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1 Introduction


- Task: Simulation of a apparatus of a complex crystal growth with heat- and thermal processes.

- Model-Problem: Multi-phase problem (solid-solid, solid-gas), multiscaling problem (anisotropical effects in the insulation) Multi-physical problem (heat-transfer, radiation, semi-transparent, magnetic-fields)

- Problems: Scaling problems (Anisotropy), Interface-Problems (steep Gradients, various material behaviors)

- Solution: Improved finite Volume methods and implicate methods.
2 Contents

- Motivation for the Crystal Growth
- Introduction to the model and the technical apparatus
- Mathematical model and equations
- Discretisation and Anisotropy
- Radiation and Semi-transparent
- Applications
- 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
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.
5 Model for the Anisotropy of the Heat-Transfer

We have the stationary heat conduction is given as:

\[- \text{div} (K_m(\theta) \nabla \theta) = f_m \quad \text{in} \; \Omega_m \quad (m \in M), \quad (1)\]

The thermal conductivity tensor is a diagonal matrix with temperature-independent anisotropy,

\[K_m(\theta) = (\kappa_{i,j}^m(\theta)), \quad \text{where} \quad \kappa_{i,j}^m(\theta) = \begin{cases} \alpha_i^m \kappa_{\text{iso}}^m(\theta) & \text{for } i = j, \\ 0 & \text{for } i \neq j, \end{cases} \quad (2)\]

\[\kappa_{\text{iso}}^m(\theta) > 0 \; \text{being the potentially temperature-dependent thermal conductivity of the isotropic case, and} \; \alpha_i^m > 0 \; \text{being anisotropy coefficients}.\]
6 Finite Volume discretisation

We use constrained Delaunay triangulation to discretize polyhedral domains and apply Voronoi-construction to define finite volumes.

Integrating (1) over $\omega_{m,v}$ and applying the Gauss-Green integration theorem yields

$$- \int_{\partial \omega_{m,v}} (K_m(\theta) \nabla \theta) \cdot n_{\omega_{m,v}} = \int_{\omega_{m,v}} f_m,$$

where $n_{\omega_{m,v}}$ denotes the outer unit normal vector to $\omega_{m,v}$.

Approximation of the isotropic part

We approximate $\kappa^m_{\text{iso}}(\theta)$ on $\gamma_{m,v,w}$ by the arithmetic mean

$$\kappa^m_{\text{iso}}(\theta) \mid_{\gamma_{m,v,w}} \approx \frac{1}{2} (\kappa^m_{\text{iso}}(\theta_v) + \kappa^m_{\text{iso}}(\theta_w)).$$
Approximation of the anisotropic part

It remains to approximate \((A_m \nabla \theta) \cdot \mathbf{n}_{\omega_{m,v}}\) on \(\gamma_{m,v,w}\), where \(A_m\) is the constant diagonal matrix

\[
A_m = (a_{i,j}^m), \quad a_{i,j}^m := \begin{cases} \alpha_{i,j}^m & \text{for } i = j, \\ 0 & \text{for } i \neq j. \end{cases}
\] (5)

For each \(\sigma \in \Sigma_{\gamma_{m,v,w}}:\)

\[
(A_m \nabla \theta) \upharpoonright_{\sigma} \cdot \mathbf{n}_{\omega_v} \upharpoonright_{\gamma_{m,v,w}} = \sum_{\tilde{v} \in V(\sigma)} \theta(\tilde{v}) (A_m \nabla \phi_{\sigma,\tilde{v}}) \cdot \frac{w - v}{\|w - v\|_2}.
\] (6)

For each \(m \in M\) and each \((v, w) \in M^2\), let \(\gamma_{m,v,w} := \partial \omega_{m,v} \cap \partial \omega_{m,w}\) denote the interface of the two Voronoï cells inside the material domain \(\Omega_m\) (of course, in general, \(\gamma_{m,v,w}\) can be empty).
To approximate the heat flux integrals
\[ \int_{\partial \omega_m,v \cap \Omega_m} (K_m(\theta) \nabla \theta) \cdot \mathbf{n}_{\omega_m,v} , \]
the set \( \partial \omega_m,v \cap \Omega_m \) is also partitioned further, namely into the interfaces with all neighboring Voronoï cells. Up to null sets with respect to \( \lambda_1 \):

\[ \partial \omega_m,v \cap \Omega_m = \bigcup_{w \in \text{nb}_m(v)} \gamma_{m,v,w}, \tag{7} \]

where \( \text{nb}_m(v) := \{ w \in V_m \setminus \{v\} : \lambda_1(\gamma_{m,v,w}) \neq 0 \} \) is the set of \( m \)-neighbors of \( v \). For example, in Fig. ??, \( \partial \omega_{1,v} \) is decomposed into \( \gamma_{1,v,u_1} \), \( \gamma_{1,v,w} \), and \( \gamma_{1,v,u_2} \).

Illustration of the decomposition of \( \partial \omega_{1,v} \).
\[ \overline{\sigma}_1 = \text{conv}\{v, w, u_1\}, \quad \overline{\sigma}_2 = \text{conv}\{v, w, u_2\} \]

\[ \overline{\Omega}_1 = \overline{\sigma}_1 \cup \overline{\sigma}_2 \]

Figure 1: Illustration of the decomposition of \( \partial \omega_{1,v} \).
7 Numerical examples for the heat-transfer

We apply the anisotropical insulations-materials in different experiments and deal with moderately anisotropic cases

a.) \((\alpha_r^1, \alpha_z^1) = (10, 1)\) (left picture, isotherms spaced at 50 K);

b.) \((\alpha_r^1, \alpha_z^1) = (1, 10)\) (middle picture, isotherms spaced at 80 K);

c.) \((\alpha_r^1, \alpha_z^1) = (10, 1)\) in top and bottom insulation parts,
\((\alpha_r^1, \alpha_z^1) = (1, 10)\) in insulation side wall (right picture, isotherms spaced at 80 K).
Results: 1. z-ani., 2. z-ani.(full), 3. z-ani.(side), r-ani.(top, bott.)
Heat-Transfer and Radiation: Modell

Heat-conduction for gas-material

\[ \rho_{Ar} \partial_t U_{Ar} - \nabla \cdot (\kappa_{Ar} \nabla T) = 0 , \quad U_{Ar} = z_{Ar} \frac{R}{M_{Ar}} T , \quad (8) \]

\( \rho_{Ar} \) is the density, \( \kappa_{Ar} \) is the thermal-conductivity, \( z_{Ar} \) is the configuration number, \( R \) is the universal gas constant, \( M_{Ar} \) is the molecular mass, \( U_{Ar} \) is the partial internal energy.

Heat-conduction for solid-material

\[ \rho_{solid} \partial_t U_{solid} - \nabla \cdot (\kappa_{solid} \nabla T) = f , \quad U_{solid} = c_{solid} T \quad , \quad (9) \]

where \( \rho_{solid} \) is the density, \( \kappa_{solid} \) is the thermal-conductivity and \( c_{solid} \) is the specific heat and \( U_{solid} \) is the partial internal energy.
Interface conditions.

\[
(\kappa \nabla T)_{Ar} \cdot \mathbf{n}_{Ar} + \mathcal{R} - J = (\kappa \nabla T)_{solid} \cdot \mathbf{n}_{Ar},
\]

where \( \mathbf{n}_{Ar} \) is the normal vector of the gas-domain.

\[
\mathcal{R} = E + J_{ref},
\]

\[
E = \sigma \epsilon T^4 \quad \text{(Stefan-Boltzmann-Equation)},
\]

\[
J_{ref} = (1 - \epsilon) J,
\]

where \( \mathcal{R} \) is the radiosity, \( E \) is the radiation and \( J_{ref} \) is the reflexed radiation and \( \epsilon \) is the emissivity.
Modelling of the Opaque case

The irradiation is defined as follows

\[ J(T) = K(R(T)) , \]  

(14)

we use the integral operator \( K \) defined by

\[ K(\rho)(x) = \int_{\Sigma} \Lambda(x, y) \omega(x, y) \rho(y) \, dy , \]  

(15)

where \( x \in \Sigma \), the visibility factor is 1 and 0, if the point \( x \) and \( y \) are mutually visible or not.

The view factor \( \omega \) is defined by

\[ \omega(x, y) := \frac{(n_g \cdot (x - y))(n_g \cdot (y - x))}{\pi((y - x) \cdot (y - x))^2} , \]  

(16)

where we have a conservation of the radiation energy.
We could reset the equation 10 by the definitions

\[ E(T) = \sigma \epsilon(T) T^4, \]  

(17)

and follow

\[ R(T) - J(T) = -\epsilon(T) \cdot (K(R(T)) - \sigma T^4). \]  

(18)

We get the the interface condition

\[ (\kappa_g \nabla T)|_{\tilde{\Omega}_g} \cdot \mathbf{n}_g - \epsilon(T)(K(R(T)) - \sigma T^4) = (\kappa_s \nabla T)|_{\tilde{\Omega}_s} \cdot \mathbf{n}_g, \text{ on } \Sigma, \]  

(19)

where the normal-vector \( \mathbf{n}_g \) belong to the gas-phase and the temperature is given as \( T \) and \( \epsilon \) is the emissivity.
Computation of the Opaque and semi-transparent case

1.) Point are viewable for the points in the same sub-domain, i.e. the negation is given as

\[ \Lambda^*((r, z), (s, y)) = 0.0, \text{ if } (s, y) \notin \partial \Omega^*_i(r, z), gas \]  \hspace{1cm} (20)

2.) For the case \((r, z) = (s, y)\) we detect the constellation for case of the self view of the point, done with the boundary-circle

\[ \Lambda^*((r, z), (s, y)) = 0.0, \text{ if } n_r(r, z) \geq 0 . \]  \hspace{1cm} (21)

3.) For the case \(z = y\), we have two circles on the level, which could see each by the following constellation

\[ \text{if } (r < s \land (n_r(r, z) \leq 0 \lor n_r(s, z) \geq 0)) \]
\[ \lor (r > s \land (n_r(r, z) \geq 0 \lor n_r(s, z) \leq 0)) \]
\[ \text{ then } \Lambda^*((r, z), (s, z)) = 0 . \]  \hspace{1cm} (22)
4.) For the case $z > y$, we have the different options for all the cases

$$
\Lambda^*((r, z), (s, y)) = \Lambda^*((s, y), (r, z)) \, , \, \forall (r, z), (s, y) \in \partial \Omega^*_{gas} . \quad (23)
$$

5.) For the case $z < y$ we use the computation

$$
\Lambda^*((r, z), (s, y)) = \Lambda^*((s, y), (r, z)) . \quad (24)
$$

For the shadowing and visibility we calculate the ray-ways based on the derived visibility angle $\theta$ with $G_{(r,z),(s,y),\theta}(\tau)$ given as

$$
G_{(r,z),(s,y),\theta}(\tau) = \begin{pmatrix}
((1 - \tau)^2 r^2 + \tau^2 s^2 + 2(1 - \tau) \tau rs \cos(\theta))^{1/2} \\
(1 - \tau)z + \tau y
\end{pmatrix}, \quad \forall \tau \in [0, \pi]
$$

$$
\text{given as } G_{(r,z),(s,y),\theta}(\tau)
$$

$$
\text{with } G_{(r,z),(s,y),\theta}(\tau)
$$
The angles $\theta$ are calculated as follows:

$$\theta^* = \theta + \theta' , \quad (26)$$

$$\cos(\theta) = \frac{z(r_{j+1} - r_j) + (r_jz_{j+1} - r_{j+1}z_j)}{r(z_{j+1} - z_j)} , \quad (27)$$

$$\cos(\theta') = \frac{z'(r_{j+1} - r_j) + (r_jz_{j+1} - r_{j+1}z_j)}{r'(z_{j+1} - z_j)} , \quad (28)$$

where $\mathbf{x} = (r, 0, z)$ and $\mathbf{x}' = (r', 0, z')$ are the coordinates.

The contact point is calculated as:

$$r_c = \frac{rr' \sin(\theta + \theta')}{r \sin(\theta) + r' \sin(\theta')} , \quad (29)$$

$$z_c = \frac{zr' \sin(\theta') + z'r \sin(\theta)}{r \sin(\theta) + r' \sin(\theta')} , \quad (30)$$

where $\mathbf{x} = (r, 0, z)$ and $\mathbf{x}' = (r', 0, z')$ are the coordinates.
The algorithm for the general radiation-cases

1.) Loop over all counter-clock-size edges

Use the connected polygons and go over the sides of the polygons.
Each point which is joint to the triangle is used

2.) Loop over all clock-size edges

Idea of adaptivity of the view-factors:

For the adaptive algorithm we interpolate the solutions of the different grids \( g_1 \) and \( g_2 \). For the interpolation we use the averaging method, i.e. we apply the coarse solutions of the view-factors and the solutions is given with the average of the two neighbor-solutions:

\[
\begin{align*}
    u_{i,1}, u_{i,2} &\rightarrow u_{i+1}. \\
    u_{i+1} &= \frac{u_{i,1} - u_{i,2}}{2}
\end{align*}
\]

(31)

(32)
We calculate the view-factor:

\[ \Lambda^* ((r, z), (s, y)) = 2 \int_0^\Pi \Lambda_{(r,z),(s,y)}(\tau)\omega_{(r,z),(s,y)}(\tau) \, d\tau. \quad (33) \]

The algorithm for the free-floating-domain is given as:

1.) The edge intersects the radiation-triangle.

2.) The edge tangential the radiation-triangle.

3.) The edge is inside the radiation-triangle, therefore we get two intervals for the visible angles.

For the inner domains we get 2 intervals:

\[ [\tau_{min_1}, \tau_{min_2}], [\tau_{max_2}, \tau_{max_1}], \]

Where \([\tau_{min_1}, \tau_{max_1}]\) is the visibility interval and is the shadowing interval \([\tau_{min_2}, \tau_{max_2}]\).

The visibility is in the range: \(0 < \tau_{min_1} < \tau_{max_1} < \pi\)
9 Numerical examples for the radiation

Test-examples:

Curved Rays with visibility intervals
Curved Rays with visibility intervals
Curved Rays with visibility intervals
10 Application in complex domains

Stationary Temperature Field

height = 85 cm

\[ \begin{align*}
T_{min} &= 888.773 \, K \\
T_{max} &= 2522.88 \, K \\
\Delta T_{max} &= 7.99299 \, K
\end{align*} \]

heat. power in cruc. = 9493.43 W
heat. power in coil = 506.568 W

prescribed power = 10000 W
frequency = 10000 Hz

coil:
5 rings
top = 0.8 m
bottom = 5.55112e-17 m

delta T[K] between isolines
Heat Source Field

height = 85 cm

PowDens_min=0 W/m^3
PowDens_max=493486 W/m^3

prescribed power = 10000 W
frequency = 10000 Hz

coil:
5 rings
top = 0.8 m
bottom = 5.55112e-17 m

delta powDens[W/m^3] between isolines

heat. power in cruc.=9493.43 W
heat. power in coil=506.568 W
11 Application in Anisotropy and Radiation

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<th>Exp.</th>
<th>Ins. regions</th>
<th>((\alpha_r^1, \alpha_z^1))</th>
<th>(T_{\text{max}}) [(K)]</th>
<th>(T_{\text{top}}) [(K)]</th>
<th>(T_{\text{bottom}}) [(K)]</th>
<th>(T_{\text{seed}}) [(K)]</th>
<th>(T_{\text{source}}) [(K)]</th>
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<td>1,2,3,4,5</td>
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<td>2711.15</td>
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<td>(b)</td>
<td>1,2,3,4,5</td>
<td>(4, 1)</td>
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<td>1970.49</td>
<td>1761.28</td>
<td>1986.69</td>
<td>1995.66</td>
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<td>(c)</td>
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Simulation of a growth apparatus with different insulations - parts

![Diagram of a growth apparatus with different insulations showing temperatures of 1600 K, 1800 K, 2200 K, and 2400 K at various parts labeled 1, 2, 3, 4, and 5.]
12 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.