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

Jari Järvinen
Silicom Ltd., Finland
http://www.silicom.fi
jari.jarvinen@silicom.fi

July 15, 2016

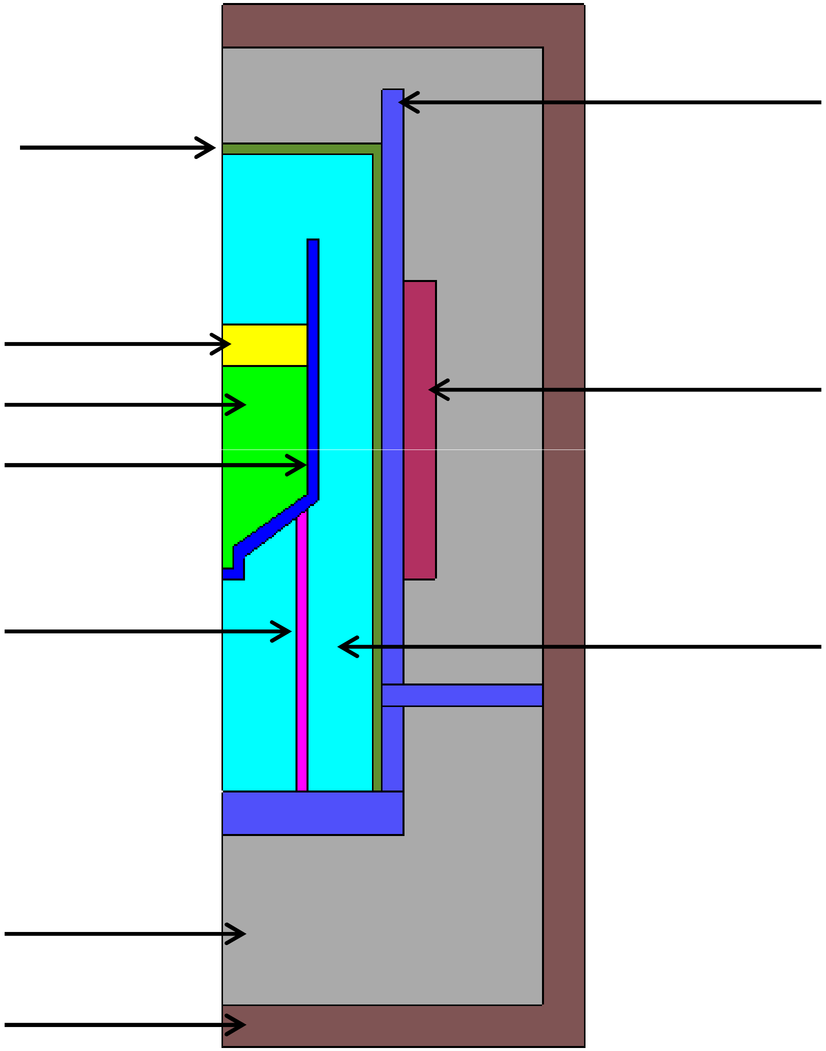
Objectives

- In this work, we demostrate the capabilities of Elmer software to simulate heat transfer and thermal stress mechanisms during the vertical gradient-freeze (VGF) growth of 3” GaAs crystal
- The work is inspired by articles in the literature; Here we follow the article of J. Amon, P. Berwian, G. Müller, Journal of Crystal Growth 198/199 (1999), p. 361-366
- 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

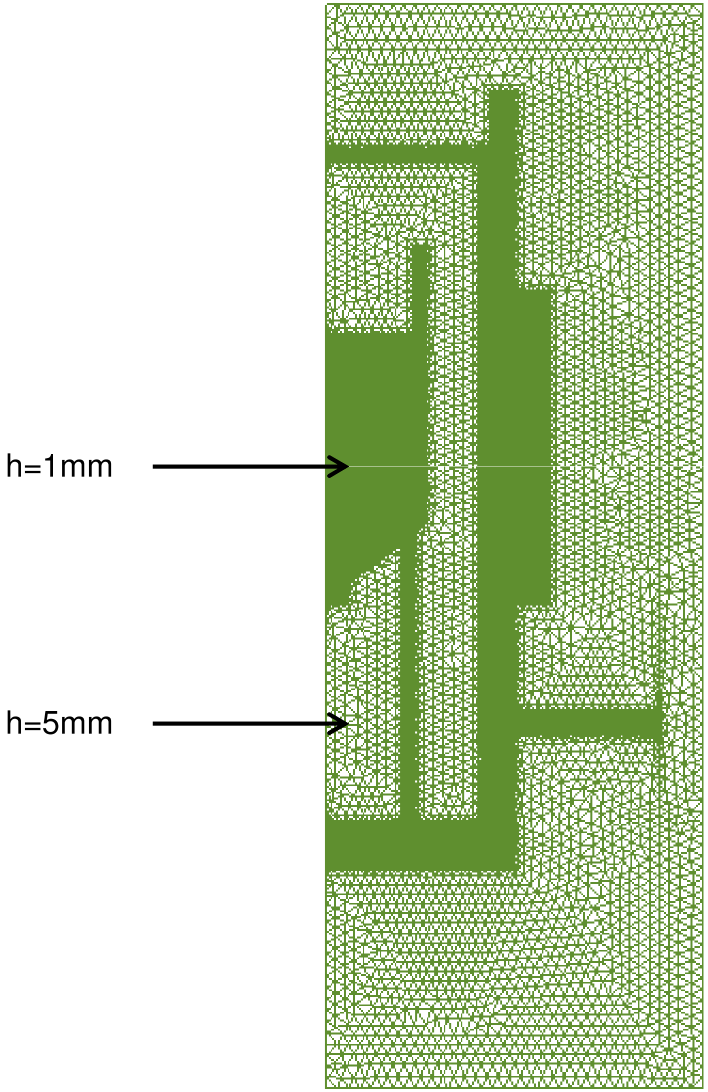
Water-cooled pressure chamber

Ceramic tube and supporting components

Heater

Gas

Finite Element Mesh



Triangular mesh created by GiD software, see http://www.gidhome.com/

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: $T=T_{fixed}$ at specific point
- Isotropic material properties in solidified crystal and crucible in thermal stress analysis

Material Properties

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

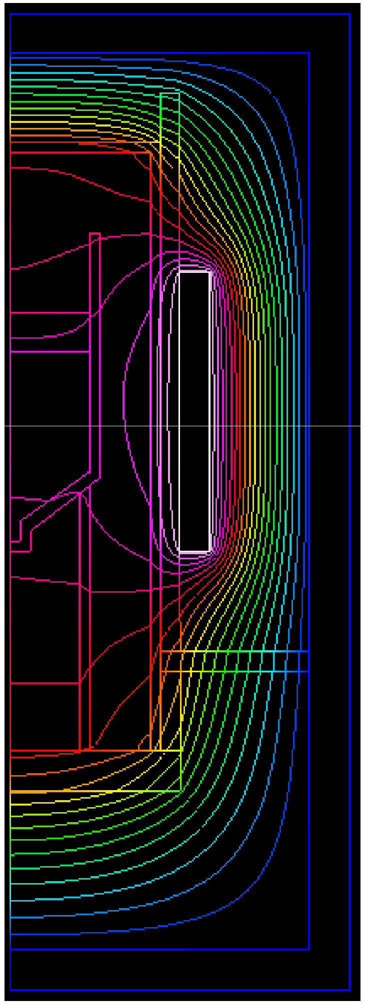
Ref. H. Weimann, J. Amon, Th. Jung, G. Müller, Journal of Crystal Growth 180 (1997), p. 560-565

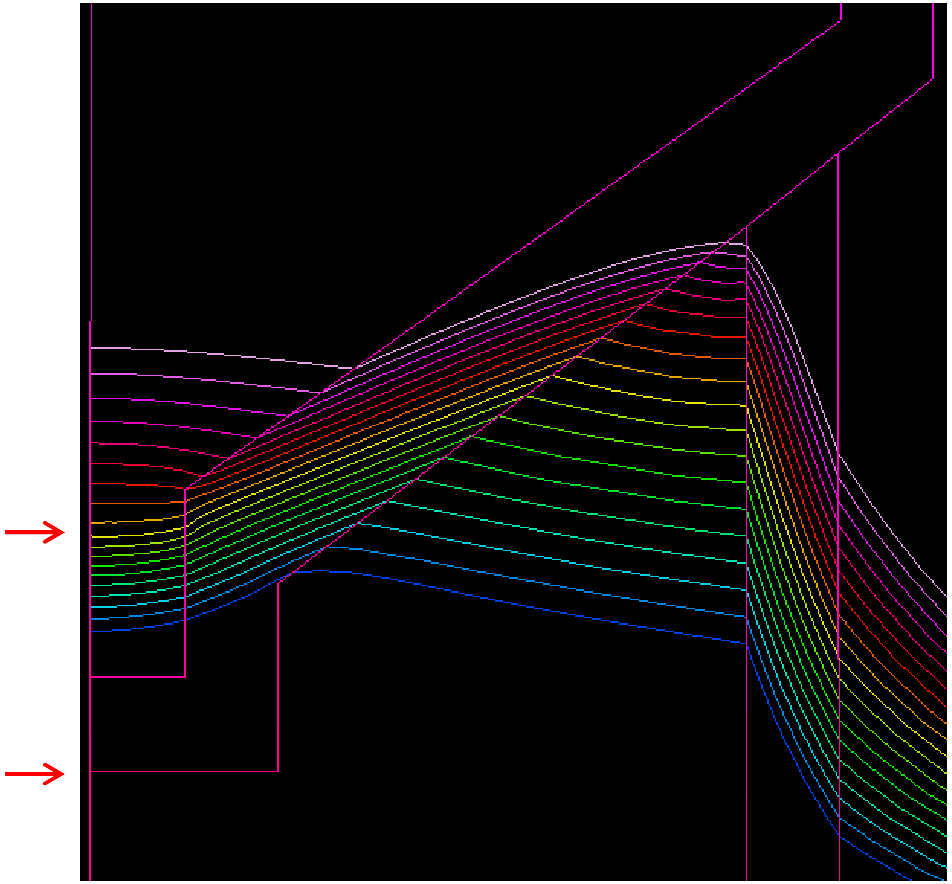
Solved Numerical Cases

- 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

Case1: Temperature Distributions

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

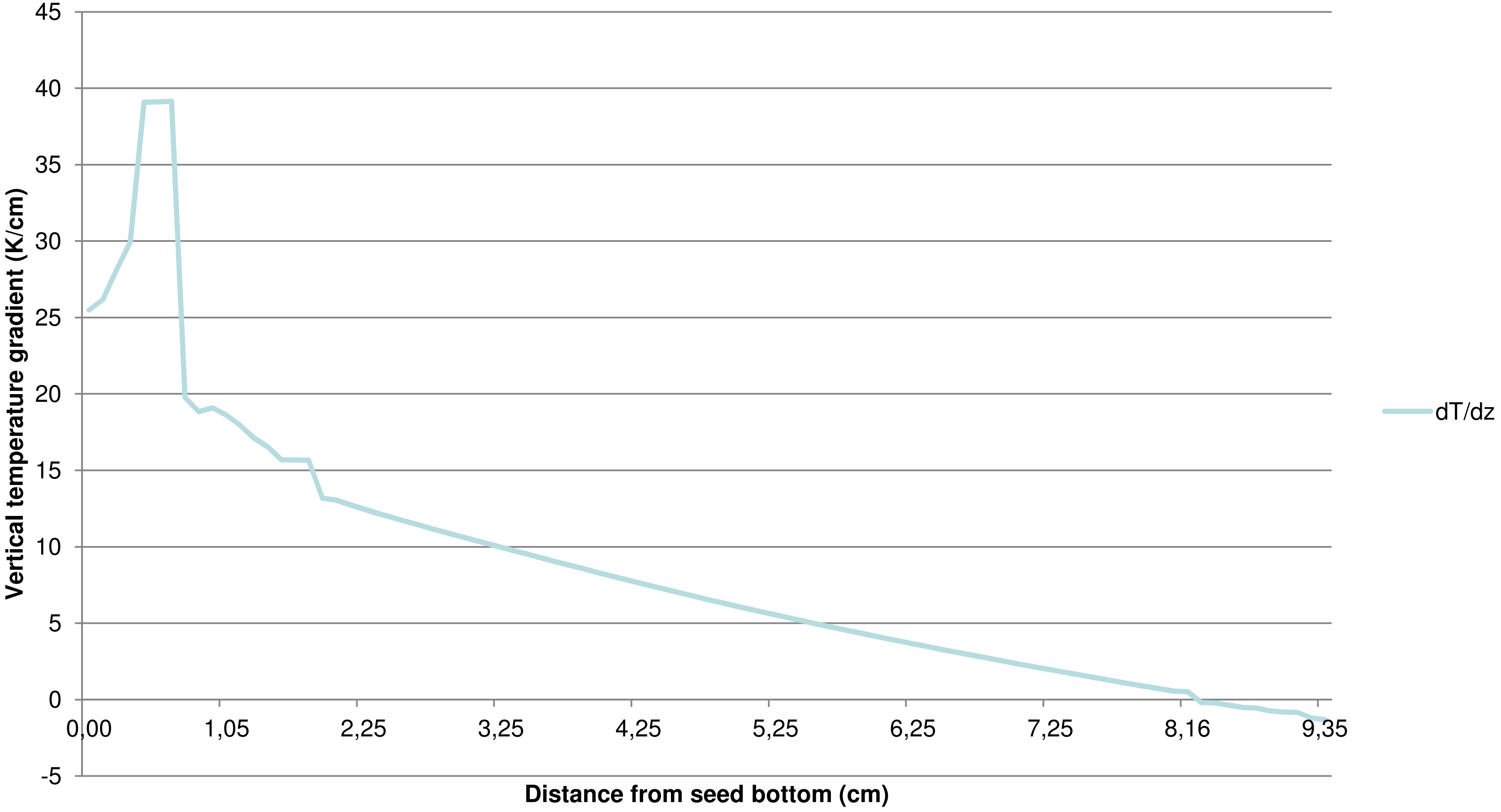




T=1510K (yellow line); Convex interface shape in seed area
Heater power adjustment such that T=1470K on horizontal crucible bottom surface

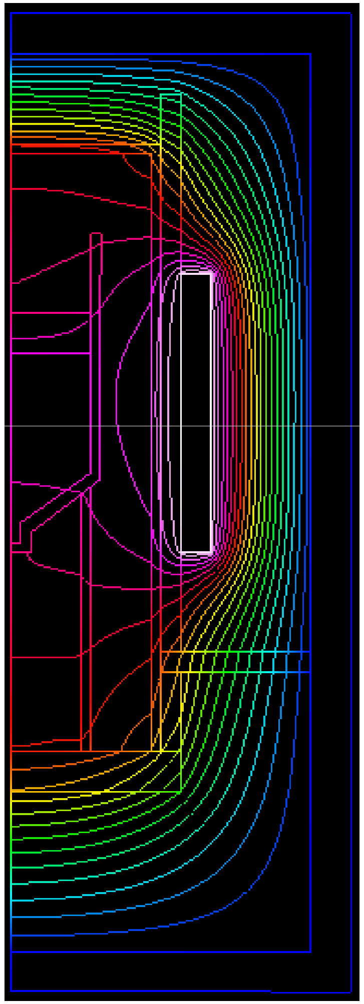
Visualizations by ElmerPost

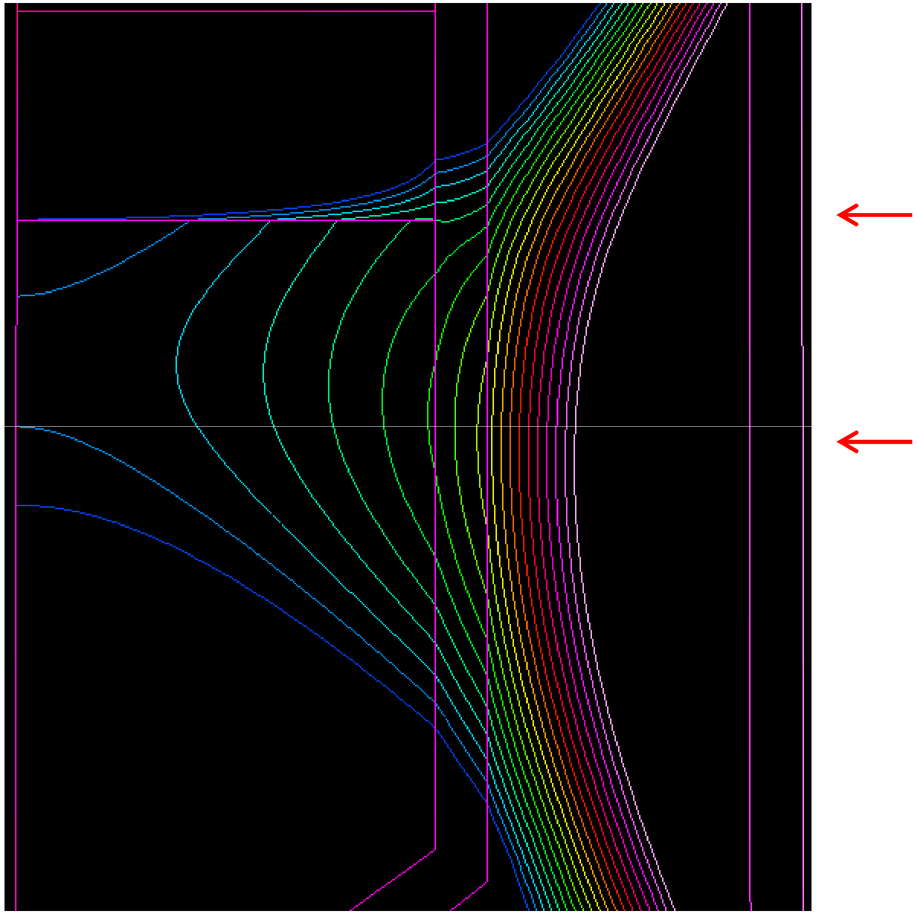
Case1: Vertical Temperature Gradient in Crystal and Melt along Symmetric-Axis



Case2: Temperature Distributions

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

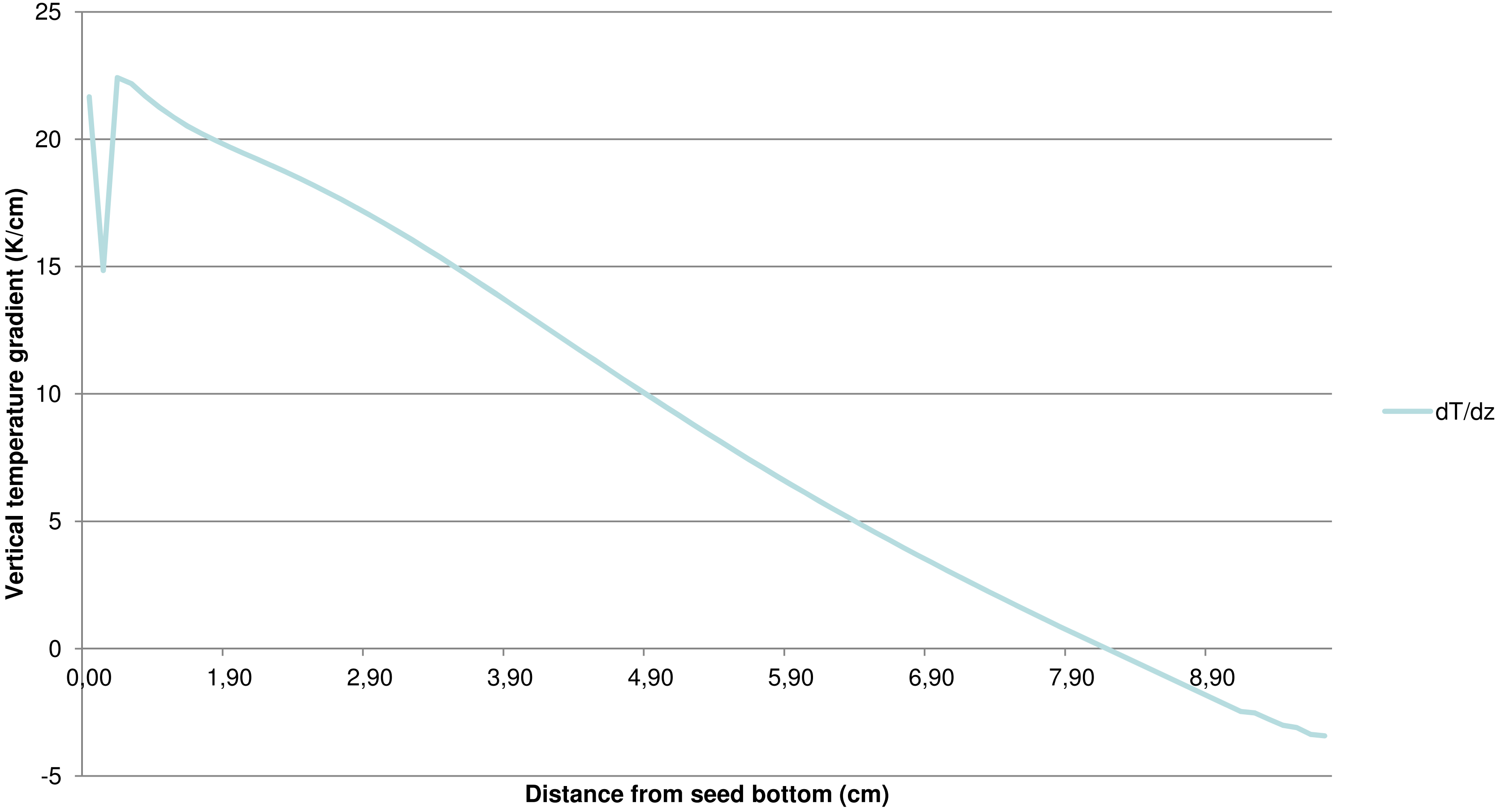




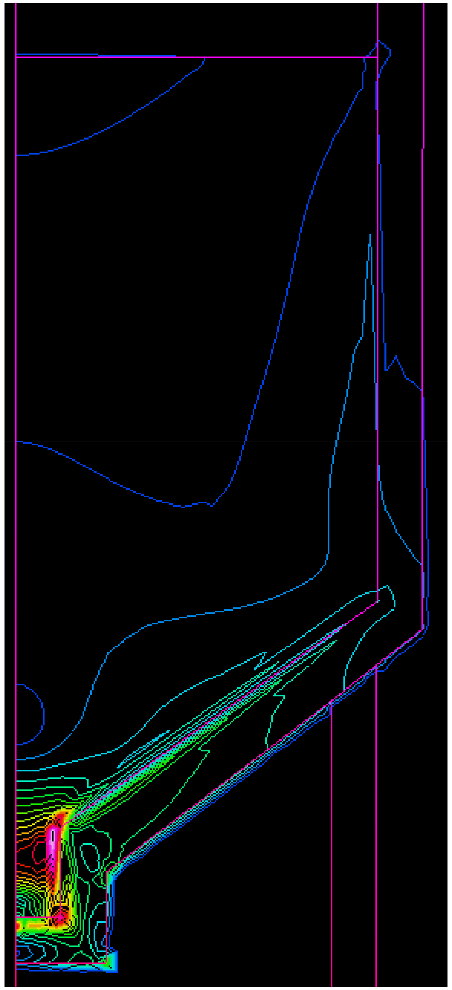
T=1510K (yellow line); Crystal completely solidified
Heater power adjustment such that T=1500K at crystal-encapsulant-crucible intersection

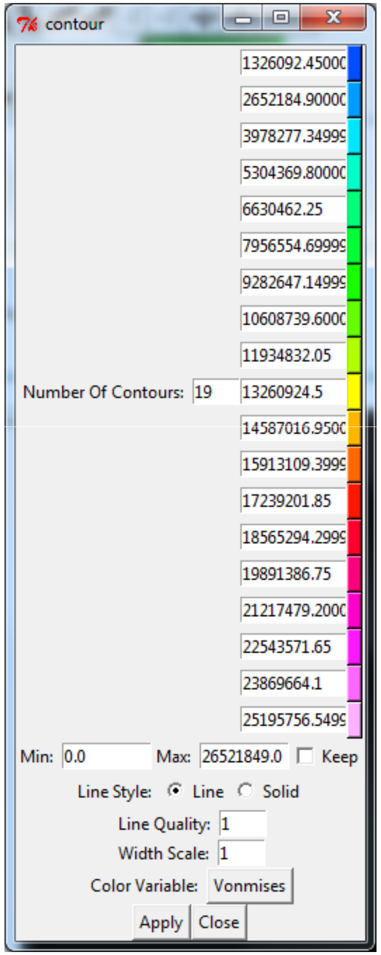
Visualizations by ElmerPost

Case2: Vertical Temperature Gradient in Crystal and Melt along Symmetric-Axis



Case2: Von Mises Stress Field in Crystal and Crucible





1326092.4500
2652184.9000
3978277.3499
5304369.8000
6630462.25
7956554.6999
9282647.1499
10608739.600
11934832.05
Number Of Contours: 19
13260924.5
14587016.950
15913109.399
17239201.85
18565294.299
19891386.75
21217479.200
22543571.65
23869664.1
25195756.549

Min: 0.0 Max: 26521849.0 ☐ Keep

Line Style: ● Line ○ Solid

Line Quality: 1

Width Scale: 1

Color Variable: Vonmises

Visualizations by ElmerPost, units in Pa

Conclusions

- We have demostrated 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