A thermomechanical study of the effects of mold topography on the solidification of Aluminum alloys

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A thermomechanical study of the effects of mold topography on the solidification of aluminum alloys at early times is provided. The various coupling mechanisms between the solid-shell and mold deformation and heat transfer at the mold/solid-shell interface during the early stages of aluminum solidification on molds with uneven topographies are investigated. The air-gap nucleation time, the stress evolution and the solid-shell growth pattern are examined for different mold topographies to illustrate the potential control of aluminum cast surface morphologies during the early stages of solidification using proper design of mold topographies. The unstable shell growth pattern in the early solidification stages results mainly from the unevenness of the heat flux between the solid-shell and the mold surface. This heat flux is determined by the size of the air-gaps formed between the solidifying shell and mold surface or from the value of the contact pressure. Simulation results show that a sinusoidal mold surface with a smaller wavelength leads to nucleation of air-gaps at earlier times. In addition, the unevenness in the solid-shell growth pattern decreases faster for a smaller wavelength. Such studies can be used to tune mold surfaces for the control of cast surface morphologies.

\textit{Keywords:} Solidification; Aluminum alloys; Mold topography; Cast surfaces

1. Introduction

The study of the development of thermal stresses and deformation during aluminum casting in the early stages of solidification is an important tool for understanding the formation of cracks, liquation or other defects in the ingot surface. In current practices surface defects formed at the early stages of solidification are later removed through expensive surface milling and scalping processes. Thus understanding the effect of mold topography on the heat extraction process and on the resulting shell growth may allow certain control of cast surface morphologies and reduce unnecessary post-casting operations needed to remove surface defects.

Theoretical studies of gap nucleation in directional solidification were carried out in [1–3] using thermo-hypoelastic perturbation theory. The gap nucleation time was calculated for different wavelengths of the sinusoidal mold topography and conclusions were drawn as to the effect of mold material and mold topology on the air-gap nucleation process. A number of simplifications were introduced in the material model, deformation mechanisms and air-gap modeling to allow the use of a linearized analytical perturbation method. Subsequent work addressed the removal of some of these limitations, e.g. in [4], the thermal capacitance of the solidifying shell is incorporated to allow a Stefan number appropriate for the solidification of metals. The solid-shell deformation subsequent to air-gap formation was not analyzed. A thermo-mechanical analysis of solidification to predict the air gap thickness was examined in [5].

The analysis of the deformation of a solidifying body is significantly different from that of a standard fixed body [6–8]. These efforts emphasize...
the need to incorporate both the initial stresses at the instant of solidification as well as the fact that the growing nature of a solidifying body leads to an incompatibility of the strain tensor.

This work provides the first numerical study of the effects of mold topography on the solid-shell growth at the early stages of solidification. It accounts for the deformation of the solid-shell and mold and in addition models the pressure and air-gap dependent thermal conditions on the mold/solid-shell interface. A study of the stress development and growth pattern after air-gap nucleation is also presented to compute the time needed for reduction of the surface unevenness resulting from the non-uniform heat extraction at the mold/solid-shell interface. Finally, conclusions as to the effect of mold topography (amplitude and wavelength) on the solid-shell growth are drawn.

2. Problem definition and governing equations

Directional solidification with sinusoidal molds of wavelength $\lambda$ and amplitude $A$ is considered as shown in Fig. 1. Since our interest is on the early stages of solidification, we assume that the top side of the computational domain is far away from the mold surface, so that temperature and pressure variations at this surface can be ignored, and that the no-slip condition for the melt flow is valid. A mold of finite dimensions is considered that however in the context of early time solidification can be considered as a semi-infinite mold. Let us assume that initially the mold cavity is filled with molten aluminum with a superheat of $\Delta \theta$. Heat is being extracted from the bottom of the cavity, and a solid-shell is formed above the upper mold surface. This solid-shell is in equilibrium under the action of the melt pressure and of the contact tractions at the sinusoidal mold surface. As temperature drops in the solid-shell, thermal stresses will develop. Therefore air-gaps between the mold and the shell may be generated, resulting in a non-uniform heat flux at the mold/solid-shell interface. In this work, the focus is to compute the effects of mold topography described by wavelength $\lambda$ and amplitude $A$ on the stress development, air-gap nucleation and growth pattern during the early stages of solidification.

![Figure 1. The solidification process with a sinusoidal mold topography. Since our interest lies in early solidification, the computational domain (solid, mushy and liquid domains) is only a small portion of the total mold domain. The $x$-displacements and the $y$ traction components in the vertical walls of the domain are taken to be zero.](image-url)

A. Definition of the thermal and flow problems

Let us denote the melt and solid-shell regions at time $t$ as $\Omega_L(t)$ and $\Omega_S(t)$, respectively, and the mold region as $\Omega_m(t)$.

In this work, the following assumptions are introduced for the transport of momentum and heat in the solidification system:

1. Constant thermo-physical and transport properties, including viscosity $\mu$, densities $\rho_s$ and $\rho_l$, thermal conductivities $k_s$ and $k_l$, heat capacities $c_s$ and $c_l$ and latent heat $L$.

2. Laminar melt flow caused by temperature-induced density variations (Boussinesq flow). The shrinkage driven flow is not modeled.

3. Permeability $K$ approximated using the Kozeny-Carman equation

$$K(\varepsilon_i) = \frac{K_0 \varepsilon_i^3}{(1 - \varepsilon_i)^2}$$

(1)
where $K_0$ is a permeability constant and $\epsilon_l$ is the liquid volume fraction.

4. Segregation is not modeled. The mixture solute concentration $C$ is expressed using the liquid fraction as

$$C = \epsilon_l C_l + (1 - \epsilon_l) C_s$$  \hspace{1cm} (2)

With the above assumptions, the volume-averaged form of the macroscopic transport equations for momentum and energy are [9,10]

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\epsilon_l \nabla p_l$$
$$+ \nabla \cdot [\mu_l \nabla(\frac{\rho}{\rho_l} \mathbf{v}) + \nabla T (\frac{\rho}{\rho_l})]$$
$$- \frac{(1 - \epsilon_l)^2 \rho}{\epsilon_l^2} \frac{v}{\rho_l K_0} - \epsilon_l \rho_0 \beta_0 (\theta - \theta_0) \mathbf{g}$$  \hspace{1cm} (3)

$$\rho \frac{\partial \theta}{\partial t} + \rho \epsilon_l c_l \mathbf{v} \cdot \nabla \theta = \nabla \cdot (k \nabla \theta)$$
$$- \rho_s [L + (c_s - c_l)(\theta - \theta_m)] \dot{\epsilon}_l$$  \hspace{1cm} (4)

where $f$ is the liquid mass fraction ($f = \epsilon_l \rho_l / \rho$), $\rho \equiv \rho_1 \epsilon_1 + \rho_s (1 - \epsilon_1)$, $\rho_c \equiv \rho_1 \epsilon_1 c_1 + \rho_s (1 - \epsilon_1) c_s$, $k \equiv k_1 \epsilon_1 + k_s (1 - \epsilon_1)$, $\theta_m$ is the melting temperature, $\beta_0$ is the coefficient of volumetric thermal expansion, and $\rho_0$ and $\theta_0$ are the reference density and temperature, respectively.

For the two limiting cases of infinitely fast and slow solute diffusion in the solid, the liquid fraction can be calculated as a function of temperature from either the Lever rule or the Scheil rule as follows:

Lever rule : $\epsilon_l = 1 - \frac{\theta - \theta_L}{(1 - k_p)(\theta - \theta_m)}$,  \hspace{1cm} (5)

Scheil rule : $\epsilon_l = \frac{\theta - \theta_m}{\theta_L - \theta_m}$,  \hspace{1cm} (6)

where $k_p$ is the partition ratio and $\theta_L = \theta_m + m_l C$ [11].

In a solidification system, heat is extracted from the solid-shell surface. The contact condition between the solid-shell and the mold surface significantly affects the growth conditions. If an air-gap forms between the growing solid-shell and the mold surface, the heat flux decreases greatly when compared to the case without an air-gap. The heat fluxes $q_g$ and $q_c$ (Fig. 1) for these two conditions are modeled as follows [1,12]:

$$q_g = \frac{h_0}{1 + \delta_{gap} h_0 / k_0} (\theta_{cast} - \theta_{mold})$$, if $\delta_{gap} > 0$ \hspace{1cm} (7)

$$q_c = \frac{1}{(R_0 + R' P)} (\theta_{cast} - \theta_{mold})$$, if $\delta_{gap} = 0$ \hspace{1cm} (8)

where $\delta_{gap}$ is the size of gap, $P$ is the contact pressure between the mold and the solid-shell, $\theta_{cast}$ and $\theta_{mold}$ are the temperatures of the solid-shell surface and the mold surface, respectively, and the parameters $R_0$, $R'$, $h_0$ and $k_0$ are taken from [1,12].

B. Definition of the deformation problem

Following [13], the mushy zone is treated as a viscoplastic porous medium saturated with liquid. The displacement vector, $\mathbf{u}$, is taken to be the primary unknown in the deformation problem. The strain measure is defined as

$$\varepsilon = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) = \varepsilon^c + \varepsilon^p + \varepsilon^\theta$$  \hspace{1cm} (9)

which is subdivided into elastic, viscoplastic, and thermal contributions. The volume-averaged model allows calculation of $\varepsilon^c$, $\varepsilon^p$ and $\varepsilon^\theta$ in the solid, liquid and mushy regions.

1. In the whole region, the stress is assumed to be given by a hypo-elastic law in the form:

$$\sigma = \mathcal{L}^c (\dot{\varepsilon}^c),$$  \hspace{1cm} (10)

where $\mathcal{L}^c \equiv 2\mu I + (\kappa - \frac{2}{3}\mu)I \otimes I$, with $\kappa$ and $\mu$ denoting the Lame parameters.

2. The thermal strain is calculated from the temperature rate $\dot{\theta}$ and the rate $\dot{g}_s$ of the solid fraction $g_s$ ($g_s \equiv 1 - \epsilon_l$) as follows:

$$\varepsilon^\theta = \frac{w}{3} \left( \beta_0 \dot{\theta} + \beta_{sh} \dot{g}_s \right) I,$$  \hspace{1cm} (11)

where $\beta_{sh}$ is the volumetric shrinkage coefficient and $w$ is a function of the solid fraction. As pointed out in [13], at low solid fractions, the bonds between the individual dendrites are relatively weak or even
non-existent. The dendrites can, therefore, contract with decreasing temperature without affecting the positions of their individual mass centers. Such solid-phase volume change would be accompanied by liquid melt feeding. Consequently, there will be no thermal strain in the solid. At high solid fractions, on the other hand, dendrites will coalesce or tangle, meaning that a change in the solid density would be reflected in a nonzero thermal strain. It was found that there exists a critical solid fraction \( g_{th} \) such that

\[
w = \begin{cases} 
0 & \text{for } g_s < g_{th} \\
1 & \text{for } g_s \geq g_{th}
\end{cases}
\]  

(12)

Eq. (12) implies that when the solid fraction \( g_s \) is less than a critical solid fraction \( g_{th} \), the body has no strength, since neither decrease of temperature and shrinkage will contribute to thermal strain. In particular, in the solid region, since \( w = 1 \) and \( g_s = 0 \) \((g_s \equiv 1)\), Eq. (11) reduces to

\[
\dot{\varepsilon}^{p} = \frac{3}{2} \frac{\dot{\varepsilon}^{p}}{\sigma} \sigma'
\]  

(13)

Because the liquid can freely feed the contraction due to decrease of temperature or shrinkage for the part of solidifying body with solid fraction below critical solid fraction \( g_{th} \), it is reasonable to apply a constraint on the stress tensor

\[
\sigma' = 0 \quad \text{if } g_s < g_{th}
\]  

(14)

where \( \sigma' \) is used here to denote the deviatoric part of the Cauchy stress

\[
\sigma' = \sigma - \frac{1}{3} \text{tr}(\sigma) I
\]  

(15)

3. The evolution of the plastic strain obeys the normality rule

\[
\dot{\varepsilon}^{p} = \frac{3}{2} \frac{\dot{\varepsilon}^{p}}{\sigma} \sigma'
\]  

(16)

where \( \dot{\varepsilon}^{p} \) is the equivalent plastic strain rate and \( \sigma \) the equivalent stress. The equivalent plastic strain evolution \( \dot{\varepsilon}^{p} \) is specified via experiments as

\[
\dot{\varepsilon}^{p} = f(\dot{\sigma}, s, \theta) = w f_0(\dot{\sigma}, s, \theta)
\]  

(17)

where \( f \) and \( f_0 \) are scalar functions and \( w \) was introduced earlier to account for the critical solid fraction. The evolution of the state variable \( s \) (resistance to plastic deformation) is also obtained from experiments and has the form

\[
\dot{s} = g(\dot{\sigma}, s, \theta) = w g_0(\dot{\sigma}, s, \theta)
\]  

(18)

Eqs. (17) and (18) give a general form of the constitutive model used in this work. Creep laws were introduced in [14,15] and are often used for solidification problems.

In this work, we assume that the solidification process is quasi-static and that the body is under equilibrium at all times. Let \( g \) be the gravity field; then the equilibrium equation of the solidifying body can be written as

\[
\nabla \cdot \sigma + \rho g = 0
\]  

(19)

As discussed in [13], the above equation is obtained from simplification of the volume-averaged momentum conservation equation given in [16] by neglecting the effect of the liquid-phase pressure upon the solid-phase momentum. In the liquid or in the mushy zone with \( g_s < g_{th} \), because \( \sigma' = 0 \), Eq. (19) will result in \( \sigma = -\rho gh I \). Note that this approach allows the initial stress of a solid particle at nucleation time to be the hydrostatic pressure of the liquid particle just before it solidifies [7].

Modeling of contact (normal traction \( t_N \) and tangential traction \( t_T \)) and air-gaps (\( \delta_{\text{gap}} \)) at the bottom of the casting surface follows the contact/friction scheme given in [17]. The mold separates the space into inadmissible (the mold region itself) and admissible (other regions) domains and is parameterized such that the normal vector \( \nu \) points into the admissible region. The gap function (\( \delta_{\text{gap}}, \) which is often denoted as \( g \))
of any point in space is defined as the shortest distance from that point to the mold. It is also assumed that the tangent traction $t_T$ can be modeled using Coulomb friction. Numerically, the contact tractions and gap size can be computed using augmentations (Uzawa’s algorithm), which will be discussed in the next section.

C. Modeling of the thermomechanical and contact problems

Let us denote the region of the solidifying body as $\Omega$, $\Gamma_s$ as the part of surface ($\Gamma_s \subset \partial \Omega$) on which a known external traction (i.e., liquid head pressure) is applied, and $\Gamma_c$ as the part of surface ($\Gamma_c + \Gamma_s = \partial \Omega$) that corresponds to regions of the body that may potentially contact the mold surface.

The weak form of Eq. (19) (principle of virtual work) is written

$$ G(u, \tilde{u}) \equiv G^{int}(u, \tilde{u}) - G^{ext}(u, \tilde{u}) - G^c(u, \tilde{u}) = 0 \quad (20) $$

for each test vector field $\tilde{u}$ with internal virtual work $G^{int}$, external virtual work $G^{ext}$ and contact virtual work $G_c$ as

$$ G^{int}(u, \tilde{u}) = \int_\Omega \sigma : \nabla \tilde{u} \, dV \quad (21) $$
$$ G^{ext}(u, \tilde{u}) = \int_{\Gamma_s} \mathbf{t} \cdot \tilde{u} \, ds + \int_{\Gamma_s} \rho g \cdot \tilde{u} \, dV \quad (22) $$
$$ G^c(u, \tilde{u}) = \int_{\Gamma_c} (\mathbf{t}_N \cdot \tilde{u} + \mathbf{t}_T \cdot \tilde{u}) \, dS \quad (23) $$

where $\mathbf{t}$ is the known applied external traction (i.e., liquid head pressure), and $\mathbf{t}_N$ and $\mathbf{t}_T$ are the unknown contact normal and tangent tractions at the mold/solid-shell interface.

One of the difficulties in solving the deformation problem is the calculation of the contact tractions $t_N$ and $t_T$. In our work, Uzawa’s augmentation algorithm is adopted with the following four steps [17]:

1. Initialize the multipliers $\lambda_N$ and $\lambda_T$.

2. Start a nested iteration to solve the displacement with contact tractions given by

$$ t_N = \lambda_N + \epsilon_N g $$
$$ t_T^{trial} = \lambda_T + \epsilon_T m_{\alpha\beta} (\varepsilon_{n+1} - \varepsilon_n) $$
$$ \Phi^{trial} = \| t_T^{trial} \| - \mu_f t_N $$

$$ t_T = \begin{cases} t_T^{trial} & \text{if } \Phi^{trial} \leq 0 \\ \mu_f t_N \frac{t_T^{trial}}{\| t_T^{trial} \|} & \text{if } \Phi^{trial} > 0 \end{cases} $$

where $\mu_f$ is the friction coefficient, $\epsilon_N$, $\epsilon_T$ are penalty parameters, and $t_T^{trial}$ is the trial tangential traction component used in the return map. Also, $\lambda_N$ and $\lambda_T$ are Lagrange multipliers, $g$ is the gap function, $\xi$ is the projection on the mold surface, $m_{\alpha\beta}$ is the metric tensor with components computed from the tangent vectors to the mold surface [17], and $\Phi^{trial}$ is the slip function used to determine whether the contact conditions correspond to slip or stick. In this work, we take $\epsilon_N = 1 \times 10^3$ and $\epsilon_T = 1 \times 10^3$.

3. Update the Lagrange multipliers.

4. Repeat the second step, until convergence occurs.

A Newton-Raphson scheme is used to solve Eq. (20) for $u$:

$$ \frac{\partial G(u^{k-1}, \tilde{u})}{\partial u} (u^k - u^{k-1}) = -G(u^{k-1}, \tilde{u}) \quad (24) $$

This linearization process requires a number of steps.

1. Linearization of the internal virtual work:

$$ \frac{\Delta G^{int}(u, \tilde{u})}{\Delta u_{br}} = \int_\Omega \tilde{u}_{ai} N_{a,j} \frac{E_{ijkl}}{2} \times \{ \delta_{kr} \delta_{is} + \delta_{is} \delta_{ks} - M_{kirs} - M_{klrs} \} N_{b,s} d\Omega, \quad (25) $$

where $N$ are the finite element shape functions, $a$ and $b$ are node indices, $i$, $j$, $k$, $l$, $r$ and $s$ are dimension indices, $u_{br}$ is the $r$ component of displacement on node $b$ and the fourth-order tensor $M$ (consistent material moduli) is defined as

$$ M_{ijkl} \equiv \frac{\partial \epsilon_{ij}}{\partial \epsilon_{kl}} = \quad (26) $$
\[
\frac{3}{2} \sigma'_{ij} \alpha \Delta t \mathcal{L}^\prime_{ijkl} \sigma'_{mn} + \frac{f}{\sigma_s} \Delta t \mathcal{L}^\prime_{ijkl} \delta_{ij} \tag{27}
\]

where \( \mathcal{L}^\prime_{ijkl} = \mathcal{L}^\prime_{ijkl} - \frac{1}{2} \mathcal{L}^\prime_{mn} \delta_{ij} \). In the formulation of \( \mathcal{M}_\varepsilon \), \( \sigma'_s \) is the trial stress, which will be defined later in this section, and the parameters \( \alpha, a_1, b_1, c \) are defined as

\[
\alpha = \frac{1 - c}{2\mu \Delta t \sigma_s^2} - \frac{3f}{2\sigma_s^2}, \\
a_1 = 1 + 3\mu \Delta t \frac{\partial f}{\partial \sigma}, a_2 = 3\mu \Delta t \frac{\partial f}{\partial s}, \\
b_1 = \Delta t \frac{\partial g}{\partial \sigma}, b_2 = 1 - \Delta t \frac{\partial g}{\partial s}, \\
c = \frac{b_2}{a_1b_2 + a_2b_1}
\]

2. The linearization of the external virtual work \( \mathcal{G}^\text{ext} \) is approximated to zero in this work with

\[
\frac{\Delta \mathcal{G}^\text{ext}(u, \dot{u})}{\Delta u_n} \approx 0
\]

3. Details of linearization for the contact virtual work \( \mathcal{G}^c \) can be found in [17].

To complete the algorithm, the radial return mapping is presented next. It provides an incremental solution to the constitutive problem with an assumed strain increment. The radial return map discussed in [18] for hyper-elastic solids is extended to address the solidification of a solidifying body. Since

\[
\sigma_n = \sigma_{n-1} + \Delta t \mathcal{L}^\prime(\dot{\varepsilon} - \bar{\varepsilon}^\theta) - \Delta t \mathcal{L}^\prime(\dot{\varepsilon}^\theta) \tag{28}
\]

we can define the trial stress as

\[
\sigma' = \sigma_{n-1} + \Delta t \mathcal{L}^\prime(\dot{\varepsilon} - \bar{\varepsilon}^\theta) \tag{29}
\]

Using Eq. (16) and taking the deviatoric part of Eq. (28), we obtain

\[
\sigma'_n = \sigma'_s - \frac{3\mu \Delta tf}{\sigma} \sigma' \tag{30}
\]

We can then take the magnitude of both sides of this equation to derive

\[
\bar{\sigma}_n - \bar{\sigma}_s + 3\mu \Delta tf = 0 \tag{31}
\]

Integration of Eq. (18) leads to

\[
s_n - s_{n-1} = g \Delta t \tag{32}
\]

By solving the above two non-linear equations iteratively for \( \sigma_n \) and \( s_n \), the radial return factor \( \eta \) can be evaluated as

\[
\eta = \frac{\bar{\sigma}_n}{\sigma_s} \tag{33}
\]

Notice that for the liquid or mushy regions where \( g_s < g_s^\text{th} \), iterations for solving Eqs. (31) and (32) are not necessary, since \( \sigma' = 0 \). The radial return factor \( \eta \) is set to 0 directly for regions with \( g_s < g_s^\text{th} \). With the radial return factor \( \eta \) calculated, we can then update the stress tensor as follows

\[
\sigma_n = \eta \sigma'_s + \frac{1}{3} \text{tr}(\sigma_s) I \tag{34}
\]

3. Numerical algorithm

The various subproblems considered here are the thermal, flow and deformation problems including phase transition and contact. The tolerance level used to define convergence in all three main solution steps is set to \( 10^{-10} \). The error criterion is based on the relative error in the solutions obtained at Newton-Raphson iterations within a time step. For example, in the heat solver, the error norm is defined as \( ||\Delta \theta||/||\theta^t|| \).

The overall algorithm is summarized below:

1. At time \( t_{n-1} \), fields such as velocity \( \mathbf{v}_{n-1} \), temperature \( \theta_{n-1} \), liquid volume fraction \( \epsilon_l \) and displacement \( \mathbf{u}_{n-1} \) are known on each node. Fields such as stress \( \sigma_{n-1} \), plastic strain \( \varepsilon_{n-1}^p \), temperature \( \theta_{n-1} \), solid fraction \( \gamma_{n-1}^s \) and state variable \( s \) are known on each element Gauss point. The air-gap size \( \delta_{gap}^{n-1} \) and contact pressure \( P_{n-1} \) are also known on each Gauss points of the mold/solid-shell boundary. These values are used as an initial guess in the update process to time \( t_n = t_{n-1} + \Delta t \).

2. Loop until the heat, flow and deformation problems are all converged:

   (a) Start a nested loop coupling only the heat and flow problems.

   i. Solve the heat transfer problem to obtain the temperature field in
both the mold and the solidifying material. This step itself is iterative because of the presence of convection and latent heat in Eq. (4). In each iteration, $e_l$ is updated using the Lever or Scheil rules. The gap size $\delta_{gap}$ and contact pressure $P_n$ are substituted into Eq. (7) to obtain the heat flux between casting and mold surface.

ii. Solve the flow problem. Since this problem is also highly nonlinear, this step also requires an iterative process.

(b) Temperature $\theta_n$ and solid fraction $g_n$ is interpolated from nodes to Gauss points, so that the thermal strain can be calculated as required in the deformation subproblem.

(c) Uzawa’s algorithm is used to solve the deformation problem with contact. By augmentations, both air-gap size $\delta_{gap}$ and contact pressure $P_n$ can be determined in this step on each Gauss point of each surface element of the solid-shell (boundary $\Gamma_c$). The deformation problem converges when $\delta_{gap}^n < 1 \times 10^{-4} A$ ($A$ is the amplitude of the mold topography).

4. Numerical investigations

In all numerical examples, the mold material properties used are tabulated in Table 1. The inelastic material model used is given in Table 2 and is based on the experimental work in [13]. The critical solid fraction has been measured for different aluminum-copper alloys [13]. These results are summarized in Fig. 2.

**Case 1: Effect of mold topography on gap nucleation time in the solidification of pure aluminum**

We assume that at the beginning of solidification, the liquid metal fully wets the sinusoidal mold and no gap is present. Gap nucleation is assumed to occur when the contact pressure falls to zero at a given location. In [1], it was shown that when the mold topography wavelength is less than a critical wavelength, gap nucleation quickly develops at the mold trough. In order to study the gap nucleation time, the time-evolution of the contact pressure before gap nucleation at the trough, $P_{tr}$, is examined. Once $P_{tr}$ reaches 0, we assume gap nucleation occurs. How gap nucleation further affects solidification is not studied in this example. Since no gaps are formed in this study, the heat flux is calculated from the contact pressure using Eq. (8) (also see [1]).

As pointed out in [7], the thermal stress in early stages of solidification can reach very high values; thus plastic deformation must be taken into account to correctly model the mechanical behavior of the solid-shell at the early stages of solidification. However, to allow comparison with the analytical results given in [1], no plastic deformation is considered in this example ($f = 0$). In this example, there is no initial superheat. Unless otherwise specified, the amplitude of the mold topography is taken as $1 \mu$m, the mold thickness is 0.5mm, the liquid pressure $P_l = 10000$ Pa and the environment temperature is applied at the bottom of the mold. All the solid or dotted lines in

**Table 1**

<table>
<thead>
<tr>
<th>Material</th>
<th>$k$ (W/m K)</th>
<th>$E$ (GPa)</th>
<th>$\nu$</th>
<th>$\rho$ (kg/m$^3$)</th>
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<td>0.37</td>
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</tr>
<tr>
<td>Iron</td>
<td>36.2</td>
<td>144</td>
<td>0.33</td>
<td>7265</td>
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<td>Lead</td>
<td>32.7</td>
<td>8.52</td>
<td>0.35</td>
<td>10665</td>
</tr>
</tbody>
</table>

**Table 2**

Constitutive law of aluminum copper alloy [13]

\[
f = \dot{\varepsilon}^p = \dot{\varepsilon}_0 \left[ \frac{\dot{\sigma}}{\sigma_0} \exp(-\delta \cdot g_x) \cdot \exp\left(-\frac{mQ}{R\theta}\right) \right]^m
\]

\[
\dot{\varepsilon}_0 \quad \sigma_0 \quad Q \quad m \quad \delta
\]

$9 \times 10^{-5}$s$^{-1}$ 5.5KPa 154J/mol 0.4 6.3
the figures below refer to the analytical results of [1–3]. In order to allow the present volume-averaged based model to simulate the solidification of pure aluminum material, we approximate the material as a dilute aluminum-copper alloy with a small copper concentration $C = 0.0001$.

The gap nucleation time is found to be affected by the mold material (mold properties given in Table 1). In general, better heat transfer in the mold leads to earlier gap nucleation. Fig. 3 shows the $P_{tr}$ evolution with the parameters $\lambda = 2 \text{ mm}$, $R_0 = 10^{-5}\text{m}^2\text{sec}\cdot\text{K}/\text{J}$ and $R' = 10^{-12}\text{m}^2\text{sec}\cdot\text{K}/\text{J}\cdot\text{Pa}$ for different molds. These parameters are selected from [2,3] to allow comparison of the present methodology with their approximate semi-analytical solution. The values of $R_0$ can in practice be controlled with mold coating or smaller-scale mold surface roughness (e.g. a high-frequency, random oscillation of topography superimposed on top of the wavy surface considered in the present work). From the curves in Fig. 3, we can see that higher the mold thermal conductivity, quicker the gaps nucleate along the mold-shell surface. This example also considers the (thermo-elastic) deformation of the mold. The agreement with the results given in [3] shown in Fig. 3 demonstrates the ability to incorporate mold deformation, which is an important contribution to gap nucleation for casting processes on thin molds. However, since this work mainly concentrates on DC casting processes involving fairly thick molds, deformation of the mold is not considered in the following examples.

Fig. 4 shows the $P_{tr}$ evolution with the parameter $R_0 = 10^{-3}\text{m}^2\text{sec}\cdot\text{K}/\text{J}$ for different wavelengths. Although the exact values are slightly different from the analytical solution in [1], both results show that a smaller wavelength leads to gap nucleation earlier. The contact pressure at the trough decreases nearly quadratically.

Figure 5 shows a linear relationship between the mean shell thicknesses at gap nucleation time and the wavelength $\lambda$ for any given liquid pressure $P_l$. A comparison with the results in [1] is shown. As pointed out in [4], the model with finite thermal capacitance leads to air-gap nucleation at a later time and to larger thickness at gap nucleation time than the model that neglects the thermal capacitance of the solidifying shell. Fig. 5 provides a comparison with the results of [1] where the Stefan number of the material is taken.
Figure 4. Evolution of $P^\text{tr}$ with time at selected $\lambda$ for pure aluminum ($P_0=8000$ Pa, $R_0 = 10^{-3}$ m$^2$ sec K/J).

Figure 5. Mean shell thickness at gap nucleation time as a function of mold wavelength for pure aluminum ($R_0 = 10^{-3}$ m$^2$ sec K/J).

as zero. This explains the higher discrepancy between the two results for high pressures.

For a given material, the value of the shell thickness at gap nucleation time is of great importance. As the thickness of the shell increases, its ability to resist distortion or warping increases as well. In many casting processes, the molten metal pressure is insufficient to prevent gap nucleation during the early stages of solidification. From this figure, one can see that high liquid pressure is preferred to obtain a thick shell at gap nucleation time. Fig. 5 can thus be useful for design purposes. For example, if the design of an aluminum casting process requires that the solid-shell should be in perfect contact with the mold while the shell thickness is less than 1 mm (in order to achieve good heat transfer until the solid-shell becomes thick enough), then one can determine the required melt pressure and mold wavelength from this figure.

Case 2: Effect of mold topography on stress development and growth pattern in the solidification of aluminum alloys

A. Unidirectional solidification of an aluminum alloy: As pointed out in [16,19], the pressure at the roots of the dendrites ($\epsilon_1 = 0.01$ or growing plane eutectic front) can be used as a hot-tearing criterion. The A-like curve in Fig. 6 shows the pressure at the roots of the dendrites for various compositions. If the Lever rule is used, the alloy composition (5.5 % copper) at the peak ($13.4 \times 10^4$ Pa) is most susceptible to hot tearing. In this calculation, for comparison purposes we use the same constitutive law as the one presented in [16]. They predicted a peak pressure of about $12.3 \times 10^4$ Pa and a corresponding alloy composition of 5.7% [16]. However, it is known that the Al-Cu alloy containing approximately 2% of copper is the most susceptible to hot tearing [16]. This difference is due to the use of the Lever rule. If, instead, a model with limited back diffusion was applied, the peak would occur at a lower concentration of copper because more eutectic would form. For example, if the Scheil rule is applied, the peak occurs at a composition of about 1% copper. Generally the Lever rule gives
the upper limit of solute concentration most susceptible to hot tearing, while the Scheil rule gives the lower limit. Since the Scheil rule predicts much better than the Lever rule, we will use the Scheil rule in all following examples.

Figure 6. Solid pressure at the roots of the dendrites for the Al-Cu system.

B. Stress development and growth pattern after gap nucleation: Figure 5 suggests the use of high melt pressure and large wavelengths as a way to suppress early air-gap formation. However, for most casting processes, the liquid pressure is not high enough to prevent gap nucleation. So investigating what happens after gap nucleation is of great importance. In the previous example studying gap nucleation time (Case 1), no plastic deformation was assumed and the solidification process was examined only before gap nucleation. However, substantial plastic deformation could be developed at early stages of solidification [7]. In this study, we use a creep law determined through experiments to describe the evolution of plastic deformation [13]. We also model the heat flux between the mold and the solid-shell satisfying Eq. (8) for the part without gap [1]. In places where the air-gap is nucleated, we model the heat flux to be related with gap size and temperature differences between the mold and the shell [12]. The heat fluxes can be then formulated using Eq. (7) in which, \( R_0 = 1 \times 10^{-5} \text{m}^2 \text{sec} \cdot \text{J/K} \), \( R' = -1 \times 10^{-12} \text{m}^2 \text{sec} \cdot \text{J/KPa} \), \( h_0 = 1.5 \times 10^8 \text{K/m}^2 \text{sec} \) and \( k_0 = 4.5 \times 10^{-2} \text{K/m} \cdot \text{sec} \). The amplitude of the mold topography is selected to be \( A = 0.232 \text{mm} \). The wavelength \( \lambda \) is selected to be 1 mm or 5 mm for allowing us to study the effects of mold topography wavelength. If not specified explicitly, a copper mold with a thickness of 5 mm is used in the calculation. The bottom of the mold is kept at 20\textdegree C, which is also the mold’s initial temperature. The casting material is an aluminum-copper alloy with 1% copper. A melt pressure of \( 10^{-2} \text{MPa} \) (about 37 cm aluminum pressure head) is applied at the top of the computational domain.

At very early stages (time = 5 ms), the growth for both wavelengths (1 mm and 5 mm) is uneven due to the unevenness of the mold topography. Fluid flow, which further leads to segregation, is developed due to the uneven front as shown in Fig. 7. For a mold with wavelength 1 mm, the growth gradually becomes uniform. At time 100 ms, the front is already flat and flow is negligible as shown in Fig. 8a. However, for a mold with wavelength 5 mm, the front unevenness keeps increasing at time 100 ms. The maximum flow velocity increases from 0.002 mm/sec at 5 ms (as shown in Fig. 7c) to 0.023 mm/sec at 100 ms (as shown in Fig. 8c). This uneven growth and flow for 5 mm wavelength mold leads to a nonuniform microstructure at the casting surface. The experimental work discussed in [2,3] has shown that both growth front and microstructure are more uniform for a smaller wavelength.

Thermal stress plays a very important role in the solid-shell growth at early stages. Because of the temperature decrease in the solid-shell and the shrinkage effects in the mushy zone, a typical gap in the order of \( \mu \text{m} \) will be formed at the trough between the mold and casting shell as shown in Fig. 9. The heat flux at the trough (where the air-gap is present) varies drastically from heat flux at the crest (where the solid-shell
contacts the mold). The drastic change in heat flux is the source of uneven growth in the early stages. A mold with a larger wavelength would increase the distance between the growing sites, which leads to more unevenness of the growth pattern. The two hills formed at the crest are growing to meet each and finally would result in a planar growth pattern. In the case of a 1 mm wavelength, the edges of the two hills start merging with each other at a time of about 5 ms, and the growth pattern completely transforms to a planar growth at time 100 ms. However, for the 5 mm wavelength, the unevenness continues increasing within the calculation time (100 ms). This shows that a small wavelength would be preferred to a larger wavelength when gap nucleation is unavoidable and the amplitude is given. Solidification with a smooth mold will also lead to results similar to those observed during solidification with a large wavelength mold.

Case 3: Effects of alloy composition, superheat, mold material and melt pressure in the solidification of aluminum alloys

A. Effects of alloy composition: Phase transition starts at a lower temperature if the solute concentration in the aluminum copper alloy is increased. However, phase transition ends at the same temperature (eutectic point) because of the eutectic formation (if Scheil rule is applied). According to our numerical results, alloy composition only has a small effect on gap evolution as shown in

Figure 7. Temperature and flow velocity at time 5 ms: (a) $\lambda = 1\,\text{mm}$ with superheat 30°C, (b) $\lambda = 5\,\text{mm}$ without superheat, (c) $\lambda = 5\,\text{mm}$ with superheat 30°C.

Figure 10. Evolution of the air-gap at the trough for different alloys ($\lambda = 5\,\text{mm}$ with 30°C superheat). The small bump around time 10 ms is due to remelting. As the air-gap is increased, the heat transfer between the mold and the shell decreases, thus leading to remelting and a sudden decrease of the air-gap size.
Figure 8. Equivalent stress and flow velocity at time 100 ms: (a) $\lambda = 1\,\text{mm}$ with superheat 30°C, (b) $\lambda = 5\,\text{mm}$ without superheat, (c) $\lambda = 5\,\text{mm}$ with superheat 30°C.

Figure 9. Temperature, flow and air-gap at time 100 ms for $\lambda = 5\,\text{mm}$ with superheat 30°C (the air-gap is magnified 20 times for easy visibility.)
Fig. 10. There is also no clear relationship between alloy composition and maximum stress in the solidifying body as shown in Fig. 11.

As pointed out in [19,16], the stress at the roots of the dendrites (1 = 0.01 or growing plane eutectic front) can be used as a hot-tearing criterion. Thus, from the study of the maximum equivalent stress evolution at the roots of the dendrites for different alloys as shown in Fig. 12, we can conclude that, using a 5 mm wavelength copper mold, aluminum alloy with about 1.8% copper is the most susceptible for hot-tearing defects.

B. Effects of superheat: Since superheat causes an additional thermal load, the shell growth velocity will be slower than the case without superheat as shown in Figs. 8b and 8c. However, the thermal load caused by superheat is small when compared to the latent heat released during phase change, and thus superheating the liquid metal will only have small effects on the growth pattern. However, superheat could lead to fluid flow, which is an important factor for segregation.

C. Effects of mold material: At the early stages of solidification, mold material determines how fast heat can be extracted away through the mold. The effect of the mold material on gap nucleation time for pure aluminum is shown in Fig. 3. Gap nucleation occurs earlier for a mold with higher conductivity. A measure of the extent to which a boundary deforms due to heat flux is the distortivity \( \delta = \frac{\mu_0 (1+\nu)}{k} \) \[3\]. For aluminum, copper, iron and lead, the corresponding distortivities are \( \delta_{Al} = 0.22\mu m/W \), \( \delta_{Cu} = 0.10\mu m/W \), \( \delta_{Fe} = 0.86\mu m/W \) and \( \delta_{Pb} = 1.53\mu m/W \). The copper mold tends to be less compliant to the evolving distortion in the aluminum shell than iron mold and lead mold. Equivalent stress and flow velocity at time 100 ms for different molds (copper, iron and lead) with the same wavelength \( \lambda = 5 \text{ mm} \) are shown in Fig. 13. At a smaller wavelength \( \lambda = 1 \text{ mm} \), the growth patterns for molds with different materials are similar. Generally the effects of mold topography is more pronounced for a mold with a larger heat conductivity.
Figure 13. Equivalent stress and flow velocity at time 100 ms, $\lambda = 5\text{mm}$ with superheat 30°C for an Aluminum alloy with 1% copper: (a) Copper mold, (b) Iron mold, (c) Lead mold.

**D. Effects of melt pressure:** In all the above examples, a melt pressure $10^{-2}\text{MPa}$ is applied at the top of the computational domain. A similar growth pattern of the solid-shell is obtained for various melt pressures varying from $10^{-3}\text{MPa}$ to $10^{-1}\text{MPa}$. This indicates that although melt pressure has a large effect on gap nucleation time (as shown in Fig. 5), its effects after gap nucleation are small. This is because the thermal stress that develops after gap nucleation is of the order of 10 MPa, which is much larger than the melt pressure.

**5. Conclusions**

A volume-averaged thermo-mechanical model was established to study the effects of mold topography on the solidification of aluminum alloys. Gap nucleation was assumed to occur when the contact pressure falls to zero. Gap nucleation time and shell thickness at gap nucleation time were calculated to illustrate the effects of mold topography. From the viewpoint of gap nucleation, a large wavelength and a high pressure is preferred to obtain better heat transfer at the early stages of solidification.

However, in most casting processes, gap nucleation is unavoidable and occurs at the very beginning of solidification. The unevenness of the heat flux between the solid-shell and the mold surface after gap nucleation leads to an unstable shell growth. From this point of view, a smaller wavelength is preferred because the growth pattern becomes stable earlier than for the case of larger wavelengths. Both the unidirectional and two-dimensional solidification examples show that aluminum copper alloy with about 1.8% copper is most susceptible for hot-tearing using the criterion suggested in [19,16] as shown in the A curve in Figs. 6 and 12. Numerical simulations show that superheating the liquid metal only slows down the solidification process. The growth pattern and the evolution of the stress are almost the same. Fluid flow caused by superheat is weak and does not significantly affect the shell growth. Generally the effects of mold topography on the growth pattern are more obvious for a mold with larger heat conductivity. Since the thermal stress that develops is of the order of 10 MPa after gap nucleation and the melt pressure is often of the order of $10^{-1}\text{MPa}$ for most casting processes, a change of melt pressure will not have a significant effect on the growth pattern at the early stages of solidification.

To facilitate the selection of mold topography for Aluminum alloys using the growth unevenness and the maximum equivalent stress in the solidifying shell as criteria, Fig. 14 summarizes some
of the studies performed in this work. As can be seen from this figure, one cannot simultaneously minimize the front unevenness and stresses in the solid-shell with only proper selection of the mold topography. However, when the mold surface wavelength is greater than a particular value (about 5 mm in the cases examined), both front unevenness and stress in the body increase. This means that for such processes mold surface wavelength should be selected with value less than 5 mm.

![Figure 14](image-url)

Figure 14. Maximum equivalent stress in the solidification body and front unevenness at an early solidification time (100 ms). The position difference of $\epsilon_1 = 0.7$ corresponding to the crest and the trough is used here as a measure of front unevenness.

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