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Modeling of SiC single crystal growth in PVT reactor

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Outline of the presentation

1. The purpose of the studies
2. The scope of the studies
3. The methods
   - Model of the reactor geometry
   - Finite Volume Method
   - Implementation of the reactions
   - Dislocation evolution model
4. Results and experimental verification
5. Summary

The purpose of the studies

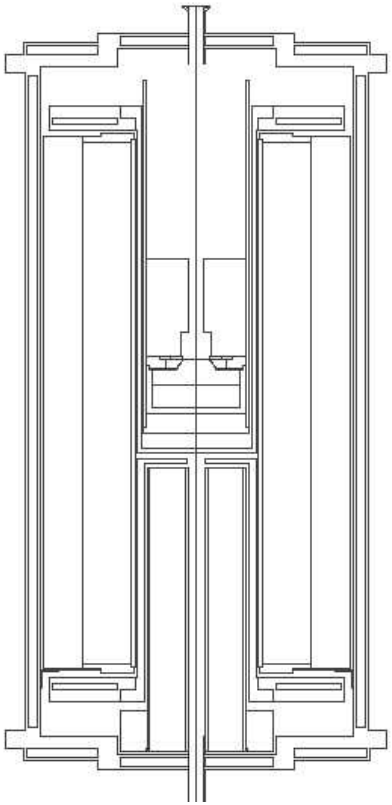
Optimization of SiC monocrystal growth process by computer modelling

Silicon carbide polycrystal (left) and monocrystalline SiC wafers (right). Source: ITME

The scope of the studies

- Optimization of the thermal conditions by modifications of the reactor geometry
  - Different solutions related with geometry of insulation
- Optimization of the process conditions
  - Temperature and temperature gradient
  - Pressure

Virtual Reactor and reactor model



- Geometry
  - Two-dimensional
  - Axisymmetric
- Boundary conditions
  - Temperatures
  - Chemical activity
- Heat transfer
  - Conductivity
  - Convection
  - radiation

Reactor model

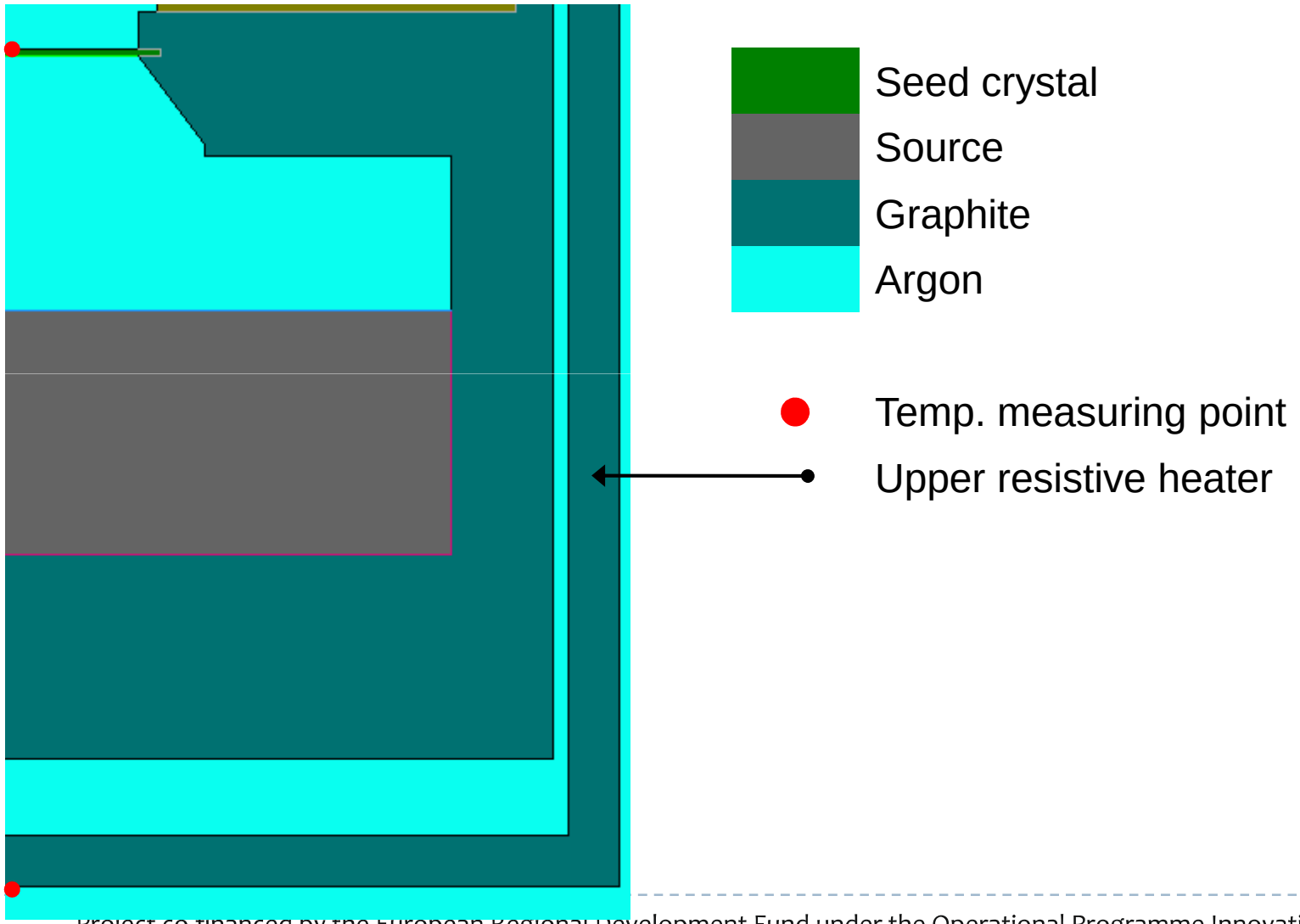
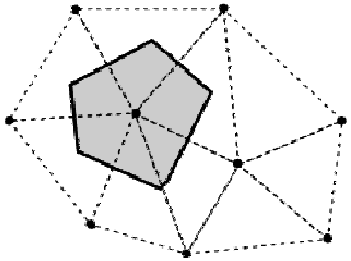


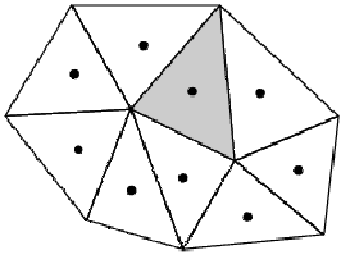
Image fromhttp://www.iue.tuwien.ac.at/phd/heinzl/node25.html

Finite Volume Method

Piecewise constant cell average for each control volume:

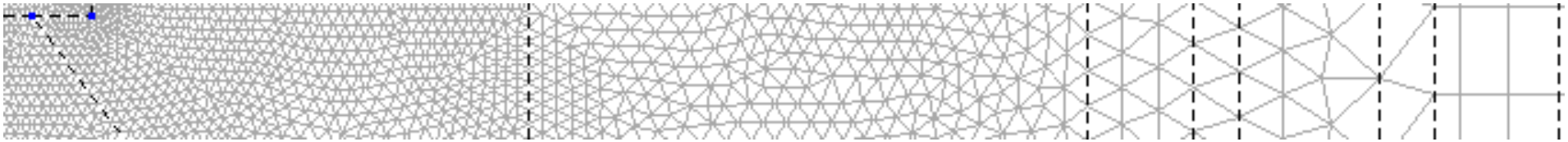
$$u_i = \frac{1}{|V_i|}\int_{V_i} u dV$$





Approximation of flux integral by a quadrature rule:

$$\int_{\partial V} f(u)\cdot dA \approx \sum_{f_{jk}\in \partial V} g_{jk}(u_j, u_k)$$



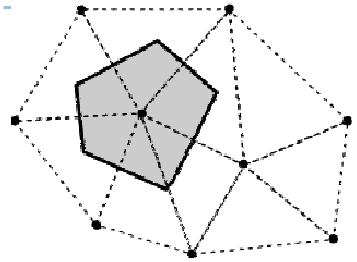
Mesh density decreases with distance from the furnace axis. Less crucial parts, like outermost thermal inslulation, are less densly covered what simplifies calculations. (VR

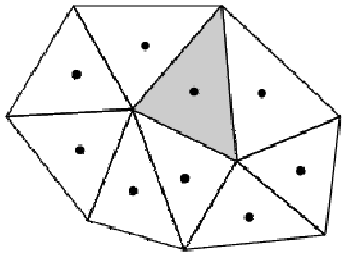
Image from http://www.iue.tuwien.ac.at/phd/heinzl/

Heat Transfer Model

Heat conduction in solids:

$$-\frac{\partial}{\partial x_i}\left(\lambda_{ik}\frac{\partial T}{\partial x_k}\right) = Q$$

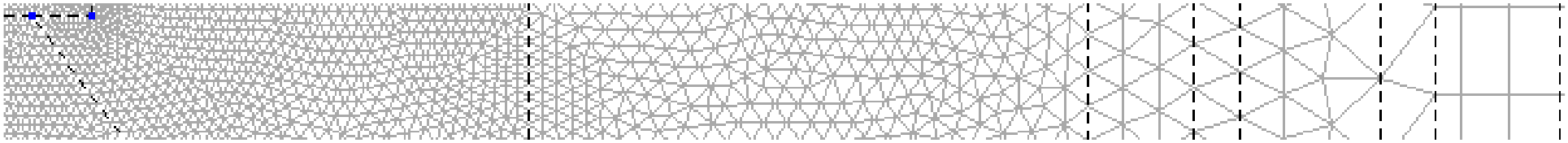




Heat flux at the ‘constant wall temperature’ boundary:

$$q_w = \lambda\frac{T_w - T_c}{dx}$$

Finite Volume Method has been utilized for heat transfer in the simulation



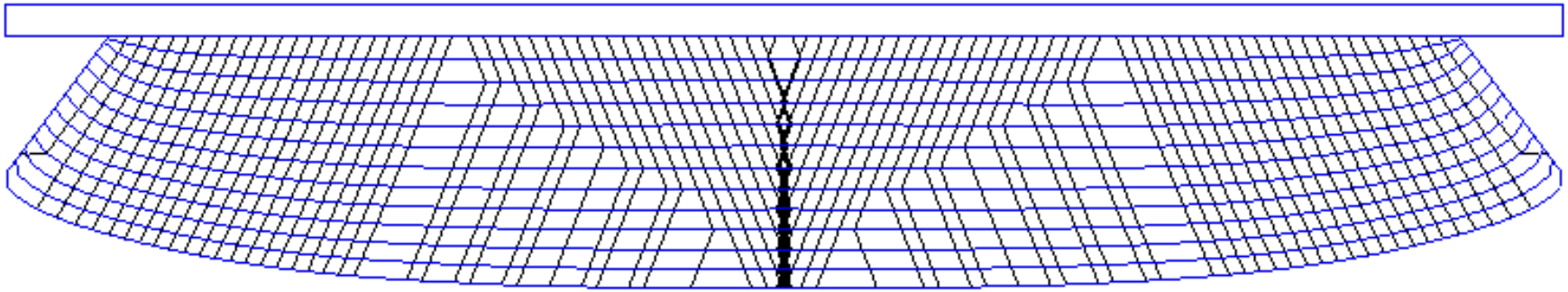
Mesh density decreases with distance from the furnace axis. Less crucial parts, like outermost thermal inslulation, are less densly covered what simplifies calculations. (VR

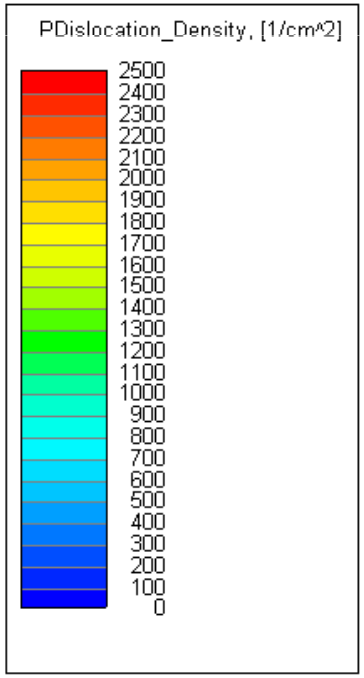
Implementation of the reactions

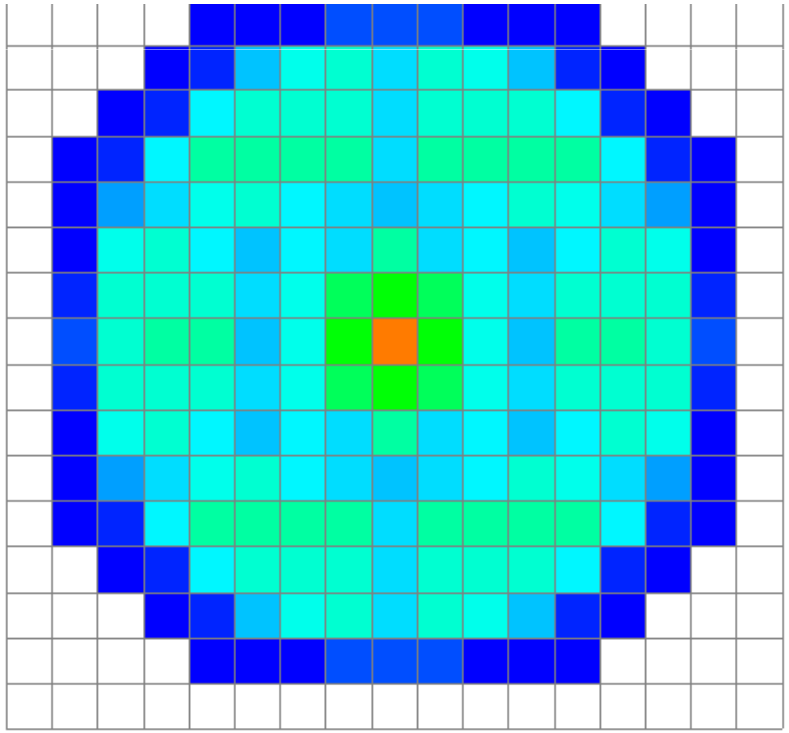
- Gas phase consists of Si, Si_2C, SiC_2 and Ar
- Reactions at crystal surface

$$SiC_2(gas) + 3Si(gas) \Leftrightarrow 2Si_2C(gas)$$
$$Si_2C(gas) + SiC_2(gas) \Leftrightarrow 3SiC(solid)$$

Dislocation evolution model





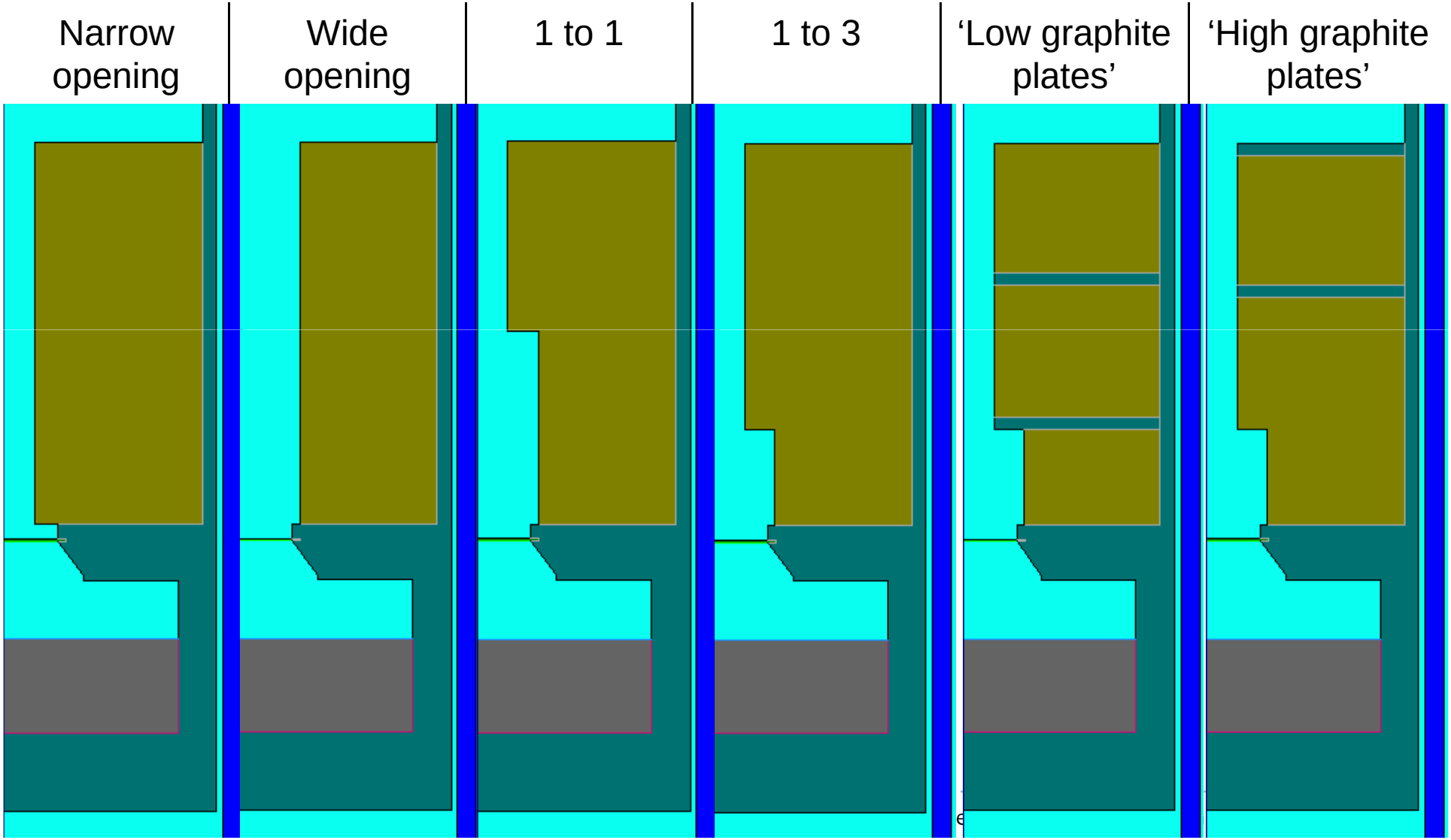


Threading dislocation traces , cut through crystal axis (above)

Threading dislocation density mapping, 7mm from the seed sufrace (left) Output from VirtualReactor

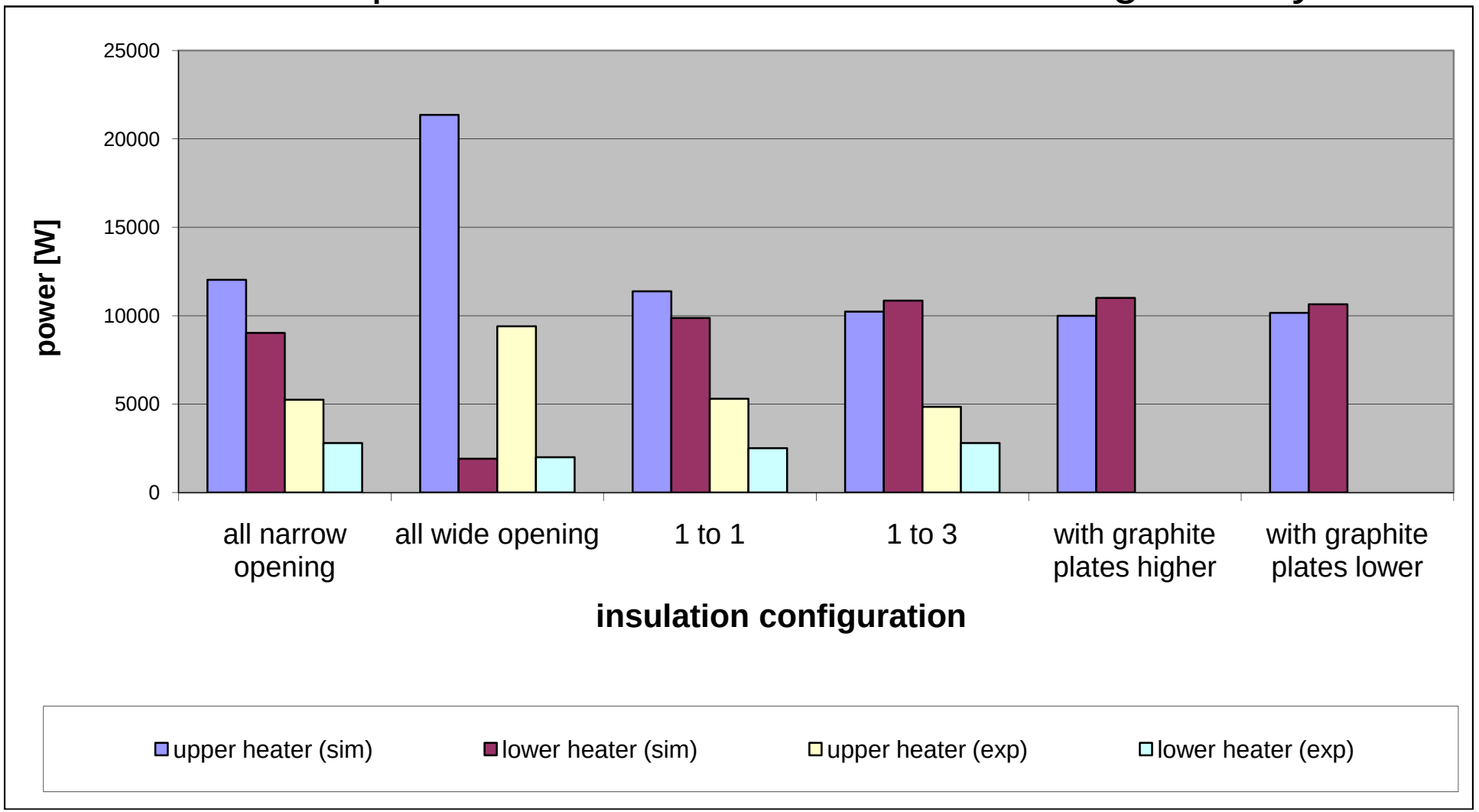
$$E_{seg} = K(\alpha)L_{seg}(\alpha)$$

Insulation geometry

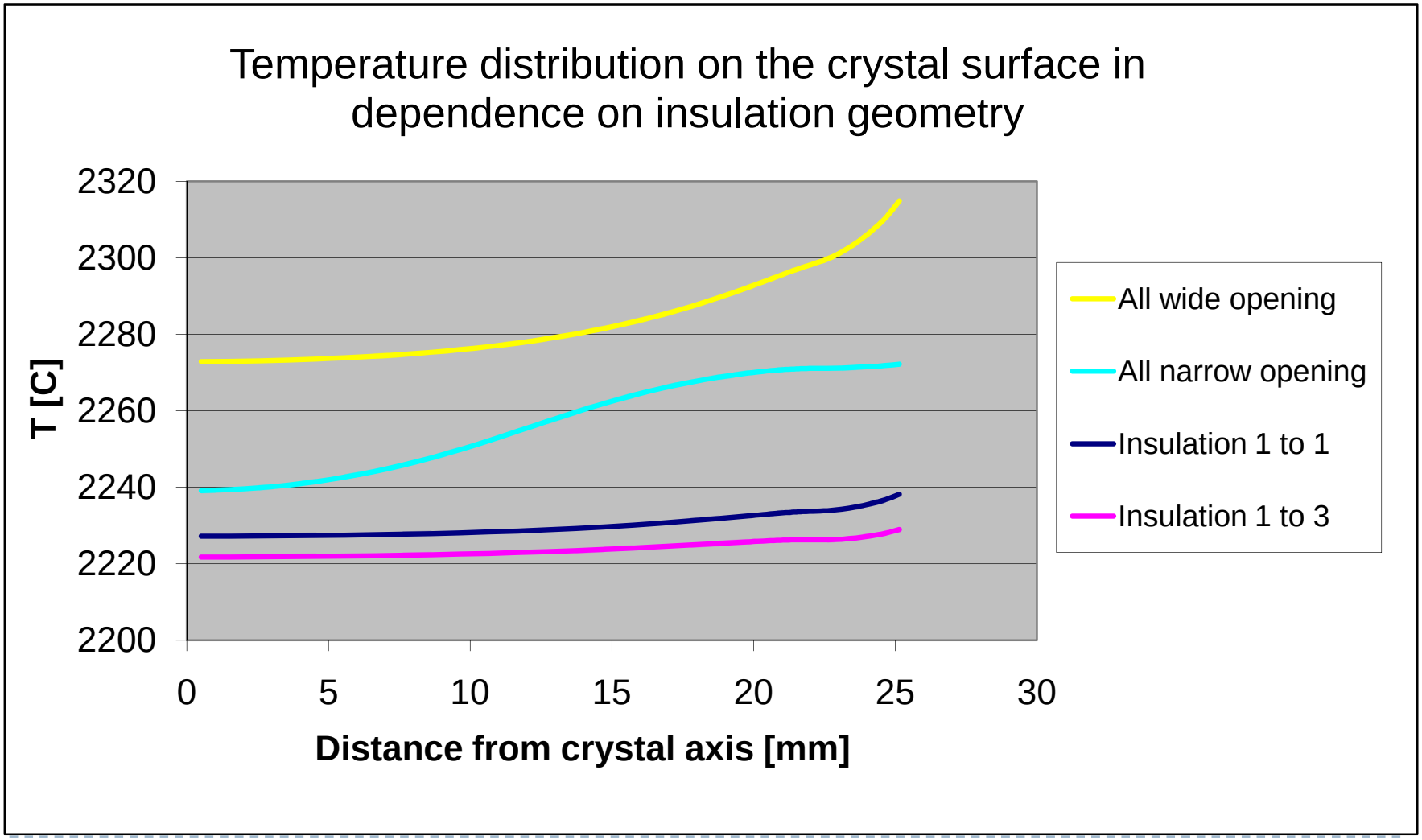


Insulation and heater power

Comparison of simulated and experimentally obtained heater power in accordance to insulation geometry



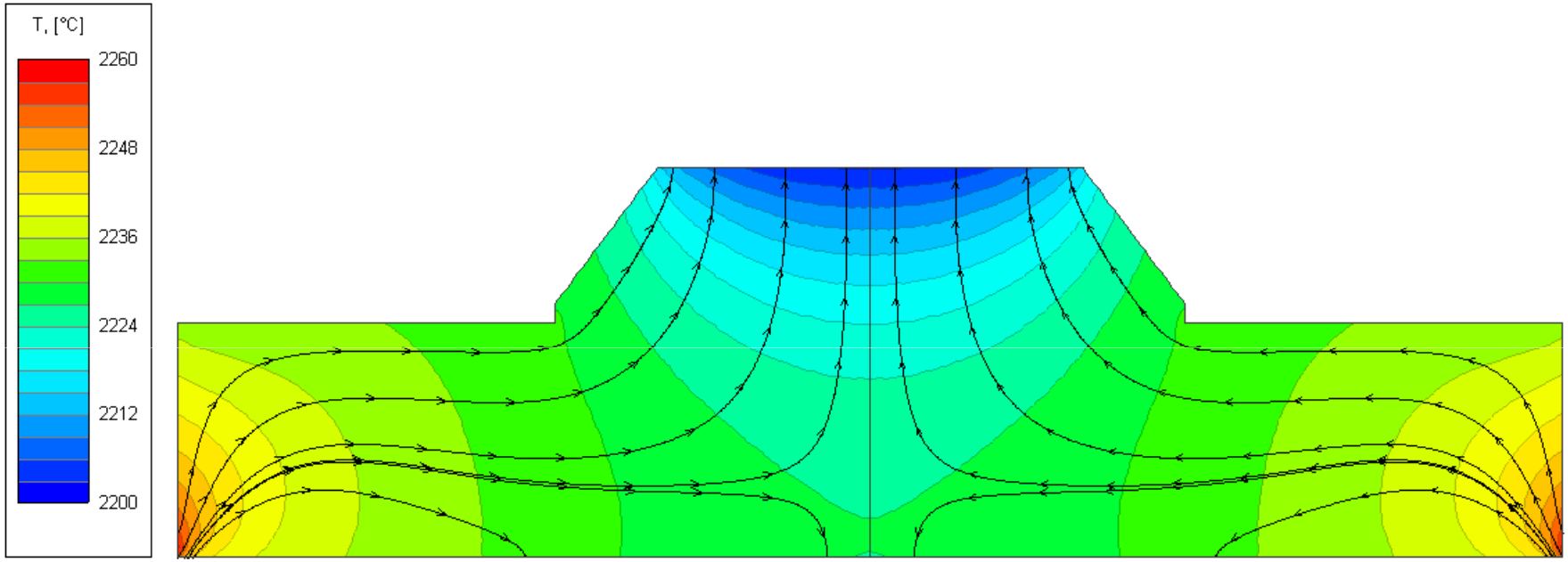
Insulation and seed temperatures



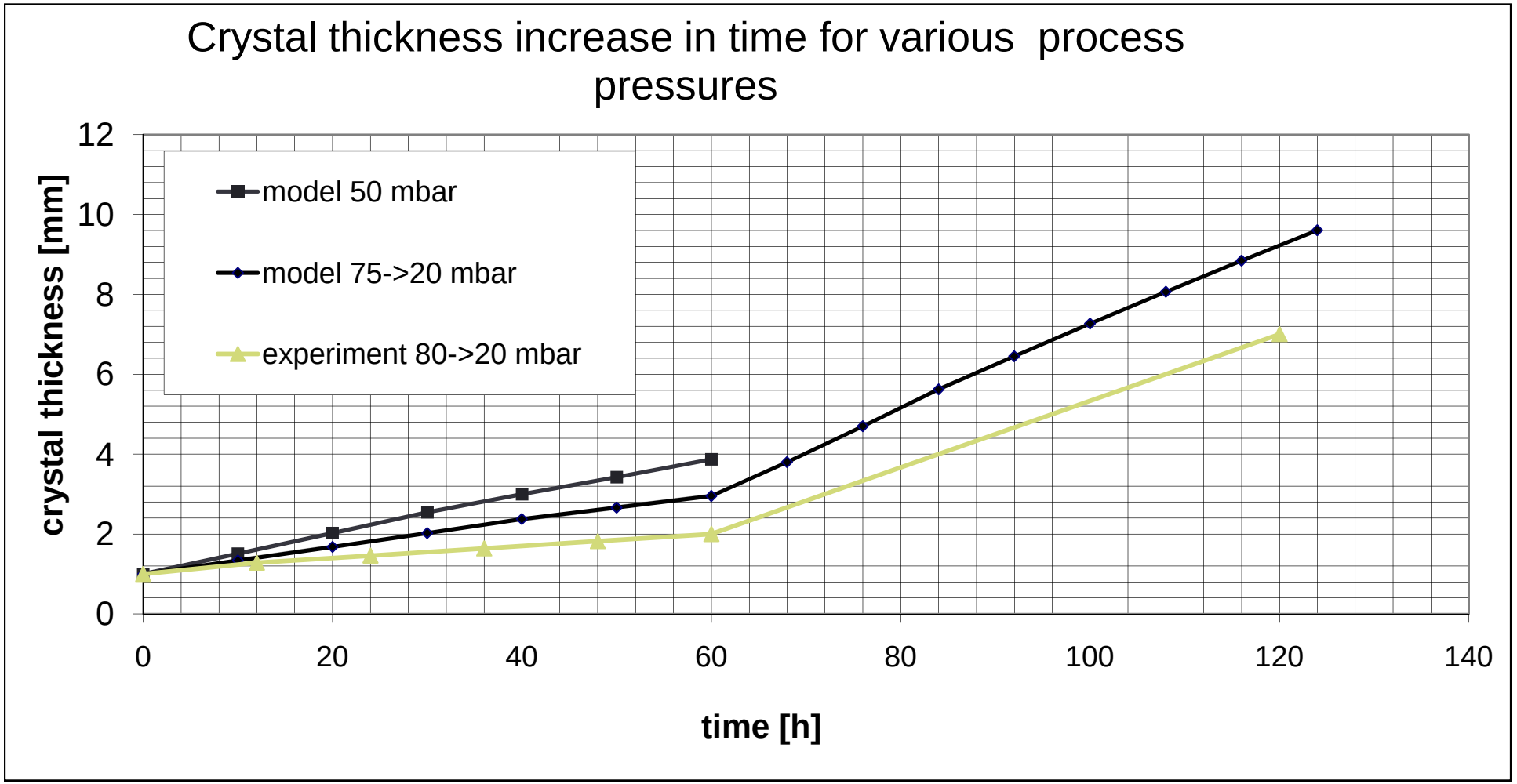
Growth rate

- The aim
  - Investigation of crystal growth rate evolution in time
  - Examination of pressure impact on growth rate
  - Examination of temperature and temperature gradient impact on growth rate

Growth rate



The effect of pressure on crystal growth



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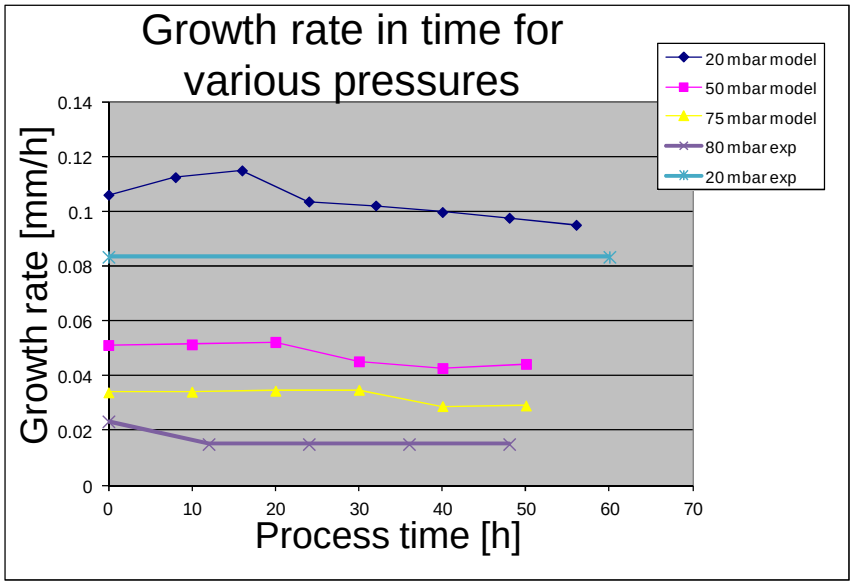
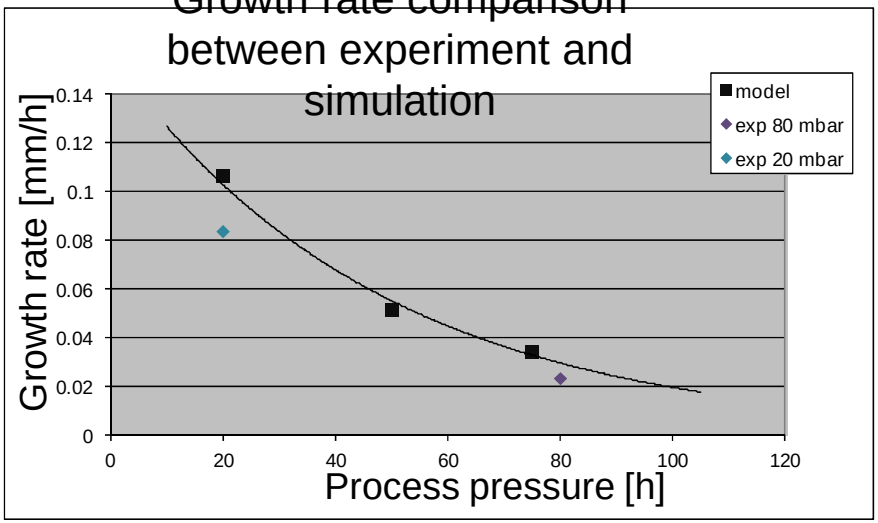
The effect of pressure on growth rate





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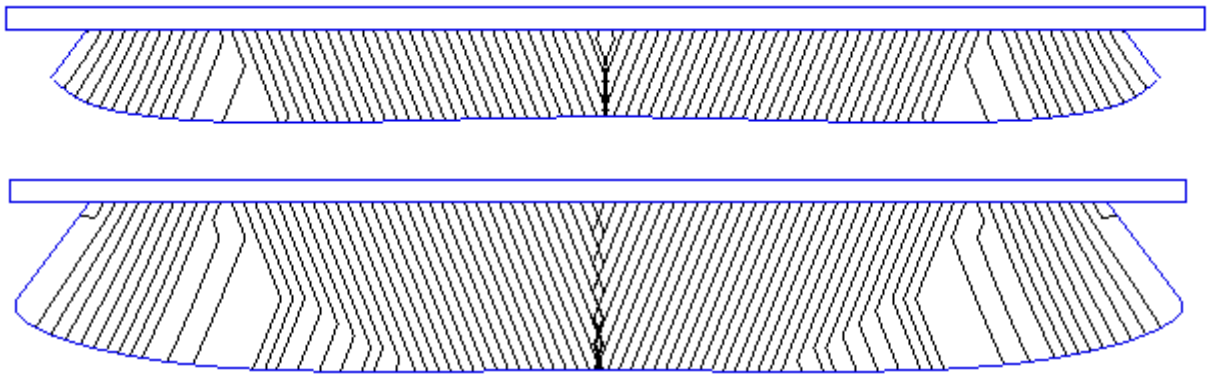
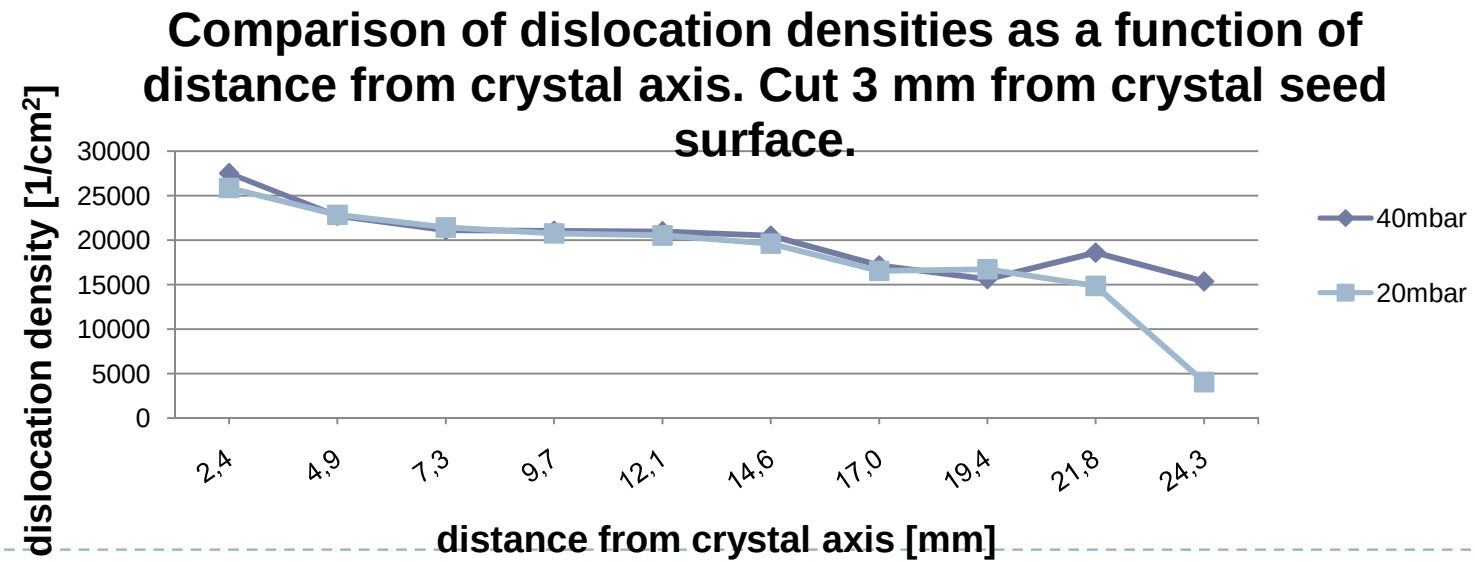
Pressure and dislocations

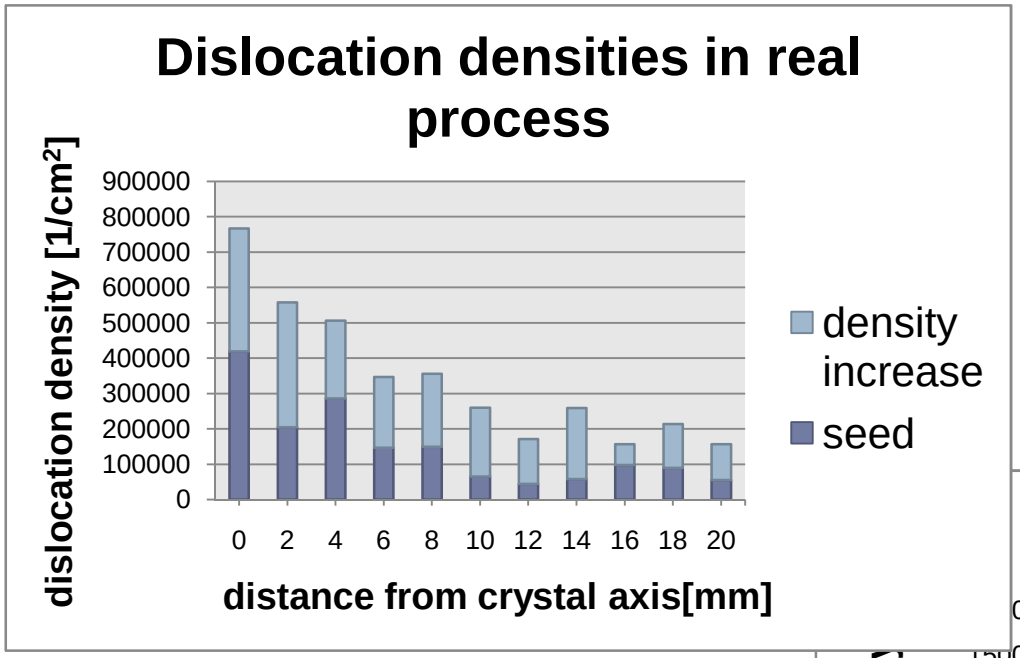


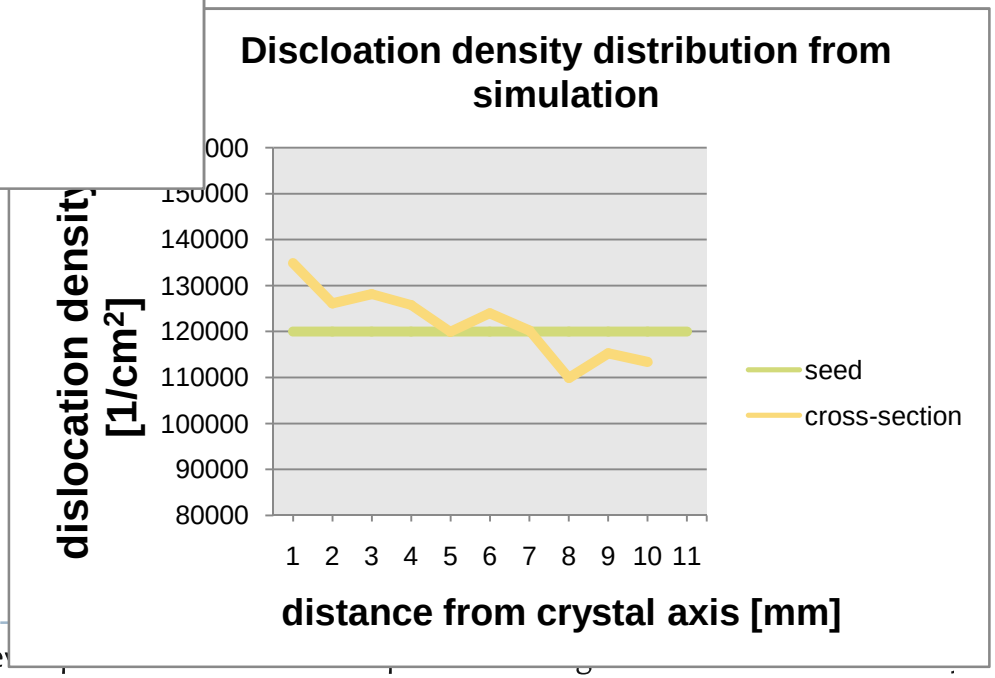
40 mbar

20 mbar

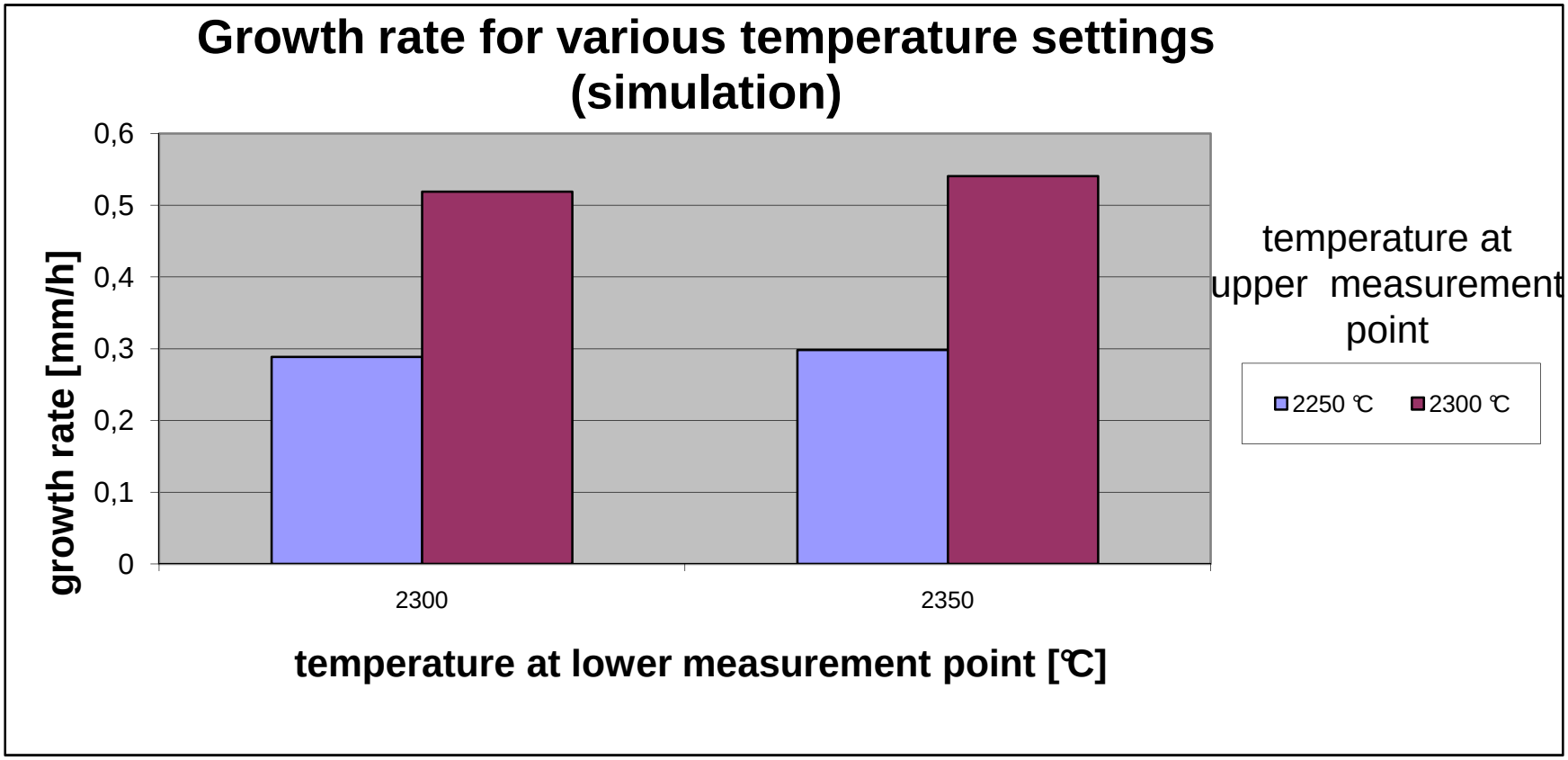


Dislocations

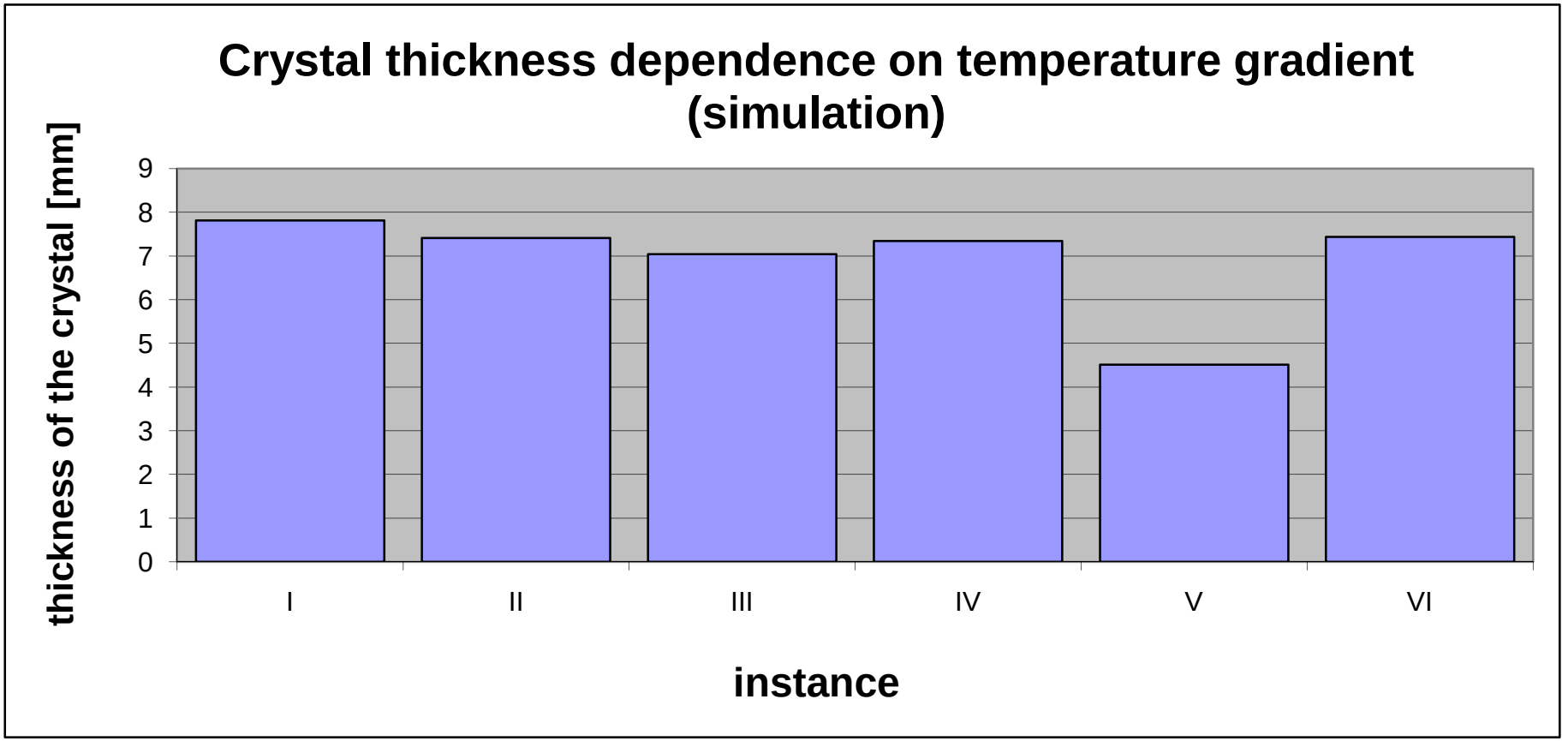




Effect of temperature on growth rate



Effect of temperature gradient on projected crystal thickness



Summary

- computer modelling is a viable tool for designing optimal conditions for SiC monocrystal growth
- modeling gives you opportunity to check the correctness of much more theories and ideas than the experiment alone
- saves time and resources

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