Optimal Contol of a PDE with Weakly Singular Integral Operator: Tuning Temperature Fields During Crystal Growth

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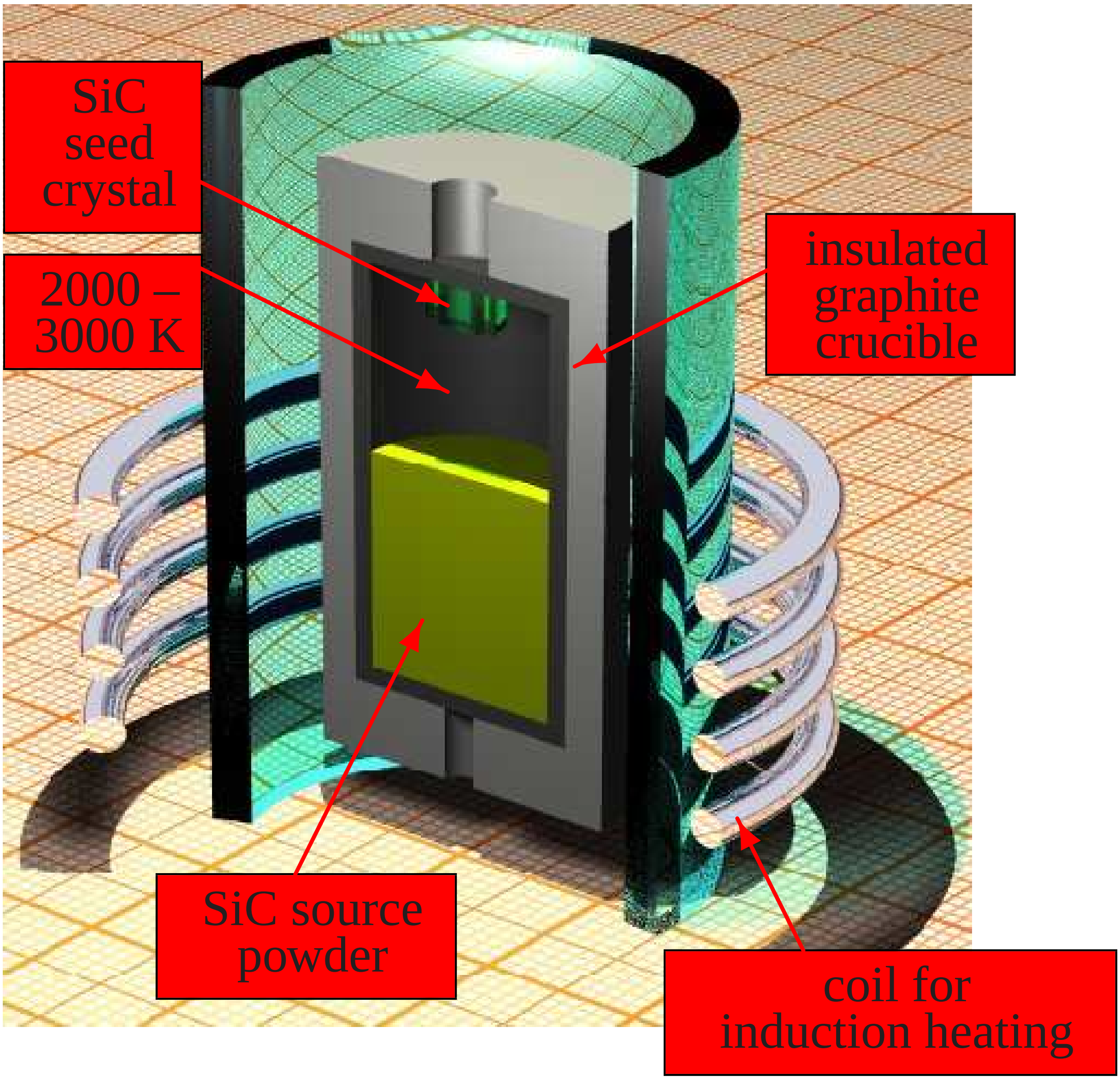
SiC growth by physical vapor transport (PVT)



- Polycrystalline SiC powder sublimates inside induction-heated graphite crucible at 2000 – 3000 K and $\approx$ 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.

Goal:

Prescribe temperature gradient in the gas phase such that it is advantageous for the growth process (e.g. radially flat near crystal surface, sufficiently large in vertical direction).

Formulation of Control Problem for Stationary Heat Transport Model

- Simplified domain:

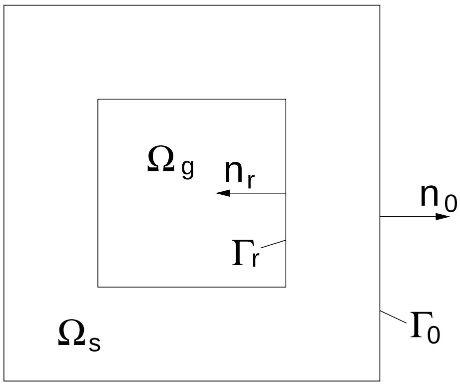


Figure 1: 2-dimensional section through an exemplary domain for nonlocal radiative heat transfer.

- Due to high temperatures: Radiative heat transfer between surfaces of cavities modelled by weakly singular integral operator.
- Control quantity with control constraints: Heat source field.

Symbols:

y: absolute temperature, ν: regularization parameter,

z: desired temperature gradient, q_{r}: radiative heat flux,

u: control (power density of heat sources), ε: emissivity,

$\kappa_{\mathrm{s}}, \kappa_{\mathrm{g}}$: thermal conductivities, y_0: external temperature,

σ: Stefan-Botzmann radiation constant.

$$
(\mathrm{P}) \quad \begin{cases}
\text{minimize} & J(y,u) := \dfrac{1}{2}\displaystyle\int_{\Omega_{\mathrm{g}}} |\nabla y - z|^2\, dx + \dfrac{\nu}{2}\displaystyle\int_{\Omega_{\mathrm{s}}} u^2\, dx \\
\text{subject to} & -\mathrm{div}(\kappa_{\mathrm{s}}\, \nabla y) = u \qquad \text{in } \Omega_{\mathrm{s}} \\
 & -\mathrm{div}(\kappa_{\mathrm{g}}\, \nabla y) = 0 \qquad \text{in } \Omega_{\mathrm{g}} \\
 & \kappa_{\mathrm{g}} \left.\dfrac{\partial y}{\partial n_r}\right|_{\mathrm{g}} - \kappa_{\mathrm{s}} \left.\dfrac{\partial y}{\partial n_r}\right|_{\mathrm{s}} = q_{\mathrm{r}} \qquad \text{on } \Gamma_{\mathrm{r}} \\
 & \kappa_{\mathrm{s}} \dfrac{\partial y}{\partial n_0} + \varepsilon\sigma\, |y|^3 y = \varepsilon\sigma\, y_0^4 \qquad \text{on } \Gamma_0 \\
\text{and} & u_a \le u(x) \le u_b \qquad \text{a.e. in } \Omega,
\end{cases}
$$

$$
q_{\mathrm{r}} = (I - K)(I - (1-\varepsilon)K)^{-1} \varepsilon\, \sigma |y|^3 y := G\, \sigma |y|^3 y,
$$

with weakly singular integral radiation operator K:

$$
(K\, y)(x) = \int_{\Gamma_{\mathrm{r}}} \omega(x, \tilde{x})\, y(\tilde{x})\, ds_{\tilde{x}}
$$

with a symmetric kernel ω (view factor):

$$
\omega(x,\tilde{x}) = \Xi(x,\tilde{x}) \frac{[n_{\mathrm{r}}(\tilde{x}) \cdot (x - \tilde{x})][n_{\mathrm{r}}(x) \cdot (\tilde{x} - x)]}{\pi |\tilde{x} - x|^4},
$$

$$
\Xi(x,\tilde{x}) = \begin{cases} 1 & \text{if } x, \tilde{x} \text{ are mutually visible,} \\ 0 & \text{otherwise.} \end{cases}
$$

Mathematical assumptions (A):

$\Omega \subset \mathbb{R}^3$, $\overline{\Omega} = \overline{\Omega}_\mathrm{s} \cup \overline{\Omega}_\mathrm{g}$, $\Omega_\mathrm{s} \cap \Omega_\mathrm{g} = \emptyset$, where each of the sets Ω, Ω_s, Ω_g, is nonvoid, bounded, open, and connected. The boundary Γ_0 of Ω is Lipschitz; the interface $\Gamma_\mathrm{r} = \overline{\Omega}_\mathrm{s} \cap \overline{\Omega}_\mathrm{g}$ is a closed Lipschitz surface that is piecewise $C^{1,\delta}$. Moreover, Γ_r is bounded away from Γ_0 (see Fig. 1).

$\sigma \in \mathbb{R}^+$, $\kappa \in L^\infty(\Omega)$, $\kappa|_{\Omega_\mathrm{s}} = \kappa_\mathrm{s}$, $\kappa|_{\Omega_\mathrm{g}} = \kappa_\mathrm{g}$, $\kappa \geq \kappa_\mathrm{min} > 0$ a.e. on Ω, $\varepsilon \in L^\infty(\Gamma_0 \cup \Gamma_\mathrm{r})$, $1 \geq \varepsilon \geq \varepsilon_\mathrm{min} > 0$ a.e. on $\Gamma_0 \cup \Gamma_\mathrm{r}$.

Semilinear state equation of (P), weak form:

$$\int_\Omega \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_\mathrm{r}} G(\sigma |y|^3 y) v \, ds + \int_{\Gamma_0} \varepsilon\sigma \, |y|^3 y \, v \, ds$$

$$= \int_{\Omega_\mathrm{s}} u \, v \, dx + \int_{\Gamma_0} \varepsilon\sigma \, y_0^4 v \, ds \qquad \forall \, v \in V, \tag{1}$$

$$V = \{v \in H^1(\Omega) \mid \tau_\mathrm{r} \, v \in L^5(\Gamma_\mathrm{r}) \, , \, \tau_0 \, v \in L^5(\Gamma_0)\}.$$

Theorem 1 [Existence (state), Laitinen, Tiihonen 2001]: For every $u \in H^1(\Omega_\mathrm{s})^*$ and $y_0 \in L^5(\Gamma_0)$, the semilinear equation (1) has a unique solution in V.

Theorem 2 [L^∞-bound, M., P., T. 2004]: If $u \in L^2(\Omega_\mathrm{s})$ and $y_0 \in L^16(\Gamma_0)$, then there exists a constant c only depending on Ω such that

$$\|y\|_{L^\infty(\Omega)} + \|y\|_{L^\infty(\Gamma_\mathrm{r} \cup \Gamma_0)} \leq c \, (1 + \|u\|_{L^2(\Omega_\mathrm{s})} + \|y_0\|_{L^4(\Gamma_0)}).$$

Theorem 3 [Minimum principle, M., P., T. 2004]: If $u(x) \geq 0$ a.e. in Ω_s and $y_0(x) \geq \vartheta > 0$ a.e. on Γ_0, then $y(x) \geq \vartheta$ a.e. on Ω and a.e. on $\Gamma_\mathrm{r} \cup \Gamma_0$.

Theorem 4 [Existence (optimal control), M., P., T. 2004]: If $y_0 \in L^{16}(\Gamma_0)$, and $y_0 \geq \vartheta > 0$, then there exists a solution $(\bar{u}, \bar{y}) \in L^\infty(\Omega_{\rm s}) \times V^\infty$ to (P).

Adjoint equation, weak form:

$$\int_\Omega \kappa \nabla p \cdot \nabla v \, dx \, + \, 4 \int_{\Gamma_{\rm r}} \sigma \, |\bar{y}|^3 \, G^*(p) \, v \, ds + 4 \int_{\Gamma_0} \varepsilon \sigma \, |\bar{y}|^3 \, p \, v \, ds$$

$$= \int_{\Omega_{\rm g}} (\nabla \bar{y} - z) \cdot \nabla v \, dx =: \langle w, v \rangle \quad \forall \, v \in H^1(\Omega). \tag{2}$$

Lax-Milgram: Ex. lin. cont. op. $B_\Omega : H^1(\Omega)^* \longrightarrow H^1(\Omega)$, $B_{\rm r} : L^2(\Gamma_r) \longrightarrow H^1(\Omega)$ such that

$$p = B_\Omega \, w + B_{\rm r} \, (-4 \, \sigma |\bar{y}|^3 \, G^*(\tau_{\rm r} p))$$

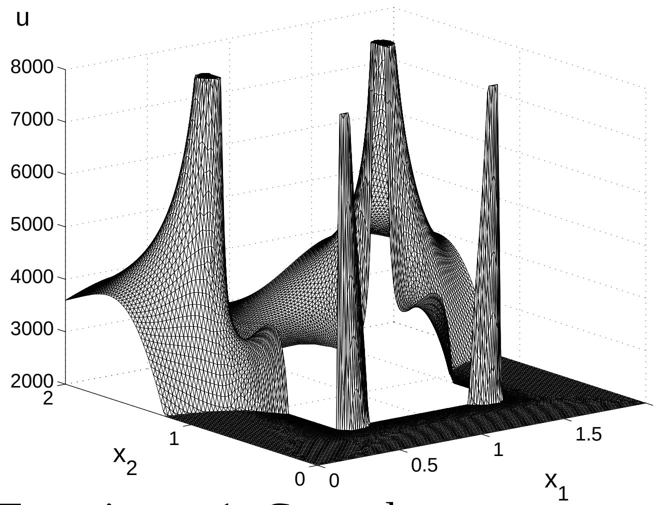
Theorem 5 [Existence (adjoint state), M., P., T. 2004]: If $\bar{y} \in V^\infty$, $\bar{y} \geq \vartheta > 0$, and $\lambda = 1$ is not an eigenvalue of $B(\bar{y})(\,\cdot\,) := -\tau_{\rm r} \, B_{\rm r}(4 \, \sigma |\bar{y}|^3 \, G^*(\,\cdot\,))$, $B(\bar{y}) : L^2(\Gamma_{\rm r}) \longrightarrow L^2(\Gamma_{\rm r})$, then to every $w \in H^1(\Omega)^*$, there exists a unique solution to (2) in $H^1(\Omega)$.

First order necessary optimality conditions:

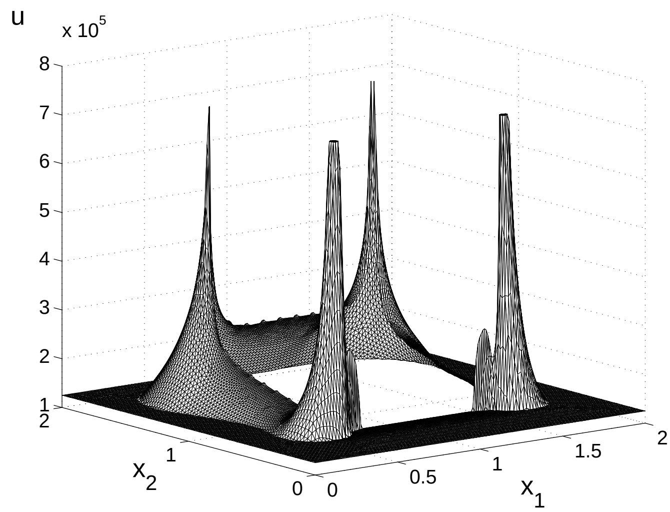
$$j'(\bar{u})(u - \bar{u}) = \int_{\Omega_{\rm s}} (u - \bar{u})(p + \nu \bar{u}) \, dx \geq 0 \quad \forall \, u \in U_{\rm ad},$$

$$\bar{u}(x) = \mathcal{P}_{[u_a, u_b]} \quad -\frac{1}{\nu} \, p(x) \quad .$$

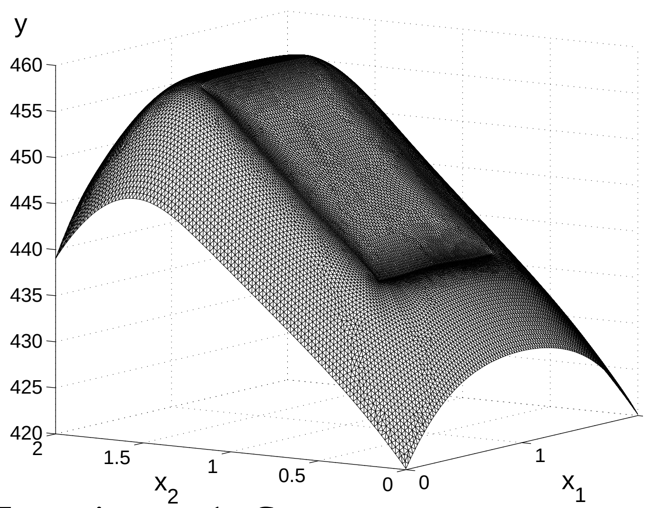
Numerical results for the simplified problem ($z = (0, 20)$):



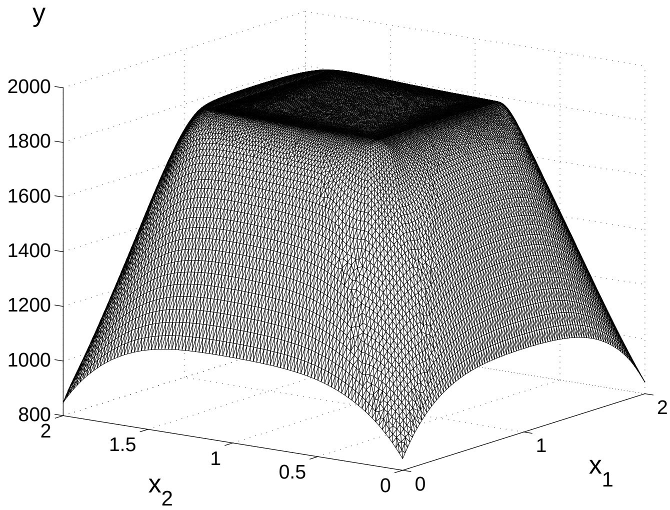
Experiment 1: Control u.



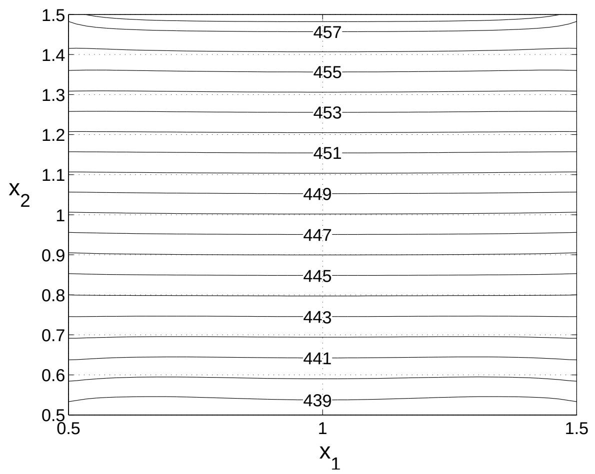
Experiment 2: Control u.



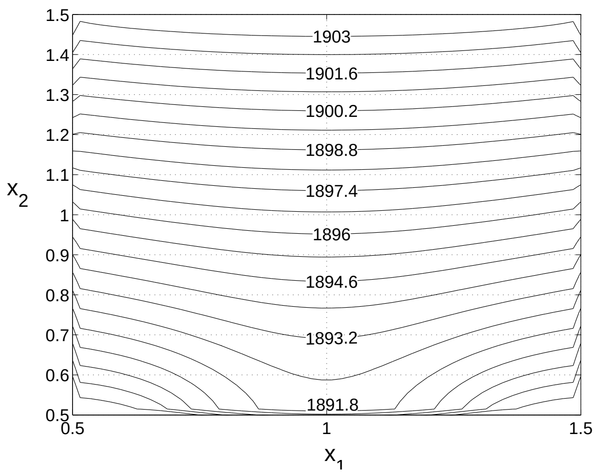
Experiment 1: State y.



Experiment 2: State y.



Experiment 1: Isotherms in Ω_{g}.

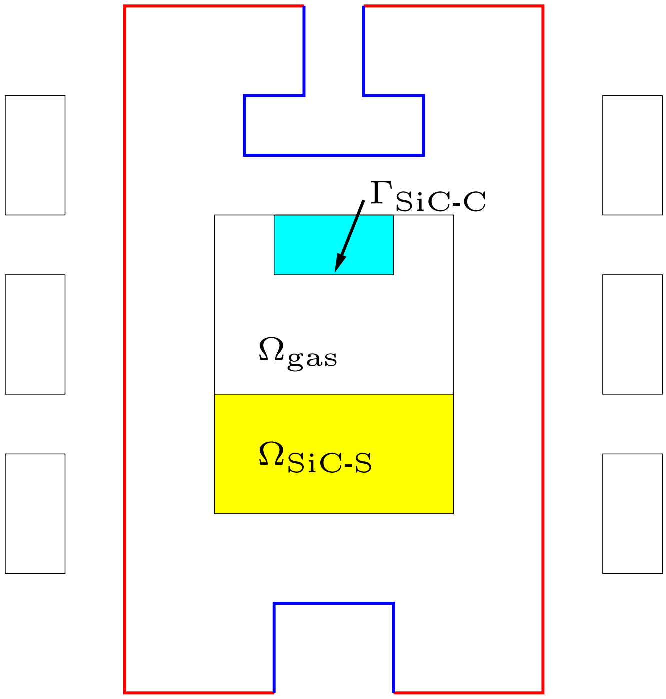


Experiment 2: Isotherms in Ω_{g}.

Experiment 1: Low temp: $u_a = 2\,\mathrm{k}$, $u_a = 8\,\mathrm{k}$, $\nu = 5 \cdot 10^{-7}$.

Experiment 2: High temp: $u_a = 125\,\mathrm{k}$, $u_a = 725\,\mathrm{k}$, $\nu = 3 \cdot 10^{-9}$.

A more complicated, realistic control problem for the temperature field: Numerical treatment



Known fact: Crystal surface forms along isotherms.

Goal: Radially constant isotherms during growth.

Control: $\displaystyle\int_{\Omega_{\text{gas}}} w(z) \left(\frac{\partial T}{\partial r}(r,z) \right)^2 \mathrm{d}(r,z) \longrightarrow \min.$

PDEs ($\mathbf{v}_{\text{gas}} = 0,\ f(x,T,P) = f(x,P)$):

$$-\operatorname{div}\ \kappa^{(\text{Ar})}(T)\,\nabla T = 0 \quad \text{in } \Omega_{\text{gas}},$$

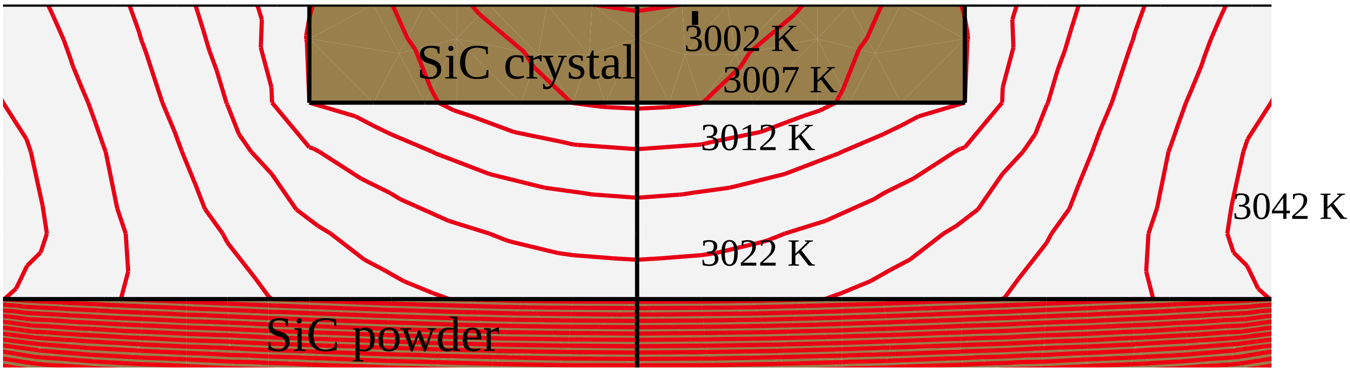
$$-\operatorname{div}\ \kappa(x,T)\,\nabla T = f(x,P) \quad \text{in } \Omega \setminus \Omega_{\text{gas}}.$$

Constraints:

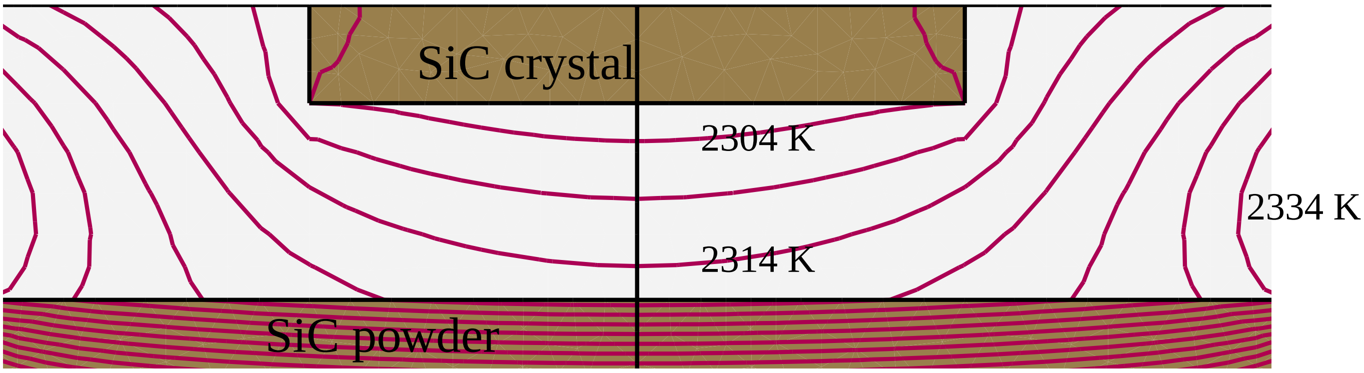
- $T_{\text{room}} \le T \le T_{\max}$ in Ω,
- $T_{\text{min,SiC-C}} \le T \le T_{\text{max,SiC-C}}$ on $\Gamma_{\text{SiC-C}}$ (need right polytype),
- $T\restriction_{\Omega_{\text{SiC-S}}} \ge T\restriction_{\Gamma_{\text{SiC-C}}} + \delta$, $\delta > 0$ (source temp. $\ge$ seed temp. $+\delta$),
- $0 \le P \le P_{\max}$ (bounds for heating power P (control parameter)).

Numerical results: Optimization of temperature field

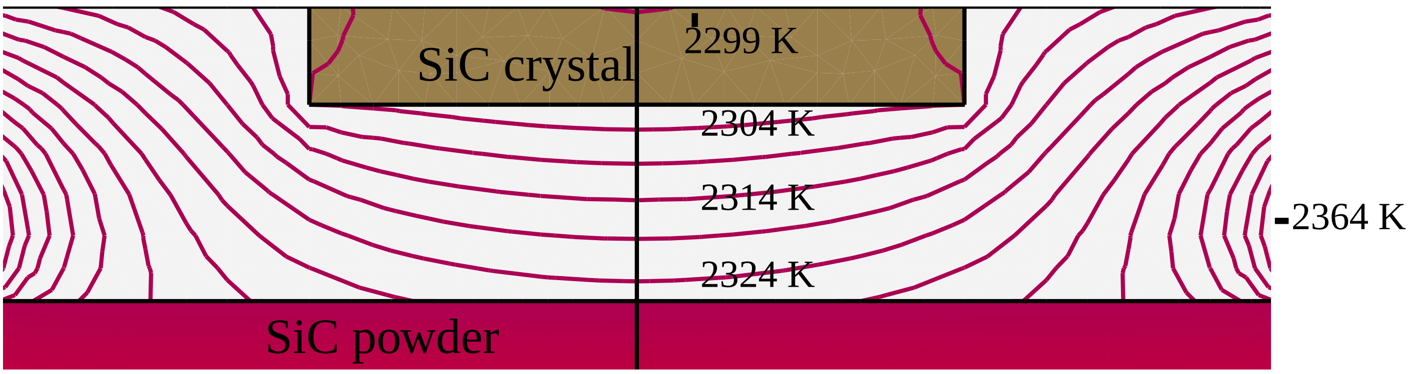
(a): $T(P = 10.0\ \mathrm{kW}, z_{\mathrm{rim}} = 24.0\ \mathrm{cm}, f = 10.0\ \mathrm{kHz})$



(b): $T(P = 7.98\ \mathrm{kW}, z_{\mathrm{rim}} = 22.7\ \mathrm{cm}, f = 165\ \mathrm{kHz})$
Nelder-Mead res. for $\mathcal{F}_{r,2}(T)$



(c): $T(P = 10.3\ \mathrm{kW}, z_{\mathrm{rim}} = 12.9\ \mathrm{cm}, f = 84.9\ \mathrm{kHz})$,
Nelder-Mead res. for $\frac{\mathcal{F}_{r,2}(T) - \mathcal{F}_{z,2}(T)}{2}$



Selected Publications

- C. Meyer, P. Philip, F. Tröltzsch: *Optimal Control of a Semilinear PDE with Nonlocal Radiation Interface Conditions.* In preparation.
- C. Meyer, P. Philip: *Optimizing the temperature profile during sublimation growth of SiC single crystals: Control of heating power, frequency, and coil position.* Preprint No. 895 of the Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin, 2003. Submitted.
- O. Klein, P. Philip, J. Sprekels: *Modeling and simulation of sublimation growth of SiC bulk single crystals*, Interfaces and Free Boundaries 6 (2004), 295–314.

More Publications / Information:

`http://www.ima.umn.edu/~philip/sic/#Publications`

`http://www.ima.umn.edu/~philip/sic/`

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