Computer Modeling and Optimization of VGF Crystal Growth process

STR Group
Saint Petersburg, Russia
www.str-soft.com
2014

1984: Start of MOCVD modeling activities at Ioffe Institute, St. Petersburg, Russia;

1993-1996: Group for modeling of crystal growth and epitaxy in University of Erlangen-Nuernberg, Germany;

STR Today:

modeling of crystal growth, epitaxy, and devices

- STR Group, Inc., Saint Petersburg, Russia
- STR, Inc., Richmond VA, USA
- STR GmbH, Erlangen, Germany
- STR K.K., Yokohama, Japan

- More than 40 scientists and software engineers, local representatives in China, South Korea and Taiwan.

Software & consulting services :

- Modeling of crystal growth from the melt and solution: CGSim
- Modeling of bulk crystal growth of SiC, AlN, GaN: Virtual Reactor
- Modeling of optoelectronic and electronic devices: SimuLED
- Modeling of deposition and epitaxy of compound semiconductors: CVDSim
- Modeling of polysilicon deposition by Siemens process: PolySim

Customer base:

- More than 170 companies and research institutes/universities worldwide
- More than 60 users of CGSim software

Main directions of process optimization

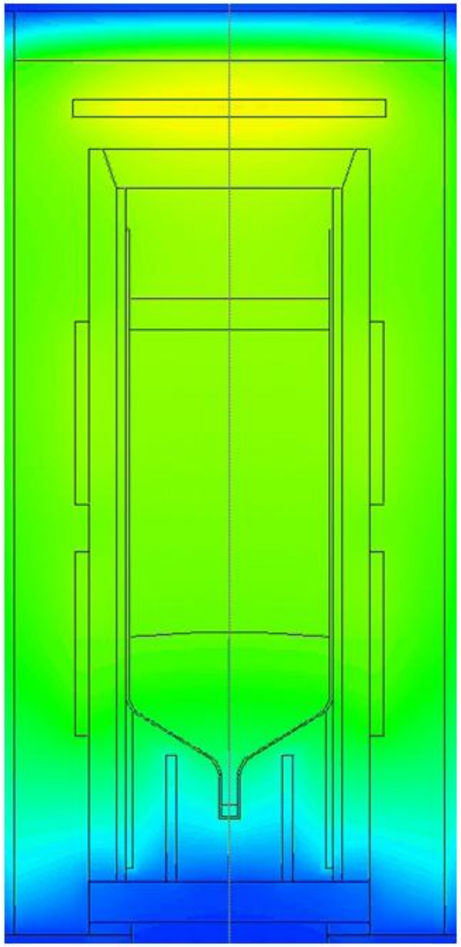
- Optimization of melt/crystal interface shape
- Reduction of probability of transition to polycrystalline material
- Reduction of dislocation density
- Better uniformity of dopant concentration
- Shorter cooling stage and process cycle
- Reduction of electricity consumption
- Development of new processes for larger and longer crystal growth

Modeling capabilities

- Heat transfer
- Gas and melt flow
- Melt/crystal interface dynamics
- Dopants transport and segregation
- Thermal stresses
- Dislocations

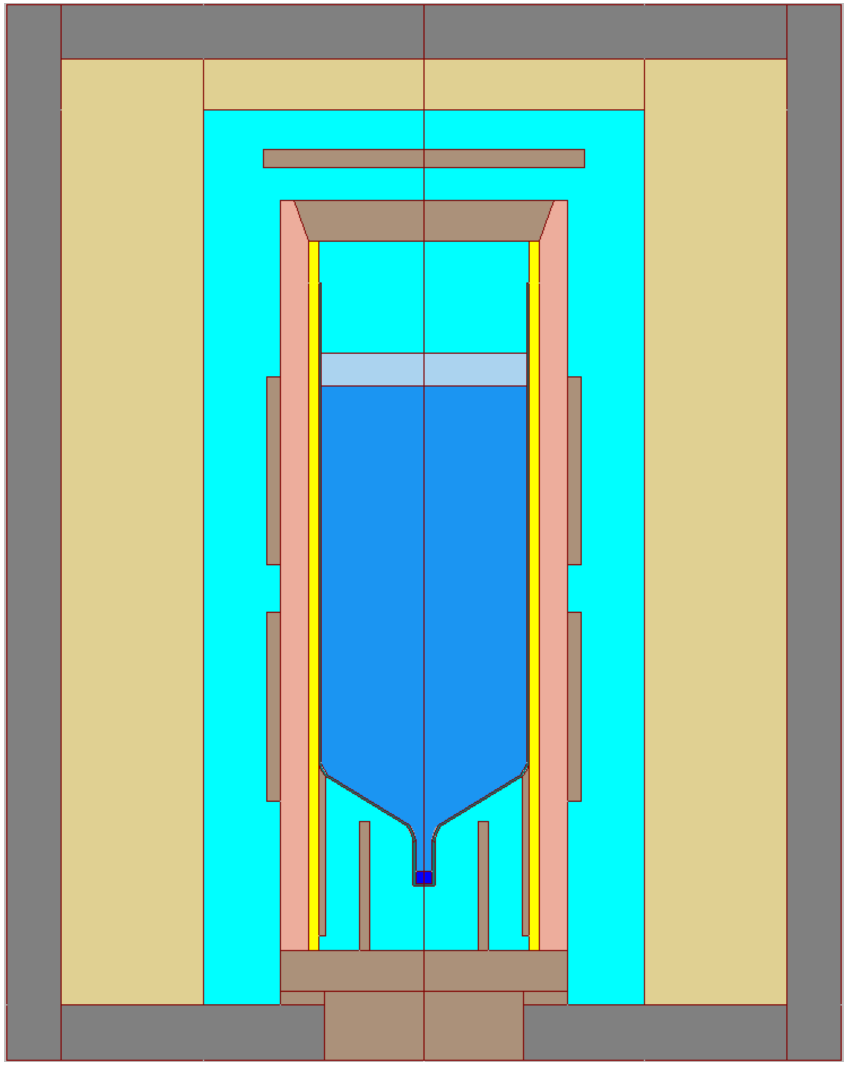
•Haasen-Alexander-Sumino model

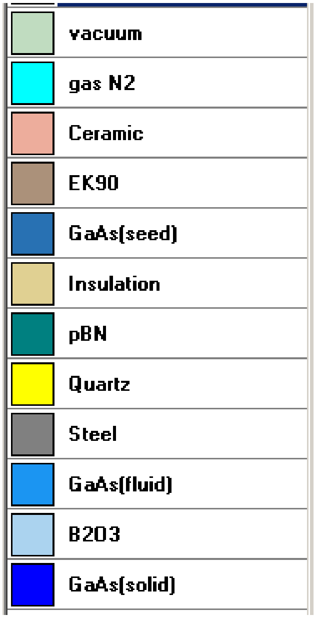
- Combined resistive and inductive heating
- Inverse heater power control
- AC magnetic fields
- Moving elements



CGSim software capabilities are regularly updated on customers' requests

Example of VGF process optimization

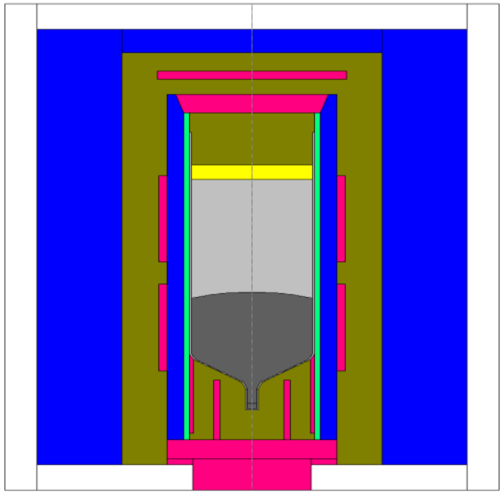


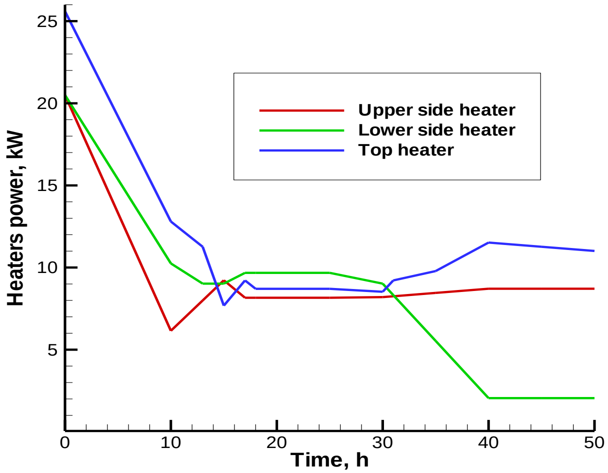


GaAs charge weight is 30 kg.

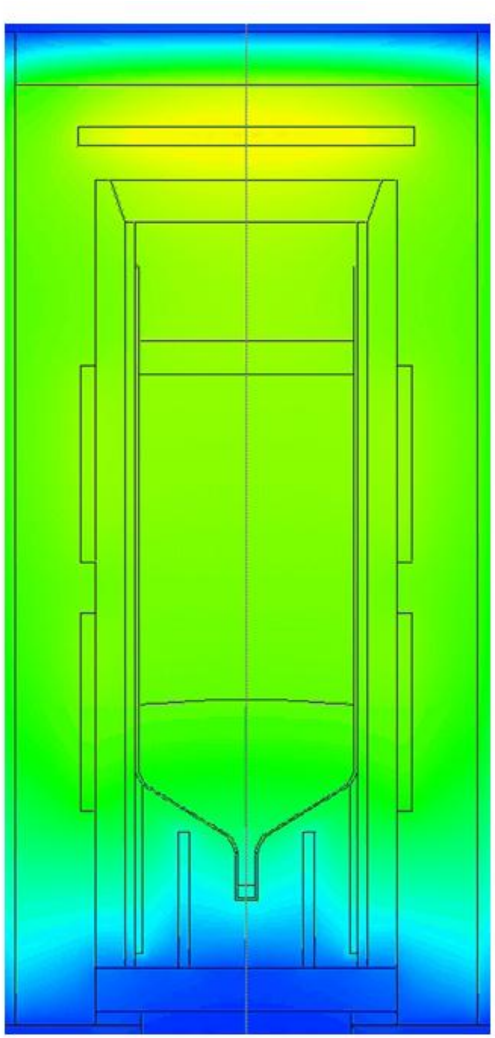
Crystal diameter is 150 mm.

Optimized process



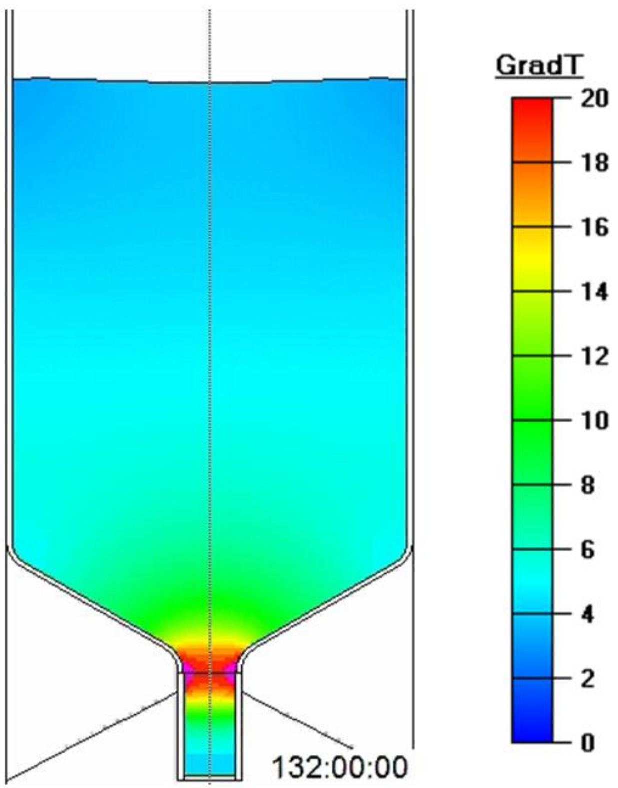


Heaters power evolution

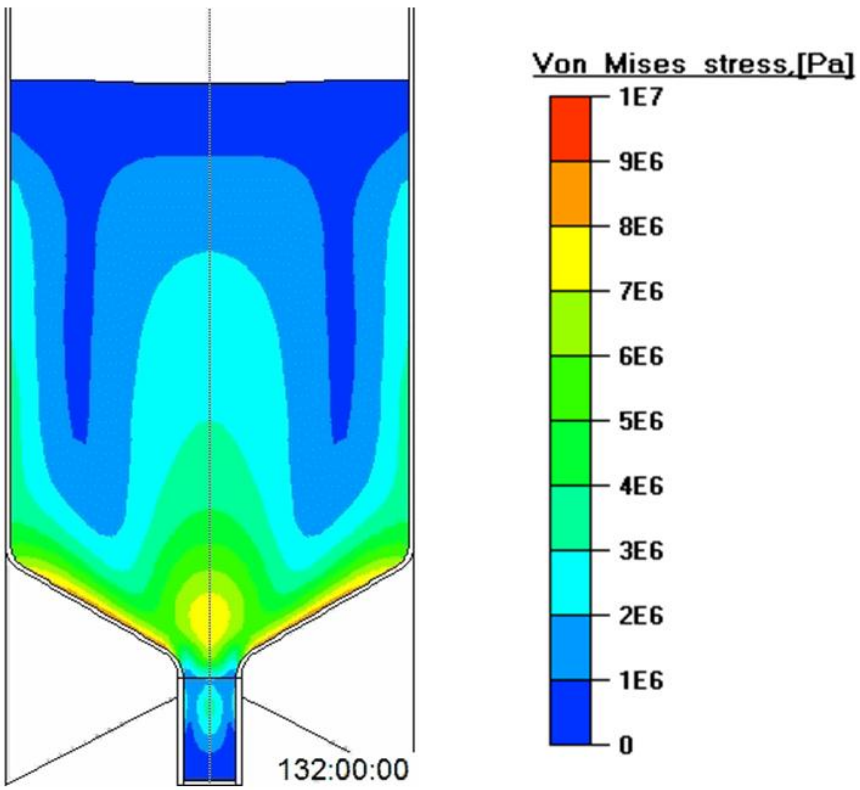


Thermal stresses

Temperature gradients



Thermal stresses



- **Direct modeling of thermal stress evolution enables more accurate process analysis and more efficient optimization**

Model of dislocation multiplication

- Haasen-Alexander-Sumino model

$$\frac{d}{dt}\varepsilon_{ij} = \frac{d}{dt}\varepsilon_{ij}^{e} + \frac{d}{dt}\varepsilon_{ij}^{T} + \frac{d}{dt}\varepsilon_{ij}^{c}$$

$$\frac{d}{dt}\varepsilon_{ij}^{c} = \frac{1}{2} b k_0 \left(\sqrt{J_2} - D\sqrt{N}\right)^{p} \exp\left(-\frac{Q}{kT}\right) N \frac{1}{\sqrt{J_2}} S_{ij}$$

$$\frac{d}{dt}N = K\, k_0 \left(\sqrt{J_2} - D\sqrt{N}\right)^{p+l} \exp\left(-\frac{Q}{kT}\right) N$$

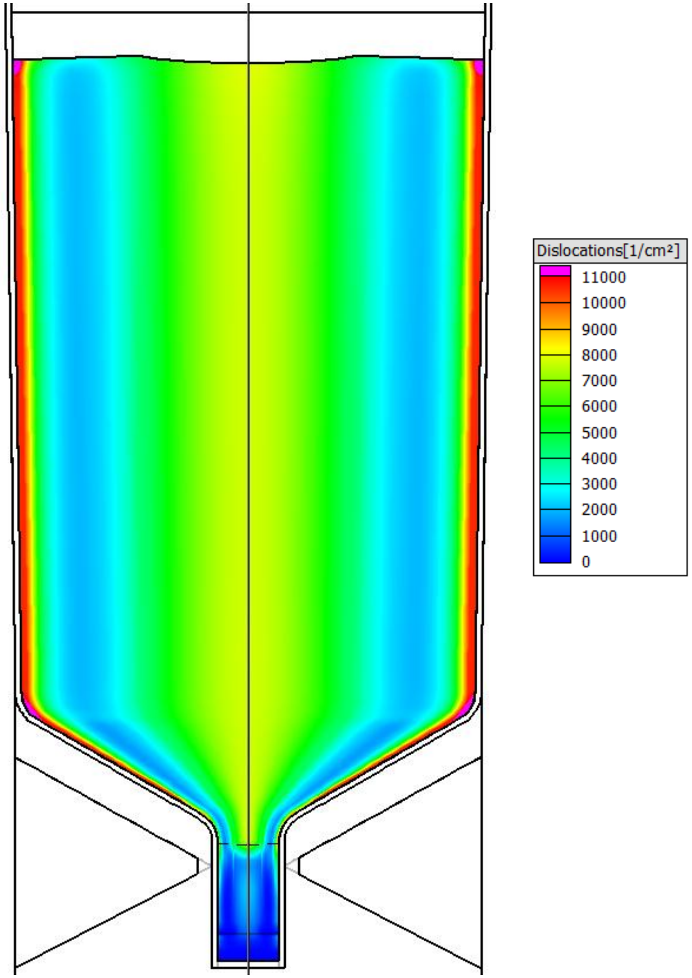
$$J_2 = \frac{1}{2}\sum_{i,j} S_{ij}^2$$

$$S_{ij} = \sigma_{ij} - \delta_{ij}\frac{1}{3}\sum_{k}\sigma_{kk}$$

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

$$\varepsilon_{ij}^{T} = \beta\left(T - T_{ref}\right)$$

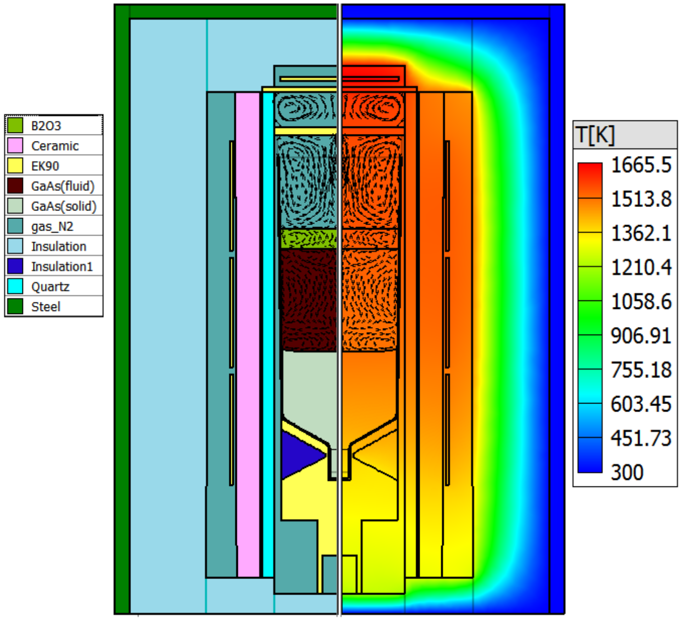
$$\sigma_{ij} = c_{ij}\varepsilon_{ij}^{e} \quad (Hook's \quad law)$$

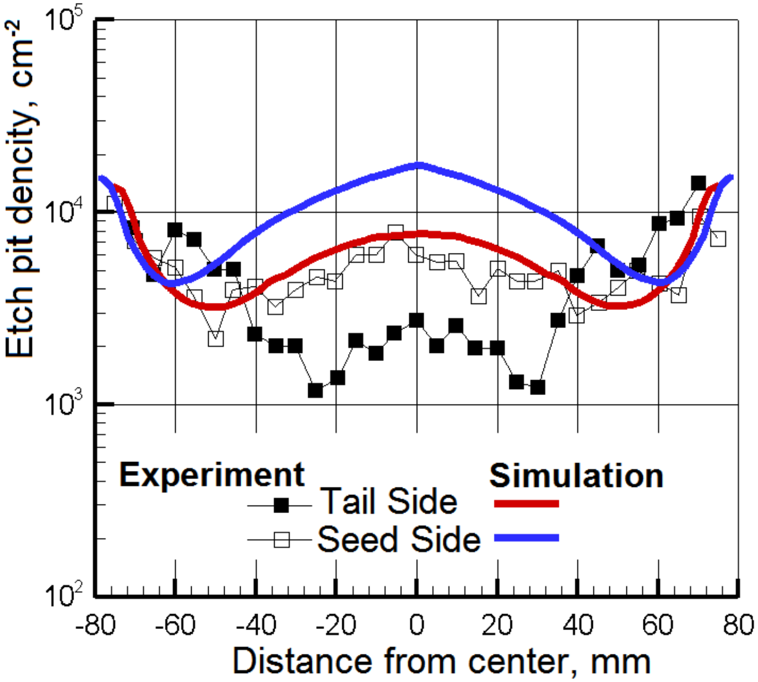


H. Alexander, P. Haasen / Solid State Physics 22 (1968) 27-158

M. Suezawa, K. Sumino, I. Yonegaga / J. Appl. Phys. 51 (1979) 217-226

Dislocations

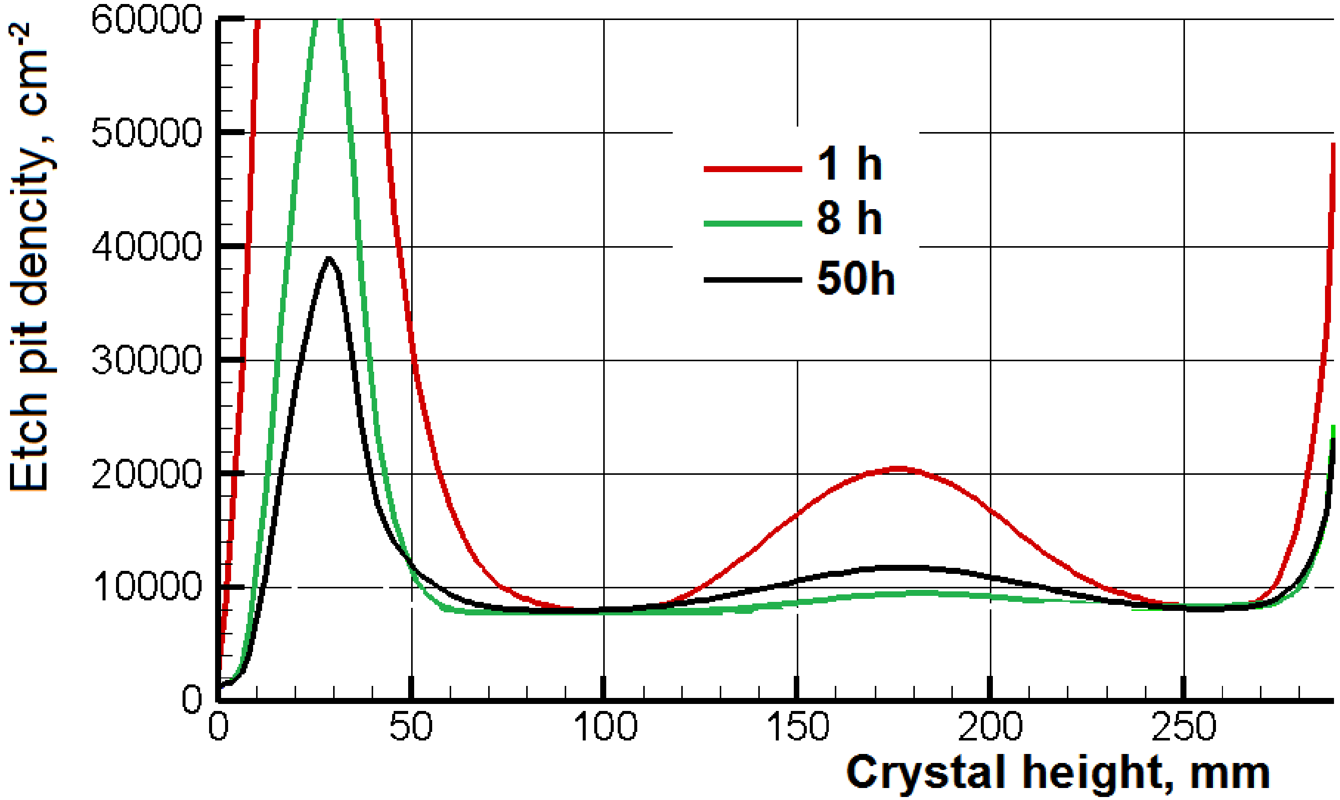




Experiment data from

T. Kawase, H. Yoshida, T.i Sakurada, at all, Properties of 6-inch Semi-insulating GaAs Substrates Manufactured by Vertical Boat Method

Dislocations



Final dislocation density distribution at the crystal symmetry axis for different heater power decrease rates

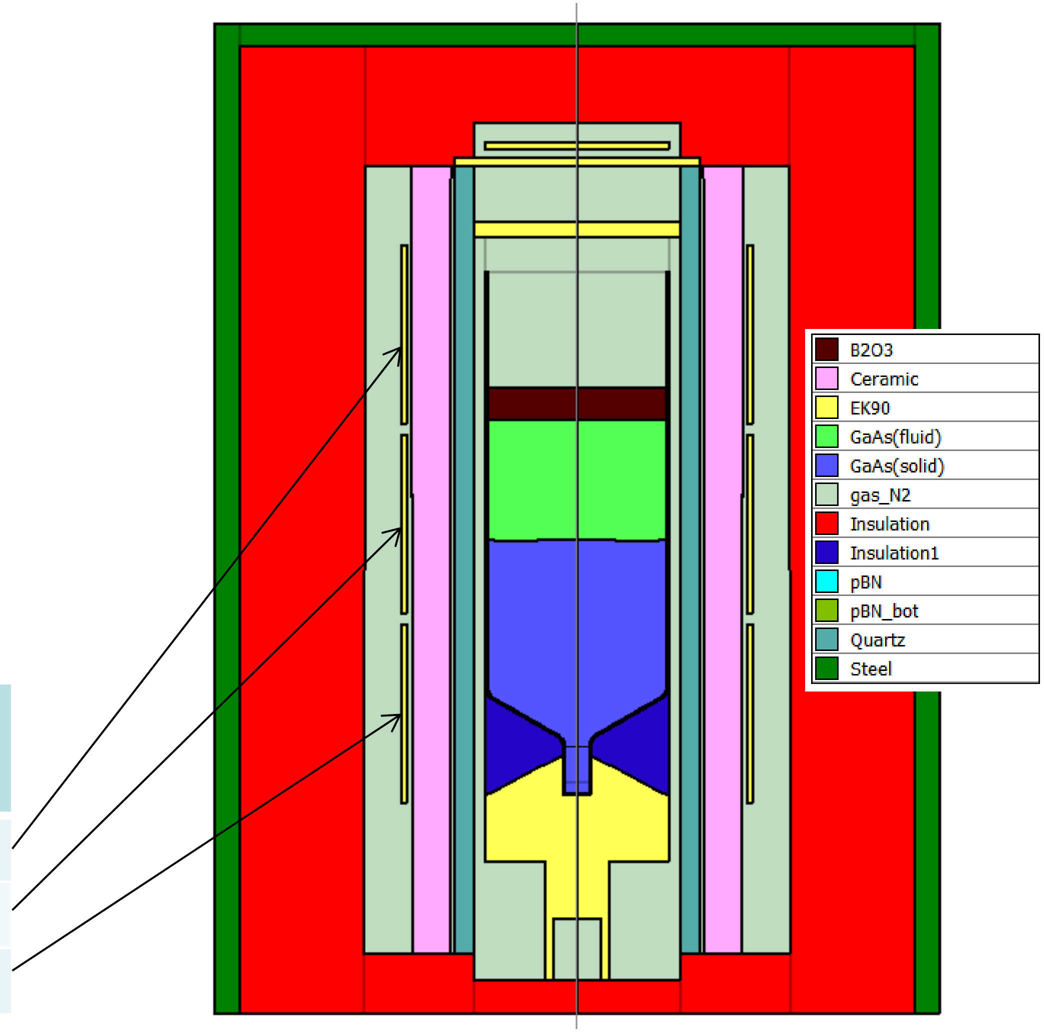
Evaluation of magnetic field effect generated by AC powered heaters on VGF GaAs crystal growth

Problem definition

- 6” crystal diameter
- 24 kg charge weight
- DC top heater
- 50 Hz AC side heater
- 1.5 mm/h growth rate
- <100> orientation

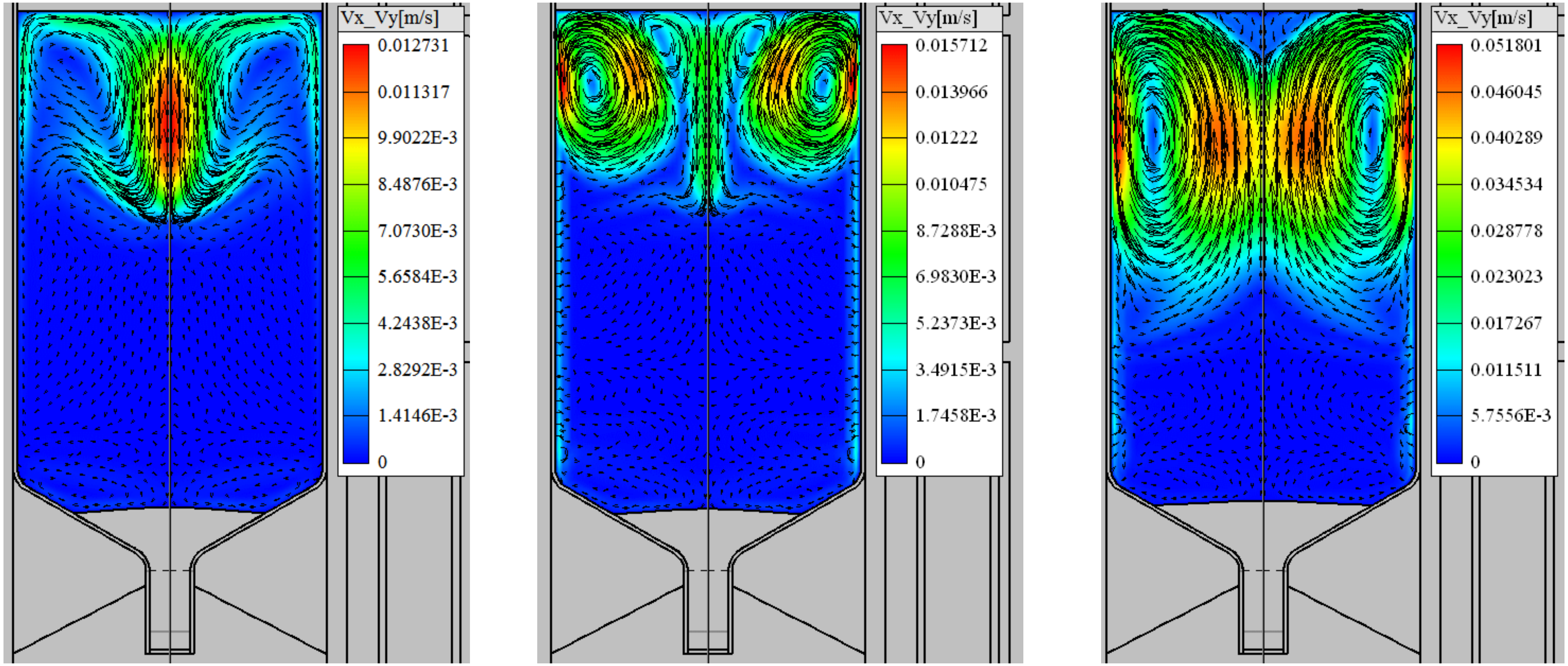
Phase definition

Heater	Downward LFs	Upward LFs
Top side	0.667	0
Middle side	0.333	0.333
Bottom side	0	0.667



Flow structure

Downward LFs



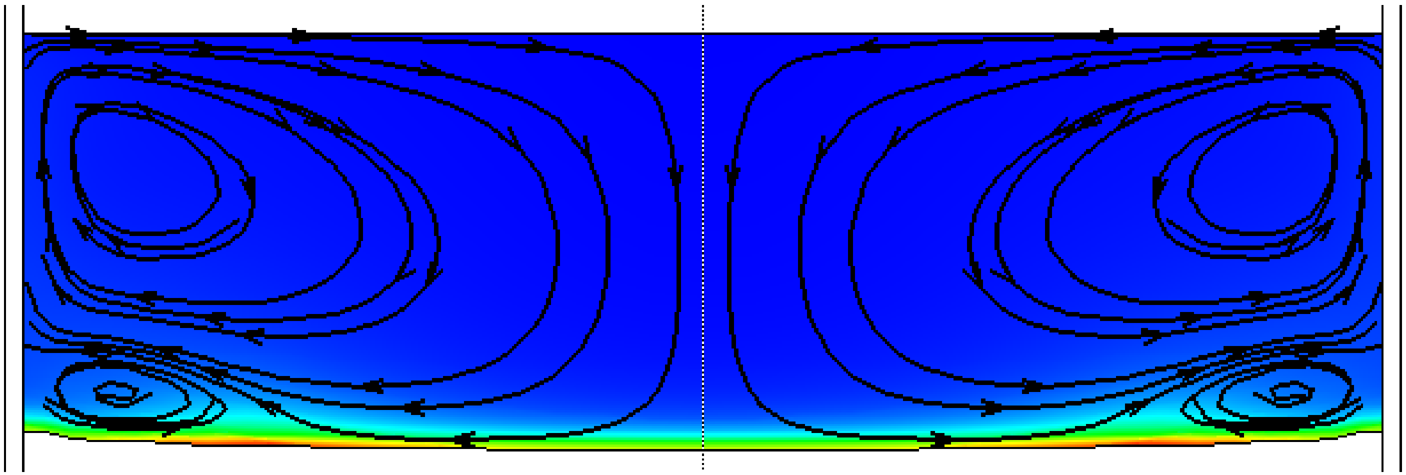
No MF | Weak MF | Strong MF

- Downward LFs generate downward melt flow along the crucible wall

Dopants transport and segregation

Dopant distribution in the crystal is governed by

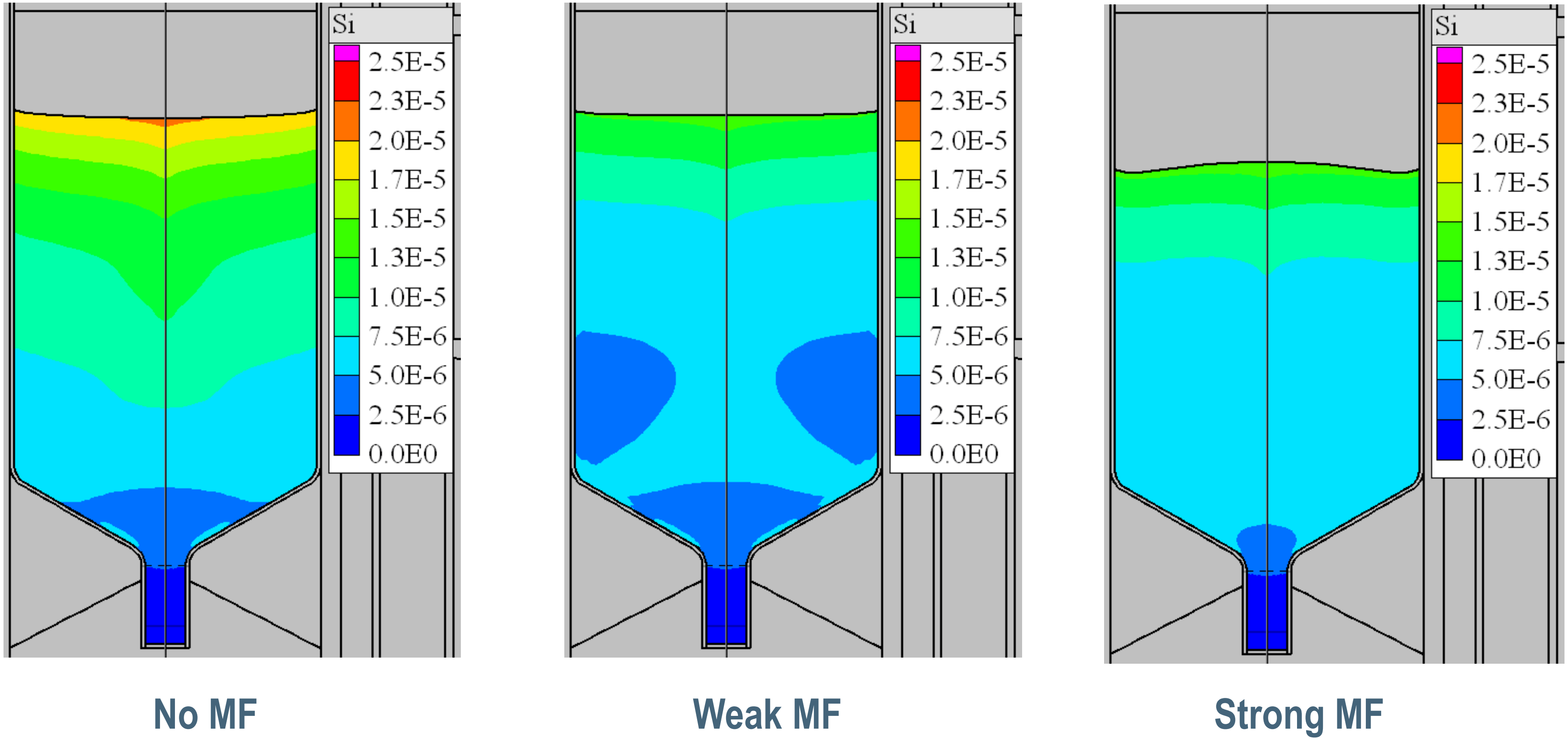
- **Dopant transport by the melt convection along the melt/crystal interface**
- **Segregation effect along the crystal height**



Modeling example of dopant transport by the melt flow

Dopants: Si

Downward LFs



- Application of AC heater with downward LFs helps to achieve more uniform dopant distribution