed to be at T_i throughout the solidification process. For

Fig. 3. Domain of the casting and mold for the solidification of an Al–Cu alloy. Also shown are the boundary conditions for the solidification problem.

Table 2

Important physical parameters for the aluminum–copper alloy

Symbol	Value	Units
k_s	192.49	$\text{W m}^{-1} \text{K}^{-1}$
k_l	82.61	$\text{W m}^{-1} \text{K}^{-1}$
c_s	1.06×10^3	$\text{J kg}^{-1} \text{K}^{-1}$
c_l	1.06×10^3	$\text{J kg}^{-1} \text{K}^{-1}$
L_f	397.5×10^3	J kg^{-1}
κ	0.17	
$\beta_{l,T}$	4.95×10^{-5}	K^{-1}
$\beta_{l,C}$	–2.0	
β_{sh}	0.10417	
ρ_s	2650	kg m^{-3}
ρ_l	2400	kg m^{-3}
μ	0.003	$\text{kg m}^{-1} \text{s}^{-1}$
T_c	821.0	K
T_m	933.0	K
T_{amb}	298.0	K
C_e	0.332	
g	9.81	m s^{-2}
m_{liq}	–337.35	K
h_0	1.5×10^3	$\text{W m}^{-2} \text{K}^{-1}$
k_0	4.5×10^{-2}	$\text{W m}^{-1} \text{K}^{-1}$
D_l	3×10^{-9}	$\text{m}^2 \text{s}^{-1}$
R_0	1×10^{-5}	$\text{K W}^{-1} \text{m}^2$
R'	-1×10^{-12}	$\text{K W}^{-1} \text{m}^2 \text{Pa}^{-1}$
H_c	0.008	m
H_m	0.005	m

the fluid flow problem, no slip and no penetration conditions are applied on all boundaries. The top surface is assumed to move downwards like a rigid lid to compensate the volume change arising due to shrinkage following the procedure in [15]. Simulations are carried out in domains similar to that in Fig. 2 and the finite element mesh is constructed with bilinear quadrilateral elements for all examples discussed in the following sections. The depth of the sinusoids is twice the amplitude, i.e. equal to $2A$.

Table 3

Mold material properties used in the numerical examples

Material	k (W/mK)	E (GPa)	ν	ρ (kg/m^3)
Copper	345.4	64	0.37	7938
Iron	36.2	144	0.33	7265
Lead	32.7	8.52	0.35	10665

Figs. 4–8 summarize results obtained for few $A - \lambda$ combinations for different process conditions with the emphasis given on early stages of solidification. The top-half corresponds to the time $t = 5$ ms, while the bottom-half corresponds to $t = 100$ ms. In all examples considered here, inverse segregation, primarily induced by shrinkage driven flow, is observed at the bottom of the cavities (Figs. 4b–8b) and is more prominent at $t = 100$ ms than at $t = 5$ ms. A zone of positive segregation is formed near the bottom of the cavity where solute enrichment occurs. This is followed by a zone of negative segregation characterized by solute depletion. Air-gap nucleation occurs at the troughs and this leads to a local reduction in heat transfer out of the solidifying shell at these locations. Consequently, remelting occurs at the troughs and solid forms earlier at the crests than at the troughs as observed in Figs. 4d–8d at $t = 100$ ms. The process parameters that are varied in these examples are wavelength of sinusoidal surfaces (λ), melt superheat (ΔT_{sup}), mold material and initial solute (Cu) concentration (C_0) of the alloy.

4.1. Effect of different sinusoid wavelengths

We first examine the effect of different mold topographies, obtained by varying wavelengths, λ , of the mold surface, on the coupled deformation and solidification process. The mold-wavelength λ is varied from 1 to 9 mm, keeping the amplitude (A) constant at 0.232 mm. The choice of the amplitude is dictated by the fact that sinusoidal molds in earlier experiments performed by ALCOA had this particular amplitude. The mold material here is copper and the melt superheat and initial solute concentration are fixed at 0°C and 5% Cu by weight, respectively. Figs. 4 and 5 show the temperature, solute concentration, equivalent stresses and liquid mass fraction along with velocity fields in the developing solid-shell at $t = 5$ and 100 ms for $\lambda = 5$ and 3 mm, respectively. At $t = 100$ ms, inverse segregation is observed at the bottom of the cavity for both cases and this is evident from Figs. 4b and 5b. Transition to a planar growth front morphology is faster for smaller wavelengths and this trend, evident from Figs. 4d and 5d, was also independently observed in [24] and [25]. Fig. 9 shows the transient variation of maximum air-gap sizes on the mold surface for different wavelengths. Initially, variation in air-gap sizes with wavelength is negligible. However, as the solid-shell develops further, air-gap sizes increase with increasing wavelength.

Fig. 10 shows the transient variation of the maximum equivalent stress for different wavelengths. The maximum equivalent stress increases sharply before decreasing with time. Initially the stresses are higher for larger wavelengths, but near $t = 100$ ms, the least value corresponds to $\lambda = 5$ mm suggesting some kind of an optimum wavelength near $\lambda = 5$ mm that leads to a reduction in equivalent stresses and air-gap sizes.

Variations in solute concentrations caused by inverse segregation are summarized in Table 4 at $t = 100$ ms. Greatest deviation from the initial concentration is obtained for the smallest wavelength ($\lambda = 1$ mm). This is because of the increase in shrinkage driven flow in the casting with decreasing wavelength. Similar observations were made in [24] for inverse segregation in a vertically solidifying Al–Cu alloy on sinusoidal surfaces.

Table 4

Comparison of variation in solute concentration for varying wavelengths at $t = 100$ ms ($A = 0.232$ mm, $C_0 = 5\%$ wt, melt superheat = 0°C , mold material—copper, N = number of nodes)

Wavelength (mm)	C_{max} wt%	C_{min} wt%	max. deviation $\max_{j=1}^N \left(100 \times \left(\frac{C_j - C_0}{C_0} \right) \right)$
1	6.031	3.743	25.14
3	5.863	4.834	17.16
5	6.127	4.806	22.54
7	6.132	4.697	22.64
9	6.138	4.832	22.76

4.2. Effect of melt superheat

Figs. 4 and 6 show the temperature, solute concentration, equivalent stress and liquid mass fraction fields for melt superheats of 0 and 3°C , respectively, at $t = 5$ ms (top-half) and 100 ms (bottom-half). In both these examples, the wavelength is fixed at 5 mm, copper is the mold material and the initial Cu concentration is 5% by weight. Inverse segregation is observed at the bottom of the cavity and is more prominent at $t = 100$ ms than at $t = 5$ ms. From Figs. 4d and 6d, it is evident that the effect of melt superheat on the solid growth front morphology is negligible. Fig. 11 shows the evolution of air-gap sizes with time for three different melt superheat values. Air gaps, which form at the troughs of the sinusoid, increase in size with decreasing melt superheat values. At any given time, the air-gap size is the highest for melt superheat of 0°C and lowest for melt superheat of 45°C . This is because, with increasing melt superheat, the size of the mushy-zone decreases and it cannot resist the liquid pressure effectively leading to better contact with the mold surface. The small perturbation near $t = 10$ ms is because of remelting. The increase in air-gap size leads to a decrease in heat transfer between the mold and shell that results in remelting. This in turn leads to decrease in the rate at which the air-gap sizes increase. Fig. 12 shows the transient variation of the maximum equivalent stress for different superheat values. Initially, higher equivalent stresses are observed with the minimum melt superheat. However, due to increased growth of the solid-shell, the differences are lower at later times. The inverse segregation given in Table 5 at $t = 100$ ms is marginally higher for higher melt superheats, but the differences here are negligible.

4.3. Effect of different initial solute concentrations

Figs. 4 and 7 show the temperature, solute concentration, equivalent stress and liquid mass fraction fields for $C_0 = 5$ and 9%, respectively, at $t = 5$ ms (top-half) and 100 ms (bottom-

Table 5

Comparison of variation in solute concentration for varying melt superheats ($A = 0.232$ mm, $C_0 = 5\%$ wt, $\lambda = 5$ mm, mold material—copper, N = number of nodes)

Superheat ($^\circ\text{C}$)	C_{max} wt%	C_{min} wt%	max. deviation $\max_{j=1}^N \left(100 \times \left(\frac{C_j - C_0}{C_0} \right) \right)$
0	6.127	4.806	22.54
30	6.135	4.729	22.70
45	6.133	4.813	22.66

Fig. 4. (a) Temperature in K (b) solute concentration (c) equivalent stress in MPa (d) liquid mass fraction and velocity vectors at (i) $t = 5$ ms ($|v|_{\max} = 0.355$ m/s) and (ii) $t = 100$ ms ($|v|_{\max} = 0.095$ m/s) for $\lambda = 5$ mm, $C_0 = 5\%$ Cu and no superheat ($A = 0.232$ mm, mold material—copper).

Fig. 5. (a) Temperature in K (b) solute concentration (c) equivalent stress in MPa (d) liquid mass fraction and velocity vectors at (i) $t = 5$ ms ($|v|_{\max} = 0.342$ m/s) and (ii) $t = 100$ ms ($|v|_{\max} = 0.090$ m/s) for $\lambda = 3$ mm, $C_0 = 5\%$ Cu and no superheat ($A = 0.232$ mm, mold material—copper).

Fig. 6. (a) Temperature in K (b) solute concentration (c) equivalent stress in MPa (d) liquid mass fraction and velocity vectors at (i) $t = 5$ ms ($|v|_{\max} = 0.382$ m/s) and (ii) $t = 100$ ms ($|v|_{\max} = 0.096$ m/s) for $\lambda = 5$ mm, $C_0 = 5\%$ Cu and 30°C superheat ($A = 0.232$ mm, mold material—copper).

Fig. 7. (a) Temperature in K (b) solute concentration (c) equivalent stress in MPa (d) liquid mass fraction and velocity vectors at (i) $t = 5$ ms ($|v|_{\max} = 0.325$ m/s) and (ii) $t = 100$ ms ($|v|_{\max} = 0.093$ m/s) for $\lambda = 5$ mm, $C_0 = 9\%$ Cu and no superheat ($A = 0.232$ mm, mold material—copper).

half). Both λ and ΔT_{sup} are fixed here with Copper being the mold material. Inverse segregation is observed at the bottom of the cavity and is more prominent at $t = 100$ ms than at $t = 5$ ms. Fig. 13 shows the transient air-gap evolution for different initial

solute concentrations. Air-gaps increase with increasing C_0 values and the difference becomes larger at later times. The magnitudes of air-gap sizes and their variation with different Cu concentrations in Fig. 13 are larger than those observed in Fig.

Fig. 8. (a) Temperature in K (b) solute concentration (c) equivalent stress in MPa (d) liquid mass fraction and velocity vectors at (i) $t = 5$ ms ($|v|_{\max} = 0.296$ m/s) and (ii) $t = 100$ ms ($|v|_{\max} = 0.057$ m/s) for $\lambda = 5$ mm, $C_0 = 5\%$ Cu and no superheat ($A = 0.232$ mm, mold material—iron).

Fig. 9. Variation of the maximum air-gap size as a function of time for different wavelengths (Cu concentration = 5%, melt superheat = 0 °C, mold material—copper).

Fig. 11. Variation of the maximum air-gap size as a function of time for different melt superheats ($\lambda = 5$ mm, Cu concentration = 5%, mold material—copper).

10 of [25] where inverse segregation was neglected. Therefore, the presence of inverse segregation at the bottom of the casting increases air-gap sizes. A perturbation, similar to that observed for different melt superheats, is observed here too at $t = 10$ ms. This is ascribed to the decrease in heat transfer between the mold and shell due to air-gap formation. Fig. 14 shows the transient variation of maximum equivalent stresses for different C_0 . Initially, higher equivalent stresses are observed for lower C_0 values. Later however, maximum equivalent stresses show lower differences for varying C_0 . Table 6 shows the inverse segregation at $t = 100$ ms for different solute concentrations and from here it is observed that the deviation is highest for $C_0 = 5\%$, while it is lower for other C_0 values.

Fig. 10. Variation of the maximum equivalent stress as a function of time for different wavelengths (Cu concentration = 5 %, melt superheat = 0 °C, mold material—copper).

Fig. 12. Variation of the maximum equivalent stress as a function of time for different melt superheat values ($\lambda = 5$ mm, Cu concentration = 5 %, mold material—copper).

4.4. Effect of different mold materials

Figs. 4 and 8 summarize results obtained with copper and iron as the mold materials, respectively. All other parameters

Table 6

Comparison of variation in solute concentration for different initial solute concentrations (C_0) ($A = 0.232$ mm, melt superheat = 0 °C, $\lambda = 5$ mm, mold material—copper, N = number of nodes)

C_0 (wt%)	$C_{\max}$ (wt%)	$C_{\min}$ (wt%)	max. deviation $\max_{j=1}^N \left(100 \times \left(\frac{C_j - C_0}{C_0} \right) \right)$
1.0	1.159	0.871	15.9
3.0	3.595	2.839	19.83
5.0	6.127	4.806	22.54
7.0	8.096	6.794	15.66
9.0	10.605	8.603	17.83

Fig. 13. Variation of the maximum air-gap size at trough as a function of time for different solute (Cu) concentrations ($\lambda = 5$ mm, superheat = 0°C , mold material—copper).

Fig. 15. Variation of the maximum air-gap size as a function of time for different mold materials (Cu concentration = 5 %, melt superheat = 0°C , $\lambda = 5$ mm).

are fixed here. The reduction in thermal conductivity of the mold material delays solid-shell growth by retarding heat transfer out of the casting. As observed in Fig. 8c, at $t = 100$ ms, the solid phase has not yet developed fully, though the preference for growth is at the crests of the sinusoids. The decrease in shrinkage driven fluid flow caused by the reduction in the phase change rate also inhibits inverse segregation, as observed in Fig. 8b. Similar results were observed for the Lead mold. Fig. 15 shows the transient evolution of air-gap sizes with Cu, Fe and Pb as the mold materials. Air-gap sizes for the Cu mold are far higher than those for Fe or Pb molds. This is because the lower thermal conductivity of Fe and Pb slows down the solid growth rate and reduces the size of the mushy-zone at a particular time, which in turn is unable to resist the liquid pressure effectively. Fig. 16

shows the transient variation of maximum equivalent stresses for mold materials discussed above and this variation is similar to those observed in Figs. 10, 12 and 14. The lower the thermal conductivity of the mold, the lower are the equivalent stresses in the solidifying body. The peak values for Fe and Pb molds are far lower than the corresponding value for the Cu mold.

The maximum equivalent stress at the dendrite roots is shown in Fig. 17 for different C_0 at $t = 100$ ms, for a fixed λ , ΔT_{sup} and mold material. Clearly, the peak value is observed for a Cu concentration of 1.8%, which makes this particular alloy most susceptible to hot-tearing. This observation was previously made in [17,18] and verified in the numerical studies of Tan and Zabaras in [25], where inverse segregation and solute transport were neglected. Non-uniform heat extraction at the metal-mold

Fig. 14. Variation of the maximum equivalent stress as a function of time for different solute (Cu) concentrations ($\lambda = 5$ mm, melt superheat = 0°C , mold material—copper).

Fig. 16. Variation of the maximum equivalent stress as a function of time for different mold materials ($\lambda = 5$ mm, Cu concentration = 5%, melt superheat = 0°C).

Fig. 17. Maximum equivalent stress at roots of the dendrites for the solidifying alloy at $t = 100$ ms ($\lambda = 5$ mm, melt superheat = 0°C , mold material—copper).

interface due to air-gap formation leads to unevenness in the solid growth front morphology. For smaller wavelengths, as discussed before, the solid growth front becomes planar faster. Fig. 18 shows the growth front unevenness and the maximum equivalent stresses at $t = 100$ ms for different λ values with C_0 , ΔT_{sup} and the mold material fixed. The trend observed here is similar to that observed in [25]. The differences arise because of inverse segregation at the casting bottom that directly affects the liquid mass fraction fields due to changes in liquidus temperature of the alloy and leads to changes in mushy-zone sizes. From Fig. 18, it is evident that the presence of inverse segregation leads to an increase in growth front unevenness. As observed in the same figure, it is difficult to simultaneously minimize the front un-

Fig. 18. Maximum equivalent stress in the solidifying alloy and front unevenness at $t = 100$ ms (melt superheat = 0°C , Cu concentration = 5 %). Following [25], the position difference of $\epsilon_1 = 0.7$ corresponding to the crest and the trough is used here as a measure of front unevenness.

evenness and equivalent stresses in the solidifying body. A wavelength less than 5 mm gives a rough optimum value. Note that the inclusion of mold deformation through coupled mold/shell distortion could cause some changes in the results given here, but the overall trend shown in Figs. 4–18 will remain the same.

5. Conclusions

A combined thermal, segregation and thermo-mechanical analysis of an Al–Cu alloy solidifying on sinusoidal mold surfaces was presented. The mold was assumed to be rigid and non-deformable. Air-gap formation was observed in all examples due to imperfect metal-mold contact and this resulted in dynamic non-uniform thermal boundary conditions at the metal-mold interface. A parametric study of air-gap formation, stress evolution and inverse segregation was performed by varying the mold surface wavelengths, melt superheat initial solute concentration and the mold material. The presence of inverse segregation at the bottom of the casting, caused by shrinkage driven fluid flow, was found to affect the magnitudes of both air-gap sizes at the mold-metal interface and equivalent stresses developing in the solidifying body. There were significant differences between the maximum air-gap sizes observed here and those observed in [25], where solute transport was neglected. The overall transient behavior of equivalent stresses was however similar to that observed in [25], but actual values of maximum equivalent stresses were different from those given in [25] due to inverse segregation near the casting bottom observed here. The presence of inverse segregation was found to increase the degree of solid growth front unevenness. With growth front unevenness and equivalent stresses as the criterion, an optimal wavelength range was obtained. The broad aim of the numerical study described here is to gain a better understanding of the process of surface defect formation in various directionally solidified aluminum castings and develop strategies to minimize these defects by designing appropriate mold surface topographies.

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