Numerical Simulation of Heat Transfer in Materials with Anisotropic Thermal Conductivity: A Finite Volume Scheme to Handle Complex Geometries

Olaf Klein[1], Jürgen Geiser[1], Peter Philip[2]

[1] Weierstrass Institute for
Applied Analysis and Stochastics (WIAS)
Berlin, Germany

[2] University of Minnesota
Institute for Mathematics and its Applications (IMA)
Minneapolis, USA

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Complex Sample Domain from Crystal Growth

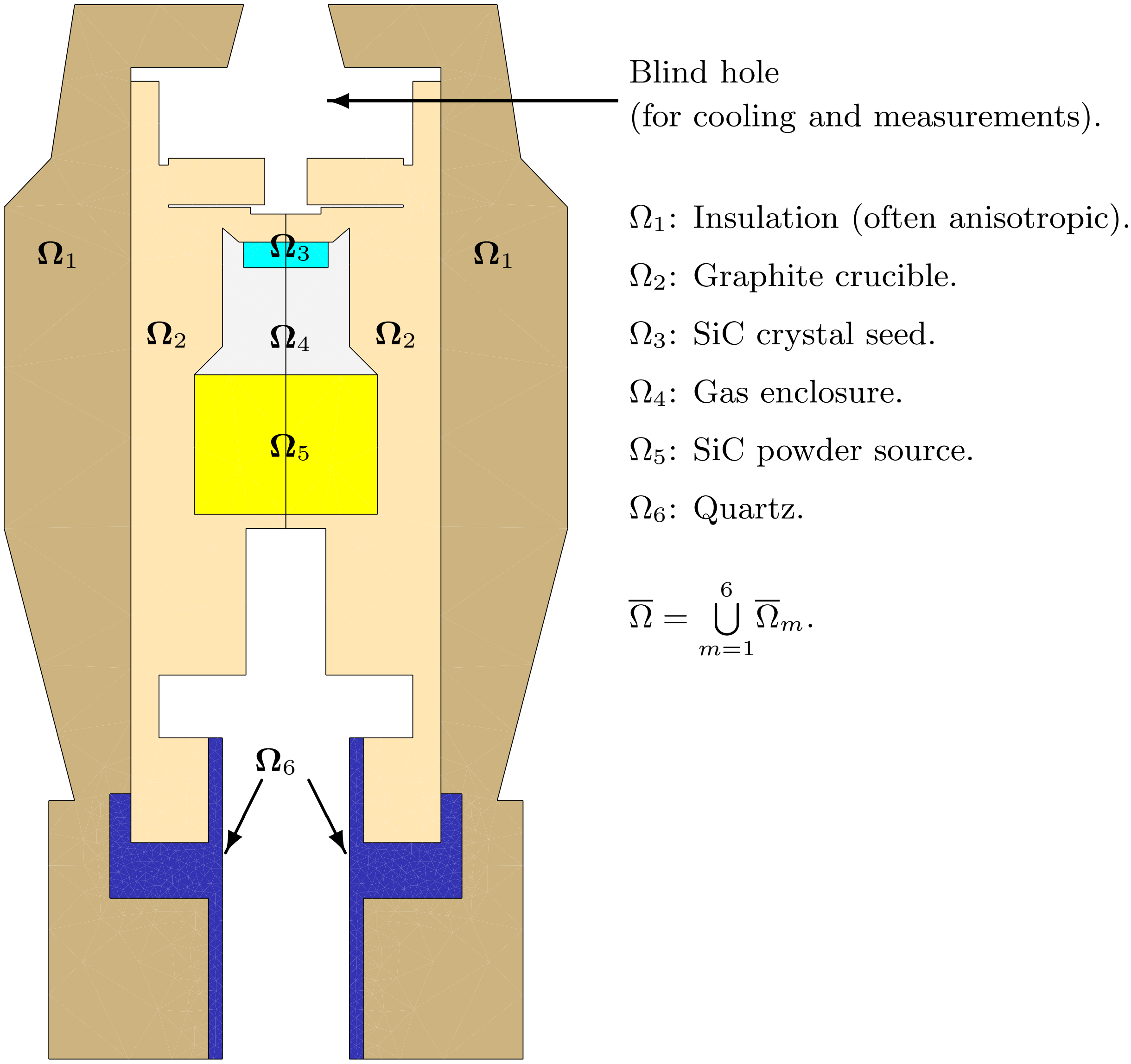


Figure 1: Axisymmetric domain representing a growth apparatus used in silicon carbide single crystal growth by physical vapor transport (PVT). The geometry is a modified version of K. Semmelroth et al., J. Phys.-Condes. Matter 16 (2004).

Model for Stationary Anisotropic Heat Conduction

$$- \operatorname{div}(K_m(\theta)\, \nabla\, \theta) = f_m \quad \text{in } \Omega_m \qquad (m \in M),$$

θ: absolute temperature, K_m: symmetric and positive definite tensor of thermal conductivity, f_m: heat sources, Ω_m: domain of material m.

Assumed form of K_m:

$$K_m(\theta) = \left(\kappa^m_{i,j}(\theta) \right), \quad \text{where} \quad \kappa^m_{i,j}(\theta) = \begin{cases} \alpha^m_i \, \kappa^m_{\text{iso}}(\theta) & \text{for } i = j, \\ 0 & \text{for } i \neq j. \end{cases}$$

Interface Conditions on $\overline{\Omega}_{m_1} \cap \overline{\Omega}_{m_2}$:

$$K_{m_1}(\theta)\, \nabla\, \theta \restriction_{\overline{\Omega}_{m_1}} \bullet\, \mathbf{n}_{m_1} = K_{m_2}(\theta)\, \nabla\, \theta \restriction_{\overline{\Omega}_{m_2}} \bullet\, \mathbf{n}_{m_1}.$$

$\restriction$: restriction, $\mathbf{n}_{m_1}$: outer unit normal vector to material m_1.

Boundary Conditions: Dirichlet, Robin

$$\theta = \theta_{\text{Dir}} \qquad \text{on } \overline{\Gamma}_{\text{Dir}},$$

$$- \left(K_m(\theta)\, \nabla\, \theta \right) \bullet\, \mathbf{n}_m = \xi_m \, (\theta - \theta_{\text{ext}}) \qquad \text{on } \Gamma_{\text{Rob}} \cap \partial\Omega_m,\, m \in M,$$

Finite Volume Discretization

$\Sigma_m = (\sigma_{m,i})_{i \in I_m}$ conforming triangulation of Ω_m satisfying the constrained Delaunay property: If γ is an interior edge of Σ_m, α and β the angles opposite to γ, then $\alpha + \beta \leq \pi$. If $\gamma \subseteq \partial\Omega_m$ is a boundary edge of Σ_m, α the angle opposite γ, then $\alpha \leq \pi/2$.

$V(\sigma_{m,i}) = \quad v^m_{i,j} : j \in \{1,2,3\} \quad$: Set of vertices.

$V := \bigcup_{m \in M,\, i \in I_m} V(\sigma_{m,i})$.

$$\omega_v := \quad x \in \Omega : \|x - v\|_2 < \|x - z\|_2 \text{ for each } z \in V \setminus \{v\} \quad ,$$

$$\omega_{m,v} := \omega_v \cap \Omega_m, \quad V_m := \{z \in V : \omega_{m,z} \neq \emptyset\}.$$

$$A_m = (a^m_{i,j}), \qquad a^m_{i,j} := \begin{cases} \alpha^m_i & \text{for } i = j, \\ 0 & \text{for } i \neq j. \end{cases}$$

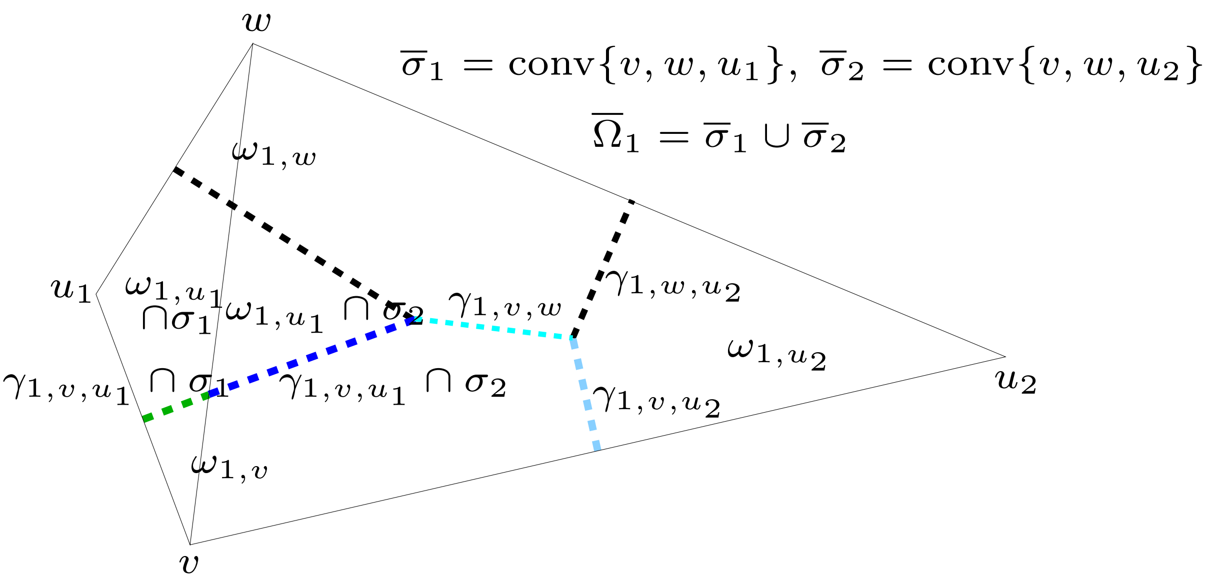


Figure 2: Illustration of the space discretization.

Approximation of Anisotropic Terms

$\phi_{\sigma,v} : \sigma \longrightarrow [0,1]$: Affine coordinates on triangle σ w.r.t. $v \in V(\sigma)$.
For each edge $[v,w]$ of some $\sigma \in \Sigma_m$:

$$\Sigma_{m,v,w} := \quad \sigma \in \Sigma_m : \{v,w\} \subseteq V(\sigma) \quad .$$

Letting

$$\Sigma_{\gamma_{m,v,w}} := \quad \sigma \in \Sigma_{m,v,w} : \lambda_1(H_{v,w,\sigma} \cap \gamma_{m,v,w}) \neq 0 \quad ,$$

decompose $\gamma_{m,v,w}$:

$$\gamma_{m,v,w} = \bigcup_{\sigma \in \Sigma_{\gamma_{m,v,w}}} \overline{\sigma} \cap \gamma_{m,v,w}.$$

Approximation:

$$(A_m \nabla \theta)\restriction_\sigma \bullet \mathbf{n}_{\omega_v}\restriction_{\gamma_{m,v,w}} \approx \sum_{\tilde{v} \in V(\sigma)} \theta(\tilde{v})\,(A_m \nabla \phi_{\sigma,\tilde{v}}) \bullet \frac{w-v}{\|w-v\|_2}.$$

Finite Volume Scheme

Find $(\theta_v)_{v \in V}$ satisfying:

$\theta_v = \theta_{\mathrm{Dir}}(v)$ for each $v \in V_{\mathrm{Dir}}$,

$$0 = \sum_{m \in M} \xi_m \quad \theta_v - \theta_{\mathrm{ext}}(v) \quad \lambda_1(\partial\omega_{m,v} \cap \Gamma_{\mathrm{Rob}})$$
$$- \sum_{m \in M} \sum_{\sigma \in \Sigma_{\gamma_{m,v,w}}} \frac{1}{2} \quad \kappa^m_{\mathrm{iso}}(\theta_v) + \kappa^m_{\mathrm{iso}}(\theta_w)$$
$$\sum_{\tilde{v} \in V(\sigma)} \theta_{\tilde{v}}\,(A_m \nabla \phi_{\sigma,\tilde{v}}) \bullet \frac{w-v}{\|w-v\|_2} \lambda_1(H_{v,w,\sigma} \cap \gamma_{m,v,w})$$
$$- \sum_{m \in M} f_{m,v}\,\lambda_2(\omega_{m,v}) \quad \text{for each } v \in V_{\neg\mathrm{Dir}} = V \setminus V_{\mathrm{Dir}}.$$

Comparison with Closed-Form Solution

Axisymmetric Single-Material Domain

$\Omega = \{(r,z) : \ 0 < r < 0.2, \ -0.2 < z < 0.2\}$:

$$-\frac{1}{r}\frac{\partial}{\partial r} \quad r\,\alpha_r \frac{\partial \theta}{\partial r} \quad - \frac{\partial}{\partial z} \quad \alpha_z \frac{\partial \theta}{\partial z} \quad = 0 \qquad \text{in } \Omega, \tag{1a}$$

$$\theta_{\mathrm{Dir}}(r,z) := \frac{1}{2}\frac{1}{\alpha_r} r^2 - \frac{1}{\alpha_z} z^2 \qquad \text{on } \partial\Omega. \tag{1b}$$

Solution: $\theta(r,z) = \frac{1}{2}\frac{1}{\alpha_r} r^2 - \frac{1}{\alpha_z} z^2 \quad$ on $\overline{\Omega}$.

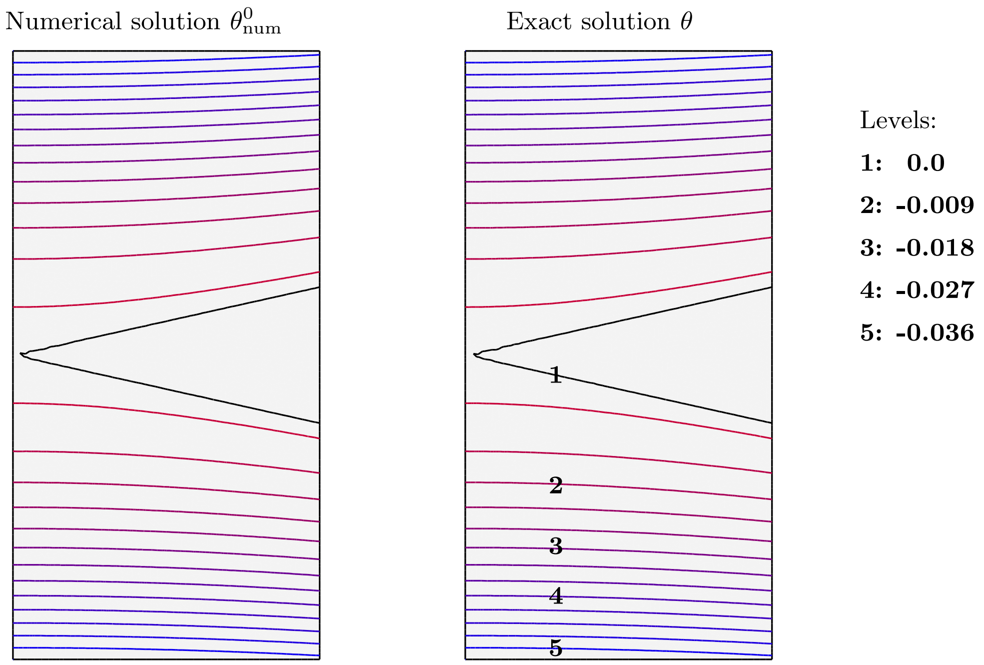


Figure 3: Solution of (1): Numerical θ^0_{num}, 3117 triangles (left); exact θ (right). Isolevel difference: 0.003.

Discrete L_1-error: $\quad \epsilon^l_{L_1} := \sum_{v \in V^l} \mathrm{vol}(\omega_v)|\theta^l_{\mathrm{num}}(v) - \theta(v)|,$

$v \in V^l$: vertices, $\mathrm{vol}(\omega_v)$: r-weighted area of Voronoï cell.

Numerical convergence rate:

$$\rho^l_{L_1} := (\ln(\epsilon^l_{L_1}) - \ln(\epsilon^{l-1}_{L_1}))/(\ln(h^l) - \ln(h^{l-1})),$$

h^l: upper bound for triangle area of level l.

Axisymmetric Multi-Material Domain

$$\Omega_1 = \{(r,z) : 0 < r < r_0,\ 0 < z < z_0\},$$
$$\Omega_2 = \{(r,z) : r_0 < r < r_{\max},\ 0 < z < z_0\},$$
$$\Omega_3 = \{(r,z) : 0 < r < r_0,\ z_0 < z < z_{\max}\},$$
$$\Omega_4 = \{(r,z) : r_0 < r < r_{\max},\ z_0 < z < z_{\max}\},$$

$$-\frac{1}{r}\frac{\partial}{\partial r}\quad r\,\alpha_{m,r}\,\frac{\partial\theta}{\partial r}\quad - \frac{\partial}{\partial z}\quad \alpha_{m,z}\,\frac{\partial\theta}{\partial z} = f_m \quad \text{in } \Omega_m, \tag{2a}$$

$$\left(\begin{pmatrix}\alpha_{m,r} & 0\\ 0 & \alpha_{m,z}\end{pmatrix}\nabla\,\theta\restriction_{\overline{\Omega}_m}\right)\bullet\,\mathbf{n}_m = \left(\begin{pmatrix}\alpha_{\tilde{m},r} & 0\\ 0 & \alpha_{\tilde{m},z}\end{pmatrix}\nabla\,\theta\restriction_{\overline{\Omega}_{\tilde{m}}}\right)\bullet\,\mathbf{n}_m \quad \text{on } \partial\Omega_m \cap \partial\Omega_{\tilde{m}}, \tag{2b}$$

$$\theta_{\mathrm{Dir},m}(r,z) := a_m\,r^2 + b_m\,z^2 + c_m \quad \text{on } \partial\Omega\cap\partial\Omega_m. \tag{2c}$$

Solution:

$$\theta(r,z) := a_m\,r^2 + b_m\,z^2 + c_m \qquad \text{on } \overline{\Omega}_m,$$
$$\theta_{\mathrm{Dir},m}(r,z) := a_m\,r^2 + b_m\,z^2 + c_m \qquad \text{on } \partial\Omega\cap\partial\Omega_m,$$

where $r_0 = z_0 = 0.1$, $r_{\max} = z_{\max} = 0.2$,

$$\begin{array}{llll}
\alpha_{1,r} = 2, & \alpha_{2,r} = 1, & \alpha_{3,r} = 4, & \alpha_{4,r} = 2,\\
\alpha_{1,z} = 1, & \alpha_{2,z} = 2, & \alpha_{3,z} = 3, & \alpha_{4,z} = 6,\\
a_1 = 1, & a_2 = 2, & a_3 = 1, & a_4 = 2,\\
b_1 = 1, & b_2 = 1, & b_3 = 1/3, & b_4 = 1/3,\\
c_1 = 0, & c_2 = -1/100, & c_3 = 2/300, & c_4 = 1/300,\\
f_1 = -10, & f_2 = -12.0, & f_3 = -18.0, & f_4 = -20.0
\end{array}$$

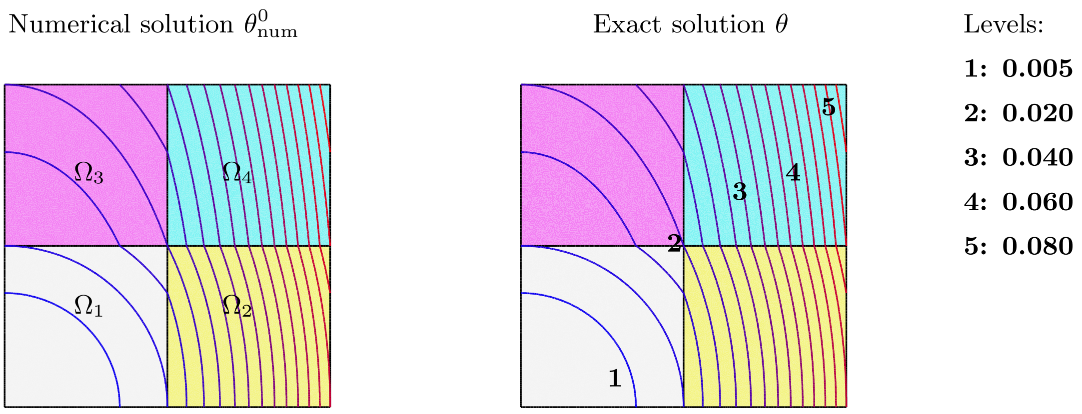


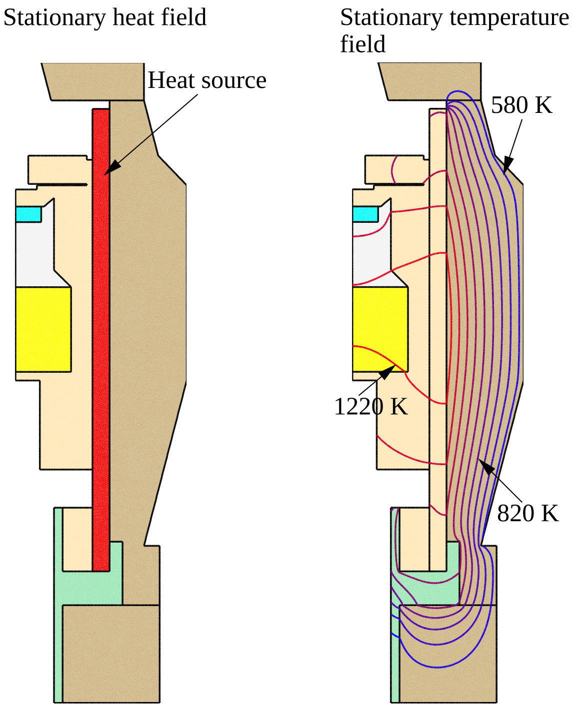
Figure 4: Solution of (2): Numerical θ^0_{num}, 3117 triangles (left); exact θ (right). Isolevel difference: 0.005.

level l	number of triangles	max area h^l	L_1-error $\epsilon^l_{L_1}$	numerical convergence rate $\rho^l_{L_1}$
0	3117	$4.0\ 10^{-5}$	$5.013\ 10^{-8}$	
1	12446	$1.0\ 10^{-5}$	$1.260\ 10^{-8}$	0.996125
2	49669	$2.5\ 10^{-6}$	$3.244\ 10^{-9}$	0.978789
3	198212	$6.25\ 10^{-7}$	$8.2815\ 10^{-10}$	0.984905
4	795195	$1.5625\ 10^{-7}$	$2.0891\ 10^{-10}$	0.993505

Table 1: L_1-error and numerical convergence rate for the numerical solution of (1) with anisotropy $(\alpha_r, \alpha_z) = (10, 1)$.

level l	number of triangles	max area h^l	L_1-error $\epsilon^l_{L_1}$	numerical convergence rate $\rho^l_{L_1}$
0	1557	$4.0\ 10^{-5}$	$2.1325\ 10^{-6}$	
1	6148	$1.0\ 10^{-5}$	$1.0669\ 10^{-6}$	0.49956
2	24813	$2.5\ 10^{-6}$	$5.259\ 10^{-7}$	0.510282
3	99428	$6.25\ 10^{-7}$	$2.638\ 10^{-7}$	0.497672
4	398130	$1.5625\ 10^{-7}$	$1.3362\ 10^{-7}$	0.490654

Table 2: L_1-error and numerical convergence rate for the numerical solution of (2).



α_r	α_z	Maximal Temperature $[K]$
1	1	1273.18
1	10	1232.15
10	10	1238.38
10	1	918.35
1	1000	1063.58
1000	1000	1030.45
1000	1	706.36

Figure 5: Left: Domain of heat sources highlighted. Right: T-field for isotropic insulation, i.e. $\alpha_r = \alpha_z = 1$.

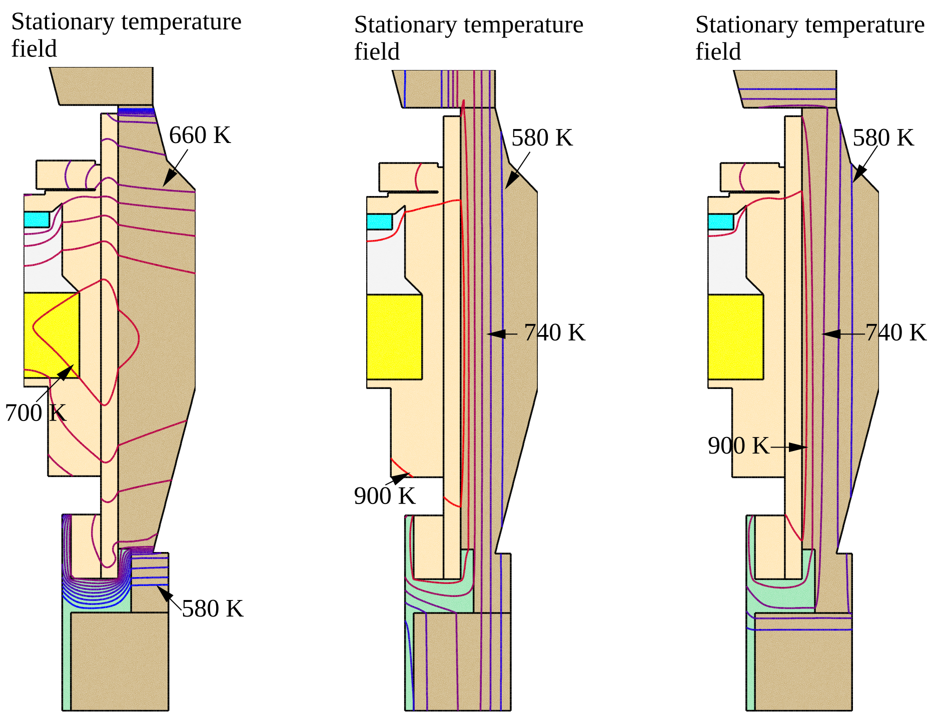


Figure 6: T-field for anisotropic insulation with $\alpha_r = 1000$ (left), with $\alpha_r = 1000$ for sides, $\alpha_z = 1000$ for top and bottom (middle), $\alpha_z = 1000$ (right).

Publications

- P. PHILIP: *Transient Numerical Simulation of Sublimation Growth of SiC Bulk Single Crystals. Modeling, Finite Volume Method, Results*, Thesis, Department of Mathematics, Humboldt University of Berlin, Germany, 2003 Report No. 22, Weierstrass Institute for Applied Analysis and Stochastics, Berlin.
- J. GEISER, O. KLEIN, P. PHILIP: *Numerical simulation of heat transfer in materials with anisotropic thermal conductivity: A finite volume scheme to handle complex geometries.* In preparation.
- J. GEISER, O. KLEIN, P. PHILIP: *Influence of anisotropic thermal conductivity in the apparatus insulation for sublimation growth of SiC: Numerical investigation of heat transfer.* In preparation.

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