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Discretisation- and Optimisation methods for a Parabolic-Equation and application on simulation in crystal growth

Lecture for Numerical Analysis and Optimisation: Technical University of Athen, Greek, December 2004, 15th December 2004
1 Introduction

Multi-dimensional and multi-physical problem in continuum mechanics for crystal growth process.

- Model: Transmission Problem of solid- and gas-phase, realized as a system of heat-equations coupled through the interface- and boundary-conditions.
- Problems: Nonlinearities for equation-parameters (e.g. material-parameters) and interface-problems with nonlinear-terms.
- Solution: Adapted discretisations and solvers for nonlinear equations.
- Methods: Finite-Volume-methods, implicit time-discretisations and direct- or iterative solvers.
2 Contents

- Motivation for the Crystal Growth
- Introduction to the technical apparatus, the production problems and the modeling
- Mathematical equations for the model
- Discretization, Solvers and Implementation
- Specifications in material (nonlinearities)
- Control for uncertain parameters (Optimization)
- Numerical Results
- Discussion and further works
3 Motivation for the Crystal Growth

The applications are: Light-emitting diodes:
Blue laser: Its application in the DVD player
SiC sensors placed in car and engines

High qualified materials with homo-gene structures are claimed.
4 Introduction to the model and the technical apparatus

SiC growth by physical vapor transport (PVT)

SiC-seed-crystal, Gas: 2000 – 3000 K, SiC-source-powder, insulated-graphite-crucible, coil for induction heating
• polycrystalline SiC powder sublimates inside induction-heated graphite crucible at 2000 – 3000 K and ≈ 20 hPa

• a gas mixture consisting of Ar (inert gas), $Si$, $SiC_2$, $Si_2C$, . . . is created

• an SiC single crystal grows on a cooled seed
Problems of the technical apparatus

SiC growth by physical vapor transport (PVT)

Good crystal with
a perfect surface
But need of high energy
and apparatus costs

Bad crystal, with
wrong parameters for the heat
and temperature
optimization-problem

Solution: Technical simulation of the process and develop the optimal control of the process-parameters.
Models for specific parts of the multi-physical processes of the Crystal-Growth

- Heat-source-field
  - Maxwell-equation
  - Heat-source
  - f (Source for the conductors)

- Temperature field
  - Heat-transfer Model
  - T (Temperature)

- Crystal growth
  - Chemical transport
  - Reaction-Diffusion
  - c (Concentration of SiC)

- Chemical processes
  - Chemical reactions
  - (Conversion)
  - c (SiC, S\textsuperscript{2}C, SiC\textsuperscript{2})

- Specification
  - Material-parameters (nonlinear functions)
  - Radiation for Gas
    - Radiation Model for the gas-phase
    - R (Radiation)
Technical Growth Apparatus

- Blind hole (for cooling of seed)
- Copper induction coil rings
- SiC crystal
- Gas
- SiC powder insulation
- Porous graphite
- Porous graphite (for cooling of seed)
5 Mathematical Equations Heat-Transfer

\[ \rho_s c_{sp} \frac{\partial_t T_s}{s} - \nabla \cdot \kappa_s \nabla T_s = f_s, \quad \text{in } \Omega_s, \quad (1) \]

\[ \rho_g \frac{z_g R_{uni}}{M_g} \frac{\partial_t T_g}{s} - \nabla \cdot \kappa_g \nabla T_g = 0, \quad \text{in } \Omega_g, \quad (2) \]

\[ -\kappa_{s_1} \nabla T_{s_1} \cdot n_{s_1} = -\kappa_{s_2} \nabla T_{s_2} \cdot n_{s_1}, \quad \text{on } \Gamma_{s_1,s_2}, \quad (3) \]

\[ -\kappa_s \nabla T_s \cdot n_s - R + J = -\kappa_g \nabla T_g \cdot n_s, \quad \text{on } \Gamma_{s,g} \quad (4) \]

\[ -(\kappa_s \nabla T_s) \cdot n_s = \sigma \epsilon (T_s^4 - T_{room}^4), \quad \text{on } \Gamma_s \quad (5) \]

\( s, s_1, s_2 \in \{1, \ldots, N\} \) (solid materials), \( g \in \{1, \ldots, M\} \) (gas materials),

\( \rho \): mass density, \( c_{sp} \): specific heat, \( T \): absolute temperature,

\( \kappa \): thermal conductivity, \( f \): power density of heat sources,

\( z \): configuration number, \( R_{uni} \): universal gas constants, \( M \): molecular mass, \( \sigma \): Boltzmann constant, \( \epsilon \): emissivity
Interface Conditions

The normal heat-flux is continuous on the interfaces between solid material and for semi-transparent materials or interfaces between solid and gas phase we add the radiosity $R$ and irradiosity $J$

$$q_{s_1} \cdot n_{s_1} = q_{s_2} \cdot n_{s_1} \quad \text{on } \Gamma_{s_1,s_2}, \quad (6)$$

$$q_s \cdot n_s - R + J = q_{semi-tr} \cdot n_s \quad \text{on } \Gamma_{s,semi-tr}, \quad (7)$$

$$q_{gas} \cdot n_{gas} - R + J = q_s \cdot n_{gas} \quad \text{on } \Gamma_{s,gas}, \quad (8)$$

where $q_{s_1} = -\kappa_{s_1} \nabla T_{s_1}$ is the heat flux, with $\kappa_{s_1}$ is the thermal conductivity, and $\Gamma_{s_1,s_2}$ is the interface between the materials $s_1$ and $s_2$ and $n_{s_1}$ is the normal vector on the solid-phase and $\Gamma_{s,gas}$ is the interface between the solid-phase $s$ and gas-phase $gas$. 
The temperature is continuous between solid materials, cf. (9) and continuous across the interface $\Gamma_{s,\text{gas}}$, cf. (10). The temperature is discontinuous, cf. (11) for the model that solid is surrounded by gas of known temperature and we have an outer boundary condition of third kind.

\begin{align*}
T_{s_1} &= T_{s_2} \quad \text{on } \Gamma_{s_1,s_2}, \\
T_s &= T_{\text{gas}} \quad \text{on } \Gamma_{s,\text{gas}}, \\
-(\kappa_{\text{gas}} \nabla T_{\text{gas}}) \cdot \mathbf{n}_{\text{gas}} &= \xi_s (T_{\text{gas}} - T_s) \quad \text{on } \Gamma_{s,\text{gas}},
\end{align*}

(9) (10) (11)
Outer Boundary Conditions

For the outer boundary condition we use the Stefan-Boltzmann law

\[-(\kappa_s \nabla T_s) \cdot \mathbf{n}_s = \sigma \varepsilon (T_s^4 - T_{room}^4),\]  \hspace{1cm} (12)

with \(\sigma\) is the Boltzmann radiation constant, \(\varepsilon\) is the emissivity, \(T_{room} = 293 K\) and we assume a black box environment (large isothermal room).

For outer boundaries receiving radiation from other parts of the apparatus we use the boundary-condition with the radiosity \(R\) and irradiosity \(J\)

\[-(\kappa_s \nabla T_s) \cdot \mathbf{n}_s - R + J = 0.\]  \hspace{1cm} (13)
Model of the Radiation in the gas-phase

The model considers an interaction between gas and radiation.

\[ R = E + J_{\text{ref}}, \]  
\[ E = \sigma \varepsilon T^4 \quad \text{(Stefan-Boltzmann equation)}, \]  
\[ J_{\text{ref}} = (1 - \varepsilon) J, \]

where \( E \) is the radiation, \( J_{\text{ref}} \) is the reflected radiation, \( \varepsilon \) is the emissivity, and \( \sigma \) is the Boltzmann radiation constant.
The radiosity is calculated as

\[ J(x) = \int_{\Gamma} \Lambda(x, y) \omega(x, y) R(y) dy. \]  

(17)

The visibility factor is calculated as

\[ \Lambda(x, y) = \begin{cases} 
1 & \text{if } x, y \text{ are mutual visible} \\
0 & \text{else} 
\end{cases} . \]  

(18)

The view-factor is calculated as

\[ \omega(x, y) = \frac{(n_{gas}(y) \cdot (x - y)) (n_{gas}(x) \cdot (y - x))}{\pi((y - x) \cdot (y - x))}. \]  

(19)
Model of the Heat Source based on Magnetic scalar potential

Heat source $f$ is denoted as $f = \frac{j^2}{\sigma}$ and $\sigma$ is the electrical conductivity, $j$ is the current density with

$$j = \begin{cases} 
  -i\omega \sigma \phi + \frac{\sigma \nu_k}{2\pi r} & \text{(inside k-th ring)}, \\
  -i\omega \sigma \phi & \text{(other conductors)}.
\end{cases}$$

where $\phi$ is the magnetic scalar potential.

Elliptic system of PDEs for $\phi$:

In insulators: $-\nu \text{div} \cdot \frac{\nabla (r \phi)}{r^2} = 0$.

In the $k$-th coil ring: $-\nu \text{div} \cdot \frac{\nabla (r \phi)}{r^2} + \frac{i \omega \sigma \phi}{r} = \frac{\sigma \nu_k}{2\pi r^2}$.

In other conductors: $-\nu \text{div} \cdot \frac{\nabla (r \phi)}{r^2} + \frac{i \omega \sigma \phi}{r} = 0$. 
Magnetic Boundary conditions

Interface condition:

\[
\left( \frac{\nu_{\text{material}_1}}{r^2} \nabla (r \phi)_{\text{material}_1} \right) \cdot \mathbf{n}_{\text{material}_1} = \left( \frac{\nu_{\text{material}_2}}{r^2} \nabla (r \phi)_{\text{material}_2} \right) \cdot \mathbf{n}_{\text{material}_1} \tag{20}
\]

Outer boundary condition: \( \phi = 0. \)

\( \nu: \) magnetic reluctivity, \( \mathbf{n}_{\text{material}_1}: \) outer unit normal of material \( 1. \)
Simulated phenomena

- **Axisymmetric heat source distribution**
  - Sinusoidal alternating voltage
  - Correct voltage distribution to the coil rings
  - Temperature-dependent electrical conductivity

- **Axisymmetric temperature distribution**
  - Heat conduction through gas phase and solid components of growth apparatus
  - Non-local radiative heat transport between surfaces of cavities
  - Radiative heat transport through semi-transparent materials
  - Convective heat transport
6 Discretization and implementation

- Implicit Euler method in time
- Finite volume method in space
  - Constraint Delaunay triangulation of domain yields Voronoi cells
  - Full up-winding for convection terms
  - Very complicated nonlinear system of equations
  - Solution by Newton’s method using Krylow subspace techniques
- Implementation tools:
  - Program package pdelib
  - Grid generator Triangle
  - Matrix solver Pardiso
7 Discretization-methods based on Finite Volume-Method

- Local Mass-conservation, Simple test-functions (box-functions).
- Un-structured Grids possible.
- Stabilization with Voronoi-boxes.

![Diagram of primary and dual grids](image)
8 Space- and Time-Discretization


We have the partition \( T = (\omega_i)_{i \in I} \) of \( \Omega \) such that, for \( m \in \{s, g\} \) (with s solid, g gas) and \( i \in I, \omega_{m,i} := \omega_i \cap \Omega_m \) defines either a void subset or a nonvoid, connected, and open polyhedral subset of \( \Omega \).

\[
\rho_m \int_{\omega_{m,i}} (U_m(T^{n+1}) - U_m(T^n)) r \, dx \\
- \Delta t^{n+1} \int_{\partial \omega_{m,i}} \kappa_m(T^{n+1}) \nabla T^{n+1} \cdot \mathbf{n}_{\omega_{m,i}} r \, ds = \Delta t^{n+1} \int_{\omega_{m,i}} f_m r \, dx,
\]

where the time interval is \( \Delta t^{n+1} = t^{n+1} - t^n \). The temperature is given as \( T^{n+1} = T(t^{n+1}, x) \), where \( x \) represents cylindrical coordinates. For the right-hand sides, we demand \( f_s := f \geq 0 \) and \( f_g = 0 \).
9 Solver methods

- **Linear Equation:**
  - Iterative methods with BiCGStab (one grid and also for unsymmetric matrices)
  - Direct solvers (symmetric matrices)

- **Nonlinear Equation:**
  - Newton-Method for scalar equations
  - Newton-Raphson-Method for systems of equations
  - Newton-Krylov-Method
10 Material Properties

For the gas-phase (Argon) we have the following parameters:

\[ \sigma_c = 0.0 \]

\[ \kappa = \begin{cases} 
1.839 \times 10^{-4} T^{0.8004} \\
-7.12 + 6.61 \times 10^{-2} T - 2.44 \times 10^{-4} T^2 + 4.497 \times 10^{-7} T^3 \\
-4.132 \times 10^{-10} T^4 + 1.514 \times 10^{-13} T^5 \\
4.194 \times 10^{-4} T^{0.671} 
\end{cases} \]

for \( T \leq 500K \),

for \( 500K \leq T \leq 600K \),

for \( 600K \geq T \).
Material Properties: Insulation

For graphite felt insulation we have the functions:

\[ \sigma_c = 2.45 \times 10^2 + 9.82 \times 10^{-2} T \]
\[ \rho = 170.0, \mu = 1.0, c_{sp} = 2100.0 \]

\[ \kappa = \left\{ \begin{array}{l}
8.175 \times 10^{-2} + 2.485 \times 10^{-4} T \\
-1.19 \times 10^2 + 0.346 T - 3.99 \times 10^{-5} T^2 + 2.28 \times 10^{-8} T^3 \\
-6.45 \times 10^{-11} T^4 + 7.25 \times 10^{-15} T^5 \\
-0.7447 + 7.5 \times 10^{-4} T
\end{array} \right. \]

\[ T \leq 1473K, \]
\[ 1473K \leq T \leq 1873K, \]
\[ 1873K \geq T, \]}
Material Properties: Graphite

For the Graphite we have the following functions:
\[ \varepsilon = \begin{cases} 
0.67 & \text{for } T \leq 1200K, \\
3.752 - 7.436 \times 10^{-3} T + 6.416 \times 10^{-6} T^2 - 2.33610^{-11} T^3 & \text{for } 500K \leq T \leq 600K, \\
-3.08 \times 10^{-13} T^4 & \text{for } 600K \geq T, \\
4.194 \times 10^{-4} T^{0.671} & \text{for } T > 600K.
\end{cases} \]

\[ \rho = 1750.0, \; \mu = 1.0, \; c_{sp} = 1/(4.41110^2 T^{-2.306} + 7.9710^{-4} T^{-0.0665}) \]
\[ \kappa = 37.715 \exp(-1.96 \times 10^{-4} T) \]
Material Properties: SiC-Crystal and SiC-Powder

For the SiC-Crystal we have the following functions:
\[\sigma_c = 10^5, \epsilon = 0.85, \rho = 3140.0, \mu = 1.0\]
\[c_{sp} = \frac{1}{(3.911 \times 10^4 T^{-3.173} + 1.835 \times 10^{-3} T^{-0.117})},\]
\[\kappa = \exp(9.892 + (2.498 \times 10^2)/T - 0.844 \ln(T))\]

For the SiC-Powder we have the following functions:
\[\sigma_c = 100.0, \epsilon = 0.85, \rho = 1700.0, \mu = 1.0, c_{sp} = 1000.0,\]
\[\kappa = 1.452 \times 10^{-2} + 5.47 \times 10^{-12} T^3\]
11 Optimization the temperature profile during sublimation growth
Stationary Equations for Optimization

\[ \text{minimize : } J(T,f) := \frac{1}{2} \int_{\Omega_g} |\nabla T - z|^2 \, dx + \frac{\nu}{2} \int_{\Omega_s} f^2 \, dx, \quad (23) \]

\[ \text{solve : } -\nabla (\kappa_s \nabla T)_s = f \text{ in } \Omega_s, \quad (24) \]
\[ -\nabla (\kappa_g \nabla T)_g = 0 \text{ in } \Omega_g, \quad (25) \]
\[ \kappa_g \frac{\partial T}{\partial n}_g - \kappa_s \frac{\partial T}{\partial n}_s = q_r \text{ on } \Gamma_r, \quad (26) \]
\[ \kappa_g \frac{\partial T}{\partial n_0} + \epsilon \sigma |T|^3 T = \epsilon \sigma T_0^4 \text{ on } \Gamma_0, \quad (27) \]
\[ \text{and } f_a \leq f \leq f_b \text{ in } \Omega, \quad (28) \]

\[ q_r(\sigma |T|^3 T) = (I - K)(I - (1 - \epsilon)K)^{-1} \epsilon (\sigma |T|^3 T)(x), \text{ where } K \text{ is the} \]
irradiation and \( y = \sigma |T|^3 T, (K y)(x) = \int_{\Gamma_r} \omega(x,z)y(z)ds_z, \nu \text{Tikhonov} \)
regularisation parameter, \( z \text{ controlled temperature Gradient}. \)
Semilinear Equations of the stationary equations with variational formulation

\[
\int_{\Omega} \kappa \nabla T \cdot \nabla v \, dx + \int_{\Gamma_0} \epsilon \sigma |\overline{T}|^3 T \, v \, ds \\
= \int_{\Omega_s} f v \, dx - \int_{\Gamma_r} q_r (\sigma |\overline{T}|^3 T) v \, ds + \int_{\Gamma_0} \epsilon \sigma T_0^4 v \, ds \quad (29)
\]

where we have the maximum principal for the semilinear PDE with \( \overline{u} \geq 0 \)

\[ q_r = (I - K)(I - (1 - \epsilon)K)^{-1} \epsilon \sigma |\overline{T}|^3 T, \] where \( K \) is the irradiation.

with \( V = \{ v \in H^1(\Omega) | \tau_r v \in L^5(\Gamma_r), \tau_0 v \in L^5(\Gamma_0) \} \), we have

\[ q_r (\sigma |\overline{T}|^3 T) v \in L^1(\Gamma_r) \] for all \( T, v \in V \).

The space \( V \) is done with the norms :

\[ ||v||_V = ||v||_{H^1(\Omega)} + ||v||_{L^5(\Gamma_r)} + ||v||_{L^5(\Gamma_0)}. \]
Optimal Conditions

PDE solution operator $S : f \rightarrow T$ from $L^2(\Omega)$ to $V^\infty$

Defining the control function as variation: $J(f, T) = J(S(f), f) = j(f)$

$$j'(\overline{f})(f - \overline{f}) = (\nabla \overline{T} - z, \nabla T)_{L^2(\Omega_g)} + \nu(\overline{f}, (f - \overline{f}))_{L^2(\Omega_s)}$$

with: $\overline{T} = S(\overline{f})$ and $T = S'(\overline{f})(f - \overline{f})$,  \hspace{1cm} (30)

solve: $-\nabla(\kappa_s \nabla T)_s = f - \overline{f}$ in $\Omega_s$, \hspace{1cm} (31)

$-\nabla(\kappa_g \nabla T)_g = 0$ in $\Omega_g$, \hspace{1cm} (32)

$$\kappa_g \left( \frac{\partial T}{\partial n} \right)_g - \kappa_s \left( \frac{\partial T}{\partial n} \right)_s - 4q_r(\sigma |\overline{T}|^3 T) = 0$$ on $\Gamma_r$, \hspace{1cm} (33)

$$\kappa_g \frac{\partial T}{\partial n_0} + 4\epsilon \sigma |\overline{T}|^3 T = \epsilon \sigma T_0^4$$ on $\Gamma_0$, \hspace{1cm} (34)

and $f_a \leq f \leq f_b$ in $\Omega$, \hspace{1cm} (35)

where $\overline{T}$ and $\overline{f}$ are the optimal values for $T$ and $f$. 

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Discretisation of the Semi-linear Equations

\[ \int_{\Omega} \kappa \nabla T^{(k+1)} \cdot \nabla v \, dx + 4 \int_{\Gamma_r} q_r (\sigma |T^{(k)}|^{3}T^{(k+1)}) v \, ds \]  

\[ + 4 \int_{\Gamma_0} \epsilon \sigma |T^{(k)}|^{3}T^{(k+1)} v \, ds \]

\[ = \int_{\Omega_s} f v \, dx + \int_{\Gamma_0} \epsilon \sigma T_0^4 v \, ds + \int_{\Gamma_0} \epsilon \sigma T_0^4 v \, ds + 3 \int_{\Gamma_r} q_r (\sigma |T^{(k)}|^{3}T^{(k)}) v \, ds \]

\[ + 3 \int_{\Gamma_0} \epsilon \sigma |T^{(k)}|^{3}T^{(k)} v \, ds \]

the PDE is linearised and \( k \) is the current iteration, where \( k + 1 \) is the next iteration.
Numerical Methods for the Optimization

Two equations are solved iteratively:

- Semi-linear discretized heat-equation
- Adjoint equation with the control-function dependent on the right-hand side and the gradients

One could control with the right-hand side $f$ the input-parameters $f_{freq}$ (frequency of the currency), $P$ power of the heater and $z_{rim}$ distance of the coil positions
Numerical Optimization

Data perturbations (uncertain parameters) and boundaries: \( f_1 < f < f_2 \)

Numerical methods (Discretisation-methods and Solvers), \( T(f) \)

Optimisation of the Parameters (Nelder-Mead, gradient gradient-methods) minimise the functional \( J(T(f)) \),
Optimization with minimizing Functionals

Optimization Problem for $f$ (frequency), $P$ (power) and $z_{rim}$ (upper coil rim):

$$\left(\overline{f}, \overline{P}, \overline{z}_{rim}\right) \in [f_{min}, f_{max}] \times [0, P_{max}] \times [z_{min}, z_{max}]$$  \hspace{1cm} (37)

and find an objective functional to minimize

$$(f, P, z_{rim}) \rightarrow J(T(f, P, z_{rim})) \text{ is minimal at } (\overline{f}, \overline{P}, \overline{z}_{rim}),$$ \hspace{1cm} (38)

where $T = T(f, P, z_{rim})$ is a solution of the stationary heat transport.
Functional to minimize

\[ J_\alpha = \alpha F_r(T) - (1 - \alpha) F_z, \quad (39) \]

where \( \alpha \) is a weighting factor, and \( F_r, F_z \) are functionals measuring the size of the absolute radial and vertical gradients of \( T \).

For example the corresponding \( F_r \) are:

\[ F_{r,\max}(T) := \max(|\frac{\partial T}{\partial r}|), \quad F_{r,2}(T) := \left( \int_{\Gamma} 2\pi r \left( \frac{\partial T}{\partial r}(r, z) \right)^2 dr \right)^{1/2}, \quad (40) \]
12 Numerical experiments for the Heat-Equation

We compute the temperature-field and heat source field for various grids. We compare the different grid-dependent solutions for the stationary cases.

The solutions for the heat equation are computed at the points $T(r_{\text{bottom}}, z_{\text{bottom}})$ and $T(r_{\text{top}}, z_{\text{top}})$ for successive grids. For the error analysis, we apply the following error differences

$$\epsilon_{\text{abs}} = |\tilde{T}_{j+1}(r, z) - \tilde{T}_j(r, z)|,$$

(41)

where $\tilde{T}_j(r, z)$ and $\tilde{T}_{j+1}(r, z)$ are solutions evaluated at the point $(r, z)$ which have been computed using the grids $j$ and $j+1$ respectively. The elements of the grid $j + 1$ are approximately $1/4$ of the elements of the grid $j$. The computational time for the finest case was about 2 h.
**Error-Analysis:**

<table>
<thead>
<tr>
<th>Level</th>
<th>Number of Nodes</th>
<th>Grid Point (0, 0.028) ($T_{\text{bottom}}$)</th>
<th>Grid Point (0, 0.173) ($T_{\text{top}}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1532</td>
<td>2408.11</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>23017</td>
<td>2409.78</td>
<td>1.67</td>
</tr>
<tr>
<td>2</td>
<td>91290</td>
<td>2410.35</td>
<td>0.57</td>
</tr>
<tr>
<td>3</td>
<td>364225</td>
<td>2410.46</td>
<td>0.11</td>
</tr>
</tbody>
</table>

Table 1: Computations on different grids for the errors analysis with absolute differences for stationary computations.
Nonlinear heat conduction for the gas material (Gas-Phase)

Heat Source Field

Height = 25 cm
PowDens_min = 0 W/m^3
PowDens_max = 7.70727e+06 W/m^3

heating power in crucible = 7546.33 W
heating power in coil = 2453.67 W

prescribed power = 10000 W
frequency = 10000 Hz
coil:
5 rings
top = 0.18 m
bottom = 0.02 m

t = 100000 s
tstep = 1e-05 s

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Temperature-source

Stationary Temperature Field

height = 25 cm

T_min = 537.517 K
T_max = 3312.53 K
delta T_max = 0 K

heating power in crucible = 7811.89 W
heating power in coil = 2188.11 W

prescribed power = 10000 W
frequency = 10000 Hz

coil:
5 rings
top = 0.18 m
bottom = 0.02 m

delta T[K] between isolines

radius = 8.4 cm

T[K]
Time-delay in the heating phase

For the growth process, the temperature difference

\[ T_{ss} = T(r_{source}, z_{source}) - T(r_{seed}, z_{seed}) \]

is crucial, but in the physical growth experiments, usually only the temperatures \( T(r_{bottom}, z_{bottom}) \) and \( T(r_{top}, z_{top}) \) is measurable.
Delay of the SiC-Powder in the heating process

Transient Temperature Field

height = 25 cm
T_min=300.026 K
T_max=1803.01 K
delTmax=40.8181 K

heating power in crucible=2997.9 W
heating power in coil=957.651 W

T_upperHole = 1393.64 K
T_lowerHole = 1661.26 K
T_lower-T_upper = 267.622 K

prescribed power = 3955.56 W
frequency = 10000 Hz

coil:
5 rings
top = 0.14 m
bottom = -0.02 m

t=4000 s
t_step=100 s

delta T[K] between isolines
Full heated SiC-Powder after 10000 sec

Transient Temperature Field

- Height = 25 cm
- $T_{\text{min}} = 504.244$ K
- $T_{\text{max}} = 3194.55$ K
- $\Delta T_{\text{max}} = 60.6559$ K

- Heating power in crucible = 7117.04 W
- Heating power in coil = 2171.85 W

- $T_{\text{upper hole}} = 2380.9$ K
- $T_{\text{lower hole}} = 2408.37$ K
- $T_{\text{lower}} - T_{\text{upper}} = 27.462$ K

- Prescribed power = 9288.89 W
- Frequency = 10000 Hz

- Coil: 5 rings
  - Top = 0.14 m
  - Bottom = -0.02 m

- $t = 10000$ s
- $t_{\text{step}} = 100$ s

- Delta $T[K]$ between isolines
13 Conclusions and future works

- Error-estimates for nonlinear parabolic-equations.
- Optimization of further terms, e.g. temperature constants for the inner heat-equation.
- Anisotropy thermal conductivity for the insulation.
- Crystal growth of the silicon-bulk with Chemical reaction in gas (diffusion-reaction-equation).
- Free boundary problems.