Introduction

- Hot tearing is a solidification defect that leads to poor product quality at best and a breakout at worst

- The averaging inherent to traditional macro-scale models prevents study of the details of hot tear formation and propagation

- This work explores the hot tearing phenomenon by combining macro-scale information with a detailed model of the morphology of the solidification front
Previous Work

Large Scales

• Simulations of entire caster

Thermomechanical model of funnel molds
Hibbeler and Thomas

Multiphysics model of beam blank
Koric, Hibbeler, Liu, and Thomas

Intermediate Scales

• Detailed simulation of a surface defect

\[ \varepsilon_c = \frac{0.02821}{\varepsilon_c^{0.3131}} \cdot \Delta T_B^{0.8638} \]

Won et al., MMTB 2000

\[ \Delta T_B = T(f_s = 99\%) - T(f_s = 90\%) \]

\[ \dot{\varepsilon} = \frac{\varepsilon(f_s = 99\%) - \varepsilon(f_s = 90\%)}{t(f_s = 99\%) - t(f_s = 90\%)} \]

\[ \varepsilon_{dmg} = \varepsilon(f_s = 99\%) - \varepsilon(f_s = 90\%) \]

\[ D = \varepsilon_{dmg} / \varepsilon_c \]

Contours of inelastic strain

H Jasti
Previous Work

Small Scales

• Semi- or Analytical models
  – Rappaz, Drezet, and Gremaud, *MMTA* 1999
  – Monroe and Beckerman, *MSEA* 2005

• Mushy zone RVE models
  – Phillion, Cockcroft, and Lee, *MSMSE* 2009

Previous Work

Room for Improvement

• Previous work covers mostly:
  – Aluminum alloys
  – Equiaxed/globular grains
  – Mushy zone frozen in time
  – Macro- or meso-scale – need liquid+solid averaging
  – Oversimplified material models – solid, liquid or both

• Present work is concerned with:
  – Commercial steel alloys
  – Entire solidification history – surface and columnar zones
  – Microscale – no averaging
  – Proper material models
  – Relate microscale information to macroscale quantities
Background

• Different break-out risk is observed during production, which is believed to be due to hot cracking in the first solid shell inside the caster: \( \underline{2} > \underline{1} \gg \underline{3} \)

<table>
<thead>
<tr>
<th>Steel grade</th>
<th>C (wt %)</th>
<th>Mn (wt %)</th>
<th>V (wt %)</th>
<th>Nb (wt %)</th>
<th>N (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LCAK</td>
<td>0.045</td>
<td>0.22</td>
<td>-</td>
<td>-</td>
<td>50</td>
</tr>
<tr>
<td>LR-HSLA</td>
<td>0.045</td>
<td>0.8</td>
<td>0.04</td>
<td>0.013</td>
<td>80</td>
</tr>
<tr>
<td>HSLA</td>
<td>0.045</td>
<td>0.8</td>
<td>0.13</td>
<td>0.013</td>
<td>130</td>
</tr>
</tbody>
</table>

Table 1: Typical chemical composition of three steel grades

This is in contradiction to the empirical finding \( \underline{2} > \underline{1} \gg \underline{3} \).

But why \( \underline{3} \ll \underline{2} \)???
Modeling Approach

**Casting Conditions**
- Mold heat transfer data under ideal taper

**Macro Slice Model**
- Bulk thermal and mechanical response

**Micro Slice Model**
- Detailed mechanical behavior in mushy zone

**Microstructure**
- Phase field calculations

**Macro Caster Model**
- Overall thermal and mechanical response, evaluate for hot tearing

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**Calibrated Heat Flux Profile**

Casting speed = 4.8 m/min

- F12l
- PV85
Microscale Domain

200,000 4-node elements, 0.3-μm square

Out-of-plane assumption: generalized plane strain \( u_z = \text{uniform} \)

Phase field calculated with MICRESS by B. Boettger

Explicit FEM

Get accelerations from force balance
\[ \nabla \cdot \sigma + b = \rho a \quad \Rightarrow a^n = M^{-1}(F^n_{\text{ext}} - F^n_{\text{int}}) \]

Integrate to get half-step velocity
\[ v^{n+\frac{1}{2}} = v^{n-\frac{1}{2}} + a^n \frac{\Delta t^{n+1} + \Delta t^n}{2} \]

Integrate at half-step to get displacement
\[ u^{n+1} = u^n + v^{n+\frac{1}{2}} \Delta t^{n+1} \]

Critical time step
\[ \Delta t < \frac{L_{\text{min}}}{c_d} \quad L_{\text{min}}, \text{ Smallest element characteristic length} \]

Dilational wave speed
\( c_d = \sqrt{\frac{\lambda + 2\mu}{\rho}} \quad \hat{\lambda} \quad \text{Effective Lame constant} \)

Efficiencies from:
- No Newton iterations (no matrix solve)
- Lumped mass matrix (no matrix solve)
- Mass scaling – make density large to increase critical step size
Modeling Issues

- Using the “traditional” quasi-static approach, the 2D simulation with previously-described conditions **always** crashes with the formation of solid material.

- An alternative approach, which explicitly integrates the full force balance, is more numerically stable:
  - Mass scaling technique increases critical time step size
  - Explicit marching scales well across processors
  - No generalized plane strain elements; must work in 3D
  - See (Koric, Hibbeler, and Thomas, IJNME 2009) for more detail

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Modeling Issues

- Imposing the generalized plane strain constraint prevents parallelization (in ABAQUS/Explicit)

- Efficient solution to this problem is to calculate the shrinkage in a macroscale model and impose time-dependent boundary conditions

\[
\text{Other BCs mimic 2D case}
\]

- Top face fixed in z
- Bottom face \( v_z = \Delta x \cdot \dot{\varepsilon}_{\text{macro}}(t) \)
- Lateral face \( v_y = W \cdot \dot{\varepsilon}_{\text{macro}}(t) \)

200,000 8-node elements, 0.3-\(\mu\)m cube
Material Models

- Liquid:
  - Elastic, perfectly plastic (500 Pa yield stress)
  - To be improved to Newtonian fluid (viscosity increases critical $\Delta t$)
- Solid: Zhu (ferrite) or Kozlowski III (austenite)

\[
\dot{\varepsilon}(s^{-1}) = 0.1 \left[ f(C)(T/300)^{-5.52} (1 + 1000\varepsilon)^n \right]
\]

\[
f(C) = 1.3678 \times 10^6 (C)^{1.555 T^{-2}}
\]

\[
m = -9.4156 \times 10^{-5} T + 0.3495
\]

\[
n = 0.1617 \times 10^{-4} T - 0.06166
\]

\[
\varepsilon(s^{-1}) = f(C) \left[ \sigma - f_c(T) \varepsilon \right] \left[ f_c(T) \right]^{\frac{1}{n(T)}} \exp \left( -\frac{4.65 \times 10^4 (K)}{T} \right)
\]

Zhu

Kozlowski

Macroscale Model

Thermal Boundary Conditions

- Insulated
- Prescribed heat flux

Mechanical Boundary Conditions

- Zero perpendicular displacement
- Equal perpendicular displacement
- Stress-Free

Material properties from CON1D
Macroscale Model – Results

Macroscale Strain History

Input this data into microscale model

Component of strain perpendicular to solidification direction

Noise corresponds to nodes turning solid
Microscale Domain

Temperature and Carbon Concentration

Microscale Deformation

Preliminary Results

- Strain concentrations in liquid regions
  - Most motion occurs in liquid

- Peak negative pressure in roots of secondary arms
  - Insufficient feeding can lead to porosity

Pressure stress

Negative pressure means material in tension
Microscale Deformation

Preliminary Results

- Consequences to be determined

Stress in vertical direction

von Mises stress

Total strain in horizontal direction

Stress in horizontal direction

LE, LE22
(Avg: 75%)

S, S22
(Avg: 75%)
Modeling Issues

- Even ABAQUS/Explicit has trouble with the formation of the first solid material, but the explanation is more evident than with /Standard:
  - *The large step-change in stiffness causes the critical time step to be violated*

- The mass scaling must be readjusted, frequently, to account for the change in stiffness as temperature and phase evolve

\[
\dot{\lambda} + 2\mu = \frac{\Delta p}{\Delta \varepsilon_{dit}} + \frac{2}{3} \frac{\Delta s}{\Delta e}
\]

\[
\begin{align*}
\Delta p & \quad \text{Pressure stress increment} \\
\Delta \varepsilon_{dit} & \quad \text{Dilational strain increment} \\
\Delta s & \quad \text{Deviatoric stress increment} \\
\Delta e & \quad \text{Deviatoric strain increment}
\end{align*}
\]

Future Work

Simulations of many dendrites will reveal statistically significant data that is usable for macroscopic models

B. Boettger
Conclusions

• Modeling effort underway to predict hot tearing from small-scale phenomena
  – Preliminary efforts look promising

• Future studies based on very large phase field simulations

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• Dr. Bernd Boettger, ACCESS e.V.
  – See (Boettger, Apel, Santillana, and Eskin, MCWASP XIII) for more detail

• National Center for Supercomputing Applications (NCSA) at UIUC – “Forge” cluster

• Dassault Systemes (ABAQUS parent company)