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.

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 the solid surface morphologies and reduce unnecessary post-casting operations needed to remove surface defects.

Theoretical studies of air-gap nucleation in directional solidification were carried out in [1-3] using thermo-hypoeelastic perturbation theory. The air-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 modelling 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 was included for realistic modelling of 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 lies in the solidification process at early times, the computational domain for the solid, mushy and liquid regions is smaller than the mold domain. The \( x \)-displacements and the \( y \)-traction components in the vertical walls of the domain are taken to be zero.

A. Definition of the thermal and flow problems

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 \( \mu_t \), 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 modelled.

3. The permeability \( K \) is approximated using the Kozeny-Carman equation

\[
K(\epsilon_l) = \frac{K_0 \epsilon_l^3}{(1 - \epsilon_l)^2},
\]

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

4. Segregation is not modelled. The mixture solute concentration \( C \) is expressed using the liquid volume fraction as

\[
C = \epsilon_l C_l + (1 - \epsilon_l) C_s.
\]
With the above assumptions, the volume-averaged form of the macroscopic transport equations for momentum and energy are [9,10]

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\epsilon I \nabla p_l + \nabla \cdot [\mu_l (\nabla (\frac{\rho}{\rho_l}) \mathbf{u}) + \nabla^T (\frac{\rho}{\rho_l})]$$

$$-\mu_l \frac{(1 - \epsilon_l)^2}{\epsilon_l^2} \frac{\rho}{\rho_l} \frac{\mathbf{v}}{K_0} - \epsilon I \rho_{\theta 0} \beta_0 (\theta - \theta_0) \mathbf{g},$$  \hspace{1cm} (3)

where $f$ is the liquid mass fraction ($f = \epsilon_l \rho_l/\rho$), $\rho \equiv \rho_l \epsilon_l + \rho_s (1 - \epsilon_l)$, $\rho_c \equiv \rho_l \epsilon_l \epsilon_l + \rho_s (1 - \epsilon_l) \epsilon_s$, $k \equiv k_l \epsilon_l + k_s (1 - \epsilon_l)$, $\theta_m$ is the melting temperature, $\beta_0$ is the coefficient of volumetric thermal expansion, and $\rho_{\theta 0}$ 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 : $\epsilon_l = 1 - \frac{\theta - \theta_L}{(1 - \epsilon_l) \theta_m + \epsilon_l \theta_0},$ \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, $\theta_L = \theta_m + m_l C$ and $m_l$ is the slope of the liquidus line in the binary alloy phase diagram [11].

The contact condition between the solid-shell and the mold surface significantly affects the solidification 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 modelled as follows [1,12]:

$q_g = \frac{h_0}{1 + \delta \delta_0 h_0/k_0} (\theta_{\text{cast}} - \theta_{\text{mold}})$, if $\delta > 0,$ \hspace{1cm} (7)

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

where $\delta$ is the size of the air-gap, $P$ is the contact pressure between the melt and the solid-shell and $\theta_{\text{cast}}$ and $\theta_{\text{mold}}$ are the temperatures of the solid-shell lower surface and the upper mold surface, respectively. 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

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

which is subdivided into elastic, viscoplastic, and thermal contributions. The volume-averaged model allows calculation of $\varepsilon^e$, $\varepsilon^\mu$ 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:

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

where $\mathcal{L}^e \equiv 2\mu \mathcal{I} + (\kappa - \frac{2}{3} \mu) \mathbf{I} \otimes \mathbf{I}$, with $\kappa$ and $\mu$ the Lame’s parameters and $\mathbf{I}$ and $\mathcal{I}$ denoting the unit second- and fourth-order tensors, respectively. In Eq. (10) and all subsequent equations, a superimposed dot on a tensor field is used to denote the corresponding rate (time-derivative) of the field.

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

$$\varepsilon^\theta = \frac{w}{3} \left( \beta_\theta \dot{\theta} + \beta_{sh} \dot{g}_s \right) \mathbf{I},$$ \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, and 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

\[
w = \begin{cases} 
0 & \text{for } g_s < g_{th}, \\
1 & \text{for } g_s \geq g_{th}.
\end{cases}
\tag{12}
\]

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 \( _{\gamma}g_s = 0 \), Eq. (11) reduces to

\[
_{\gamma}\varepsilon = \frac{1}{3}\beta_0\theta I.
\tag{13}
\]

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

\[
\sigma' = 0 \quad \text{if} \quad g_s < g_{th},
\tag{14}
\]

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

\[
\sigma' \equiv \sigma - \frac{1}{3}tr(\sigma)I.
\tag{15}
\]

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

\[
\varepsilon^p = \frac{3}{2} \frac{\varepsilon^p}{\sigma'}
\tag{16}
\]

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

\[
\varepsilon^p = f(\bar{\sigma}, s, \theta) = w f_0(\bar{\sigma}, s, \theta),
\tag{17}
\]

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

\[
\dot{s} = g(\bar{\sigma}, s, \theta) = w g_0(\bar{\sigma}, s, \theta).
\tag{18}
\]

Eqs. (17) and (18) give a general form of the constitutive model used in this work. Simpler creep laws were also introduced in [14,15] for modelling 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 \( \mathbf{g} \) be the gravity field; then the equilibrium equation of the solidifying body can be written as

\[
\nabla \cdot \sigma + \rho g = 0.
\tag{19}
\]

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 \( \sigma = -\rho g h I \). Note that this approach allows the initial stress of a solid particle at nucleation time to be the hydrostatic pressure of the corresponding liquid particle just before it solidified [7].

Modelling of contact (normal traction \( t_N \) and tangential traction \( t_T \)) and air-gaps (\( \delta_{gap} \)) 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 domain, and is parameterized such that the normal vector \( \nu \) points into the admissible domain. The gap function (\( \delta_{gap} \), which in the contact problem literature 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 modelled 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. Modelling of the thermomechanical and contact problems
Let us denote the region of the solidifying body as \( \Omega \), \( \Gamma_\sigma \) as the part of surface (\( \Gamma_\sigma \subset \partial \Omega \)) on which a known external traction (i.e., liquid head pressure) is applied, and \( \Gamma_c \) as the part of surface of the body (\( \Gamma_c + \Gamma_\sigma = \partial \Omega \)) that may potentially contact the mold surface.

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

\[
\mathcal{G}(\mathbf{u}, \mathbf{\hat{u}}) = \mathcal{G}^{\text{int}}(\mathbf{u}, \mathbf{\hat{u}}) - \mathcal{G}^{\text{ext}}(\mathbf{u}, \mathbf{\hat{u}}) - \mathcal{G}^{\text{c}}(\mathbf{u}, \mathbf{\hat{u}}) = 0, \tag{20}
\]

for each test vector field \( \mathbf{\hat{u}} \) with the internal virtual work \( \mathcal{G}^{\text{int}} \), external virtual work \( \mathcal{G}^{\text{ext}} \) and contact virtual work \( \mathcal{G}^{\text{c}} \) defined as

\[
\mathcal{G}^{\text{int}}(\mathbf{u}, \mathbf{\hat{u}}) = \int_\Omega \sigma : \nabla \mathbf{u} \, dV, \tag{21}
\]

\[
\mathcal{G}^{\text{ext}}(\mathbf{u}, \mathbf{\hat{u}}) = \int_{\Gamma_\sigma} \mathbf{t} \cdot \mathbf{\hat{u}} \, dS + \int_\Omega \rho g \cdot \mathbf{\hat{u}} \, dV, \tag{22}
\]

\[
\mathcal{G}^{\text{c}}(\mathbf{u}, \mathbf{\hat{u}}) = \int_{\Gamma_c} (\mathbf{t}_N \cdot \mathbf{u} + \mathbf{t}_T \cdot \mathbf{\hat{u}}) \, dS, \tag{23}
\]

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

\[
t_N = \lambda_N + \epsilon_N g > 0, \quad t_{trial}^T = \lambda_T + \epsilon_T m_{\alpha \beta} (\xi_{N} - \xi_{z-1}), \quad \Phi_{trial} = \mu_{f} t_{N}, \quad t_{T} = \begin{cases} t_{T_{trial}}^T, & \text{if } \Phi_{trial} \leq 0, \\ \mu_{f} t_{N}, & \text{if } \Phi_{trial} > 0, \end{cases}
\]

where \( \mu_f \) is the friction coefficient, \( \epsilon_N, \epsilon_T \) are penalty parameters, and \( t_{T_{trial}}^T \) 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 point on the mold surface, \( m_{\alpha \beta} \) is the metric tensor with components computed from the tangent vectors to the mold surface, and \( \Phi_{trial} \) is the slip function used to determine whether the contact conditions correspond to slip or stick [17].

In this work, we take \( \epsilon_N = 1 \times 10^4 \) 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 \( \mathbf{u} \):

\[
\frac{\partial \mathcal{G}(\mathbf{u}_n^{k-1}, \mathbf{\hat{u}})}{\partial \mathbf{u}} (\mathbf{u}_n^k - \mathbf{u}_n^{k-1}) = -\mathcal{G}(\mathbf{u}_n^{k-1}, \mathbf{\hat{u}}). \tag{24}
\]

This linearization process requires a number of steps.

1. Linearization of the internal virtual work:

\[
\frac{\Delta \mathcal{G}^{\text{int}}(\mathbf{u}, \mathbf{\hat{u}})}{\Delta \mathbf{u}_{br}} = \int_\Omega \mathbf{\hat{u}}_{ar} \mathbf{N}_{a\beta} \frac{\mathcal{L}^e_{ijkl}}{2} dV, \tag{25}
\]

where \( \mathbf{N} \) are the finite element shape functions, \( a \) and \( b \) are node indices, \( i, j, k, l \) are the fourth-order tensor \( \mathbf{M} \) is defined as

\[
\mathbf{M}_{ijkl} \equiv \frac{\partial \mathbf{\hat{e}}^e_{ij}}{\partial \mathbf{\hat{e}}_{kl}} = \frac{3}{2} \{ \sigma_{ij} \alpha \Delta t L^e_{mnkl} \sigma_{mn} + \frac{f}{\sigma_s} \Delta t L^e_{ijkl} \}, \tag{26}
\]

where \( L^e_{ijkl} = L^e_{ijkl} - \frac{1}{3} L^e_{mnkl} \delta_{ij} \). In the definition of \( \mathbf{M}, \sigma_{ij} \) is the trial stress, which will be defined later in this section, and the parameter \( \alpha, a_1, b_1 \) and \( c \) are defined as

\[
\alpha = \frac{1 - c}{2 \mu \Delta t \sigma_s^2} - \frac{3f}{2 \sigma_s^2},
\]
\[
\begin{align*}
a_1 &= 1 + 3\mu\Delta t \frac{\partial f}{\partial \sigma}, \\
b_1 &= \Delta t \frac{\partial g}{\partial \sigma}, \\
c &= \frac{b_2}{a_1 b_2 + a_2 b_1}.
\end{align*}
\]

2. The linearization of the external virtual work \( \mathbf{G}^{ext} \) is approximated to zero in this work with \( \frac{\Delta \mathbf{G}^{ext}(\mathbf{u}, \mathbf{u})}{\Delta \mathbf{u}} \approx 0 \).

3. Details of linearization for the contact virtual work \( \mathbf{G}^c \) 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

\[
\mathbf{\sigma}_n = \mathbf{\sigma}_{n-1} + \Delta t \mathbf{L}^c(\mathbf{\dot{e}} - \mathbf{\dot{e}}^g) - \Delta t \mathbf{L}^c(\mathbf{\dot{e}}^P),
\]

we can define the trial stress as

\[
\mathbf{\sigma}^1 = \mathbf{\sigma}_{n-1} + \Delta t \mathbf{L}^c(\mathbf{\dot{e}} - \mathbf{\dot{e}}^g).
\]

Using Eq. (16) and taking the deviatoric part of Eq. (27), we obtain

\[
\mathbf{\sigma}'_n = \mathbf{\sigma}^1 - \frac{3\mu\Delta t f}{\sigma} \mathbf{\sigma}'.
\]

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

\[
\mathbf{\dot{e}}_n - \mathbf{\dot{e}}_s + 3\mu\Delta t f = 0.
\]

Integration of Eq. (18) leads to

\[
s_n - s_{n-1} = g_1 \Delta t.
\]

By solving the above two non-linear equations iteratively for \( \mathbf{\dot{e}}_n \) and \( s_n \), the radial return factor \( \eta \) can be evaluated as

\[
\eta = \frac{\mathbf{\dot{e}}_n}{\mathbf{\dot{e}}_s}.
\]

Notice that for the liquid or mushy regions where \( g_s < g_s^h \), iterations for solving Eqs. (30) and (31) are not necessary, since \( \mathbf{\sigma}' = 0 \). The radial return factor \( \eta \) is set to 0 directly for regions with \( g_s < g_s^h \). With the radial return factor \( \eta \) calculated, we can then update the stress tensor as follows

\[
\mathbf{\sigma}_n = \eta \mathbf{\sigma}^1 + \frac{1}{3} \text{tr}(\mathbf{\sigma}_n) \mathbf{I}.
\]

3. Numerical algorithm

The various subproblems considered here are the thermal, flow and deformation problems including phase transition and contact. The flow problem that was not described in the earlier section follows the methodology in [9]. 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 \( \| \Delta \theta^t \| / \| \theta^t \| \). 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 \( \mathbf{\sigma}_{n-1} \), plastic strain \( \mathbf{\varepsilon}^p_{n-1} \), temperature \( \theta_{n-1} \), solid fraction \( g_s^{n-1} \) 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 point 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, \( \epsilon_l \) is updated using the Lever or Scheil rules. The air-gap size \( \delta_{gap}^{n} \) and contact pressure \( P_{n} \) are substituted into Eq. (7) to obtain the
heat flux at the solid-shell/mold interface.

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

(b) Temperature $\theta_n$ and solid fraction $g^n_s$ 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. Using augmentations, both the air-gap size $\delta^n_{gap}$ and the contact pressure $P_n$ can be determined in this step on each Gauss point of each surface element at the solid-shell boundary $\Gamma_c$. Augmentations are stopped when the gap function (for points in contact) becomes less than $10^{-4}A$, where $A$ is the mold amplitude.

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

Table 1

<table>
<thead>
<tr>
<th>Material</th>
<th>$k$ (W/mK)</th>
<th>E (GPa)</th>
<th>$\nu$</th>
<th>$\rho$ (kg/m³)</th>
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<tbody>
<tr>
<td>Copper</td>
<td>345.4</td>
<td>64</td>
<td>0.37</td>
<td>7938</td>
</tr>
<tr>
<td>Iron</td>
<td>36.2</td>
<td>144</td>
<td>0.33</td>
<td>7265</td>
</tr>
<tr>
<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]

\[
f = \dot{\varepsilon}^p = \dot{\varepsilon}_0 \left( \frac{\dot{\varepsilon}}{\sigma_0} \exp(-\delta \cdot g_s) \cdot \exp(-\frac{mQ}{R\theta}) \right)^\frac{1}{n}
\]

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>$\dot{\varepsilon}_0$</td>
<td>$\sigma_0$</td>
<td>$Q$</td>
<td>$m$</td>
</tr>
<tr>
<td>$9 \times 10^{-3}$s⁻¹</td>
<td>5.5KPa</td>
<td>154J/mol</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Figure 2. The critical solid fraction for different Aluminum alloys [13].

We assume that at the beginning of solidification, the liquid metal fully wets the sinusoidal mold and no air-gaps are 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 air-gap nucleation at the trough, $P_{tr}$, is examined. Once $P_{tr}$ reaches 0, we assume that air-gap nucleation occurs. How air-gap nucleation further affects solidification is not studied in this example. Since
no air-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 and plastic deformation must be taken into account to correctly model the mechanical behavior of the solid-shell. 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 $0.5 mm$, the liquid pressure $P_l = 10000 \text{ Pa}$ and room temperature is applied at the bottom of the mold. All the solid or dotted lines in 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 air-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 air-gap nucleation. Fig. 3 shows the $P_{tr}$ evolution with the parameters $\lambda = 2 \text{ mm}$, $R_0 = 10^{-5} \text{ m}^2 \text{ sec} \text{ K/J}$ and $R' = 10^{-12} \text{ m}^2 \text{ sec} \text{ K/J Pa}$ 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 the higher the mold thermal conductivity, the quicker the air-gaps nucleate along the mold-shell interface. 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 $R_0 = 10^{-3} \text{ m}^2 \text{ sec} \text{ K/J}$ 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 air-gap nucleation at earlier times. The contact pressure at the trough decreases nearly quadratically.

Fig. 5 shows a linear relationship between the mean shell thickness at air-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 a larger solid-shell thickness at air-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 as zero. This explains the higher discrepancy between the two results for high pressures.

For a given material, the value of the solid-
shell thickness at air-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 air-gap nucleation during the early stages of solidification. From Fig. 5, one can see that high liquid pressure is preferred to obtain a thick shell at air-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 ($\epsilon_i = 0.01$ 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 ($13.4 \times 10^3$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 $12.3 \times 10^3$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.

![Graph of pressure vs. concentration of copper](image.png)

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

**B. Stress development and growth pattern after air-gap nucleation:** Fig. 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 air-gap nucleation. So investigating what happens after air-gap nucleation is of great importance. In the previous example studying air-gap nucleation time (Case 1), no plastic deformation was assumed and the solidification process was examined only before air-gap nucleation. 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 air-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, \( R_0 = 1 \times 10^{-5}\text{m}^2\text{sec/J/K} \), \( R' = -1 \times 10^{-12}\text{m}^2\text{sec/J/ Pa} \), \( h_0 = 1.5 \times 10^5\text{K/m}^2\text{sec/J} \) and \( k_0 = 4.5 \times 10^{-2}\text{K/m sec/J} \). 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°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 0.002mm/sec at 5 ms (as shown in Fig. 7c) to 0.023mm/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 stresses play 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
Figure 7. Temperature and flow velocity at time 5 ms: (a) $\lambda = 1\text{mm}$ with superheat $30^\circ\text{C}$, (b) $\lambda = 5\text{mm}$ without superheat, (c) $\lambda = 5\text{mm}$ with superheat $30^\circ\text{C}$.

pattern. The two hills formed at the crest are growing to meet each other and finally would result in a planar growth pattern. In the case of a $1\text{mm}$ 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 $5\text{mm}$ 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 air-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 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 [16,19], the stress at the roots of the dendrites can be used as a hot-tearing cri-
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.)
Figure 11. Evolution of maximum equivalent stress in solid-shell for different alloys ($\lambda = 5$ mm with $30^\circ$C superheat).

teron. 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, the mold material determines how fast heat can be extracted away through the mold. The effect of the mold material on air-gap nucleation time for pure Aluminum is shown in Fig. 3. Air-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 $\delta = \frac{\beta s (1+\nu)}{k}$ [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 the iron or lead molds. Equivalent stress and flow velocity at time 100 ms for different molds (copper, iron and lead) with the same wavelength $\lambda = 5$ mm are shown in Fig. 13. At a smaller wavelength $\lambda = 1$ mm, the growth patterns for molds with different materials are similar. Generally the effect of mold topography is more pronounced for a mold with a larger heat conductivity.

**D. Effects of melt pressure:** In all of the above examples, a melt pressure $10^{-2}$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 $10^{-3}$MPa.
to $10^{-1}$ 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. Air-gap nucleation was assumed to occur when the contact pressure falls to zero. Air-gap nucleation time and shell thickness at air-gap nucleation time were calculated to illustrate the effects of mold topography. From the viewpoint of air-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, air-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 air-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 [16,19] 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 $10^{-1}$ 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 sur-

Figure 13. Equivalent stress and flow velocity at time 100 ms, $\lambda = 5 mm$ with superheat 30°C for an Aluminum alloy with 1% copper: (a) Copper mold, (b) Iron mold, (c) Lead mold.
face 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. Maximum equivalent stress in the solidifying body and front unevenness at an early solidification time (100 ms). The position difference of $\epsilon_l = 0.7$ corresponding to the crest and the trough is used here as a measure of front unevenness.](image)

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