GaAs Crystal Growth with Vertical Gradient-Freeze Technique: Simulation of Heat Transfer and Thermal Stresses

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Objectives

- In this work, we demonstrate the capabilities of Elmer software to simulate heat transfer and thermal stress mechanisms during the vertical gradient-freeze (VGF) growth of 3” GaAs crystal.
- Elmer is an open-source software, developed by CSC – IT Center for Science in Finland: Further details: https://www.csc.fi/web/elmer
Assumptions

- Axi-symmetric furnace geometry
- Steady-state analysis
- Melt and gas convections neglected (Melt/gas flow play a minor role in VGF with bottom seeding)
Furnace Geometry

- Silica ampoule
- Boric oxide
- GaAs crystal/melt
- pBN crucible
- Crucible holder
- Thermal insulation
- Water-cooled pressure chamber
- Ceramic tube and supporting components
- Heater
- Gas
Finite Element Mesh

Triangular mesh created by GiD software, see [http://www.gidhome.com/](http://www.gidhome.com/)

Number of triangular elements: 43825
Number of nodes: 22120
Heat Transfer and Thermal Stress Mechanisms

• Heat transfer by conduction in solid materials, gas and GaAs crystal/melt
• Diffuse-gray radiation between surfaces within the ampoule
  – Solid materials considered as opaque materials
  – Gas: Non-participating medium
• Tracking of crystal-melt interface: Enthalpy method
• Automatic heater power adjustment: $T = T_{\text{fixed}}$ at specific point
• Isotropic material properties in solidified crystal and crucible in thermal stress analysis
## Material Properties

<table>
<thead>
<tr>
<th>Material</th>
<th>Material Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs crystal/melt</td>
<td>Density: 5710 kg/m³ (crystal), 5300 kg/m³ (melt)</td>
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<tr>
<td></td>
<td>Heat cap.: 420 J/kgK (crystal), 420 J/kgK (crystal)</td>
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<td></td>
<td>Heat cond.: 7.12 W/mK (crystal), 17.8 J/kgK (crystal)</td>
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<td></td>
<td>Latent heat: 726000 J/kg, Phase change interval: [1510; 1512K]</td>
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<tr>
<td></td>
<td>Poisson ratio: 0.31, Young’s modulus: 8.55e10 Pa</td>
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<tr>
<td></td>
<td>Heat expansion coefficient: 5.2e-6 1/K</td>
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<tr>
<td>Encapsulant (Boric oxide)</td>
<td>Heat cond.: 0.5 W/mK, Emissivity: 0.3</td>
</tr>
<tr>
<td>Crucible (pBN)</td>
<td>Heat cond.: 4.0 W/mK, Emissivity: 0.4</td>
</tr>
<tr>
<td></td>
<td>Poisson ratio: 0.21, Young’s modulus: 1.95e10 Pa</td>
</tr>
<tr>
<td></td>
<td>Heat expansion coefficient: 1.0e-6 1/K</td>
</tr>
<tr>
<td>Crucible support, quartz ampoule, ceramics</td>
<td>Heat cond.: 2.0 W/mK, Emissivity: 0.35</td>
</tr>
<tr>
<td>Gas</td>
<td>Heat cond.: 2.0 W/mK</td>
</tr>
<tr>
<td>Heater</td>
<td>Heat cond.: 85.0 W/mK</td>
</tr>
<tr>
<td>Insulation</td>
<td>Heat cond.: 1.0 W/mK</td>
</tr>
<tr>
<td>Chamber</td>
<td>Heat cond.: 15.0 W/mK</td>
</tr>
</tbody>
</table>

Solved Numerical Cases

- Case1: Seed solidification - Heater power adjustment such that $T=1470K$ at the outer edge of horizontal crucible bottom surface
- Case2: Crystal (complete) solidification - Heater power adjustment such that $T=1500K$ at the crystal-encapsulant-crucible intersection
**Case 1: Temperature Distributions**

- **Global temperature distribution;**
- **On external chamber wall**
- **T=300K**
- **T=1510K (yellow line); Convex interface shape in seed area**
- **Heater power adjustment such that T=1470K on horizontal crucible bottom surface**

Visualizations by ElmerPost
Case 1: Vertical Temperature Gradient in Crystal and Melt along Symmetric-Axis

![Graph showing vertical temperature gradient vs distance from seed bottom](Graph.png)
Case2: Temperature Distributions

Global temperature distribution;
On external chamber wall
T=300K

T=1510K (yellow line); Crystal completely solidified
Heater power adjustment such that T=1500K at crystal-encapsulant-crucible intersection

Visualizations by ElmerPost
Case 2: Vertical Temperature Gradient in Crystal and Melt along Symmetric-Axis

![Graph showing vertical temperature gradient (dT/dz) vs. distance from seed bottom (cm). The graph plots the gradient values over a range of distances, indicating a descending trend.]
Case 2: Von Mises Stress Field in Crystal and Crucible

Visualizations by ElmerPost, units in Pa
Conclusions

• We have demonstrated Elmer capabilities in solving GaAs crystal growth in Vertical Gradient Freeze (VGF) process; The same procedure can be applied for other materials used in VGF, like InP and Ge
• We have considered only opaque materials in the model; Encapsulant and silica parts can also be considered as transparent materials
• In the current configuration, axial temperature gradient may be too high for reliable and reproducible seeding; The model can be used in optimizing thermal boundary conditions to reach low thermal stresses and constant growth rate
• The model would also allow multi-zone heater set-up