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Numerical Simulation and Control of Sublimation Growth of SiC Bulk Single Crystals: Modeling, Finite Volume Method, Analysis and Results

Peter Philip

Show & Tell at IMA

Minneapolis, September 15, 2004

Joint work with:

- Jürgen Geiser, Olaf Klein, Jürgen Sprekels, Krzysztof Wilmański
  (Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin) (modeling, finite volume method)
- Christian Meyer, Fredi Tröltzsch
  (TU Berlin, Department of Mathematics) (optimal control)

Cooperation with:

- Klaus Böttcher, Detev Schulz, Dietmar Siche
  (Institute of Crystal Growth (IKZ), Berlin) (growth experiments)

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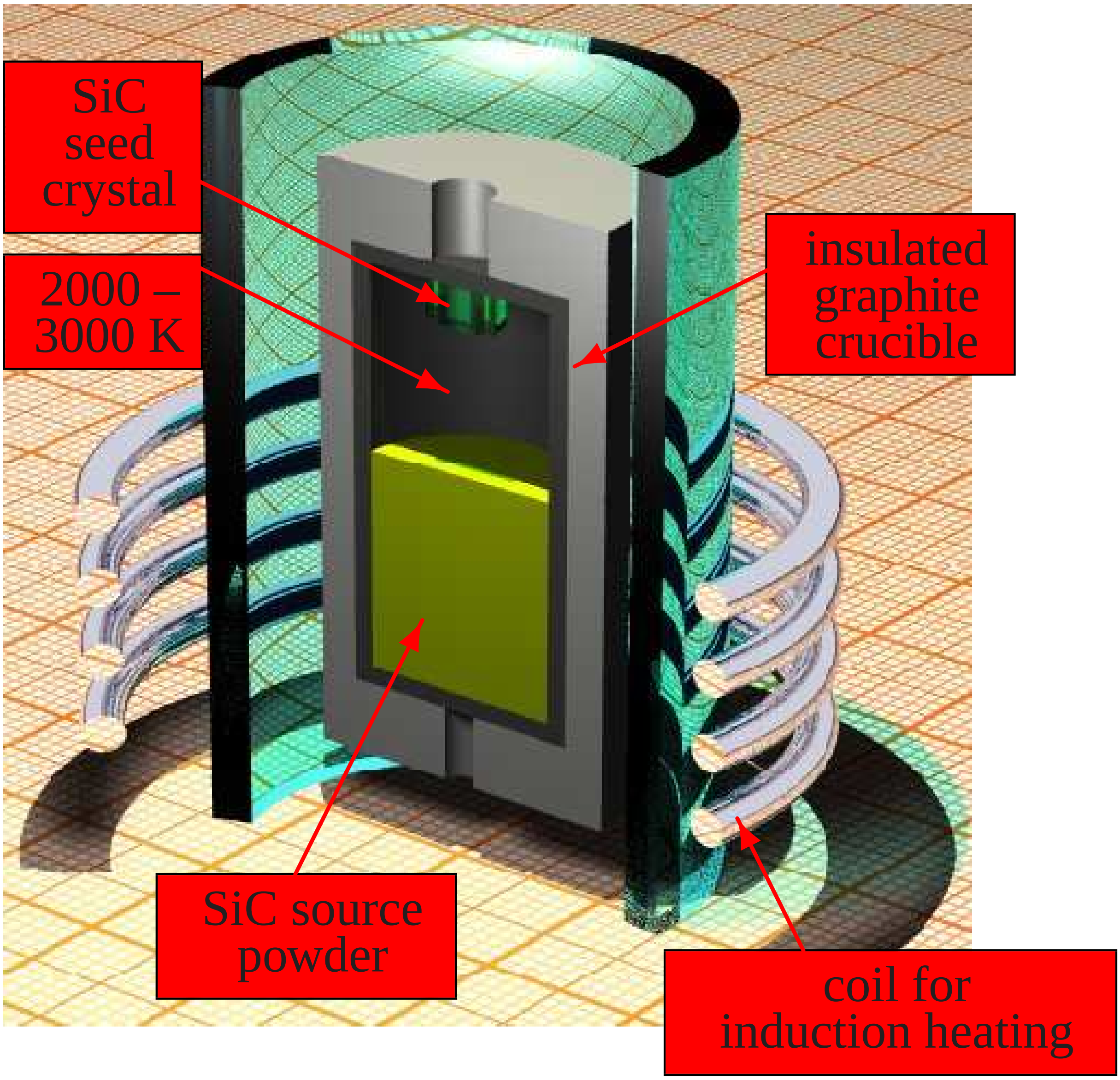
SiC growth by physical vapor transport (PVT)



- 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, $\ldots$ is created
- an SiC single crystal grows on a cooled seed

Goal:

Stationary and transient optimal control of process, using mathematical modeling, numerical simulation.

Heat Transport Model

Nonlinear heat conduction in material j:

$$\frac{\partial \varepsilon_j}{\partial t} + \operatorname{div} \mathbf{q}_j = f_j, \qquad \mathbf{q}_j = -\kappa_j \nabla T,$$

ε_j: internal energy, T: absolute temperature,

$\mathbf{q}_j$: heat flux, κ_j: thermal conductivity,

f_j: power density of heat sources (induction heating).

Interface Conditions

Continuity of the heat flux:

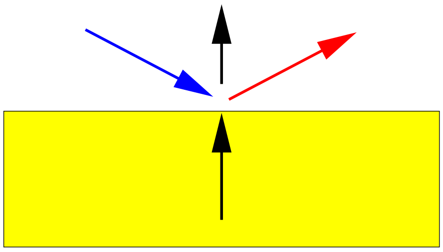
Between solids: $\mathbf{q}_{j_1} \bullet \mathbf{n}_{j_1} = \mathbf{q}_{j_2} \bullet \mathbf{n}_{j_1}$ on γ_{j_1,j_2}.

Between gas and solid j:

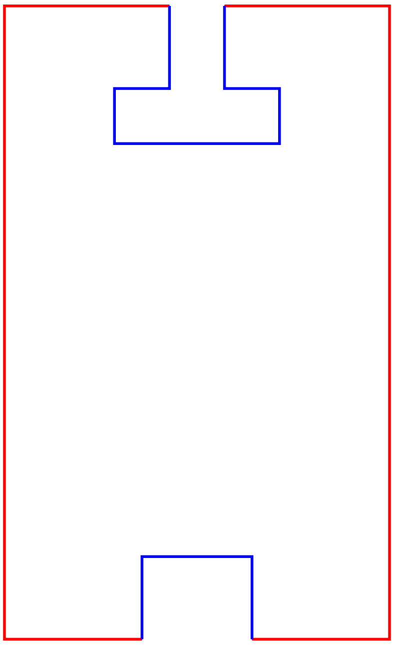
$$\mathbf{q}_{\mathrm{gas}} \bullet \mathbf{n}_{\mathrm{gas}} - R + J = \mathbf{q}_j \bullet \mathbf{n}_{\mathrm{gas}} \text{ on } \gamma_{j,\mathrm{gas}},$$

$\mathbf{n}_j$, $\mathbf{n}_{\mathrm{gas}}$: outer unit normal, R: radiosity, J: irradiation.

Continuity of temperature throughout apparatus.



Outer Boundary Conditions



Emission according to Stefan-Boltzmann law:

$$-\left(\kappa_j \nabla T\right) \bullet \mathbf{n}_j = \sigma \epsilon_j(T)\left(T^4 - T_{\text{room}}^4\right),$$

ϵ_j: emissivity, $T_{\text{room}} = 293$ K.

On surfaces of open cavities:

$$\mathbf{q}_j \bullet \mathbf{n}_j - R + J = 0.$$

Finite Volume Scheme

General theory for finite volume methods for systems of nonlinear evolution equations in space-time domains $\Omega \times [0, t_{\rm f}]$, $\Omega = \bigcup_{j=1}^{N} \Omega_j$, with disjoint polytopes (bounded polyhedral sets) Ω_j. Type and/or form of the PDEs may vary from subdomain to subdomain. Typical form:

$$\partial_t b_j(u_j, x, t) + \nabla \bullet \mathbf{v}_j(u_j, x, t) - \nabla \bullet (k_j(u_j, x, t) \nabla u_j) = f_j(u_j, x, t).$$

The unknown functions u_j on Ω_j are connected by interface conditions between adjacent subdomains.

Typical example: $u_j = T_j =$ temperature on the subdomain Ω_j (gas, different solid components of the growth apparatus).

Possible interface conditions between $\Omega_{j_1}, \Omega_{j_2}$:

- $u_{j_1} = u_{j_2}$ (continuity)
- $-k_{j_1}(u_{j_1}, x, t) \nabla u_{j_1} \bullet \mathbf{n}_{p_{j_1}} = \xi_{\{j_1, j_2\}} \cdot (u_{j_1} - u_{j_2})$, $\xi_{\{j_1, j_2\}} > 0$ (jump condition)
- $k_{j_2}(u_{j_2}, x, t) \nabla u_{j_2} \bullet \mathbf{n}_{p_{j_2}} - k_{j_1}(u_{j_1}, x, t) \nabla u_{j_1} \bullet \mathbf{n}_{p_{j_1}} = \mathcal{A}_\gamma(u_1, \ldots, u_N)(x)$ (nonlocal operator; typically: radiation)

Outer boundary conditions (on $\partial\Omega$):

Dirichlet, Neumann, Robin, emission, nonlocal radiation.

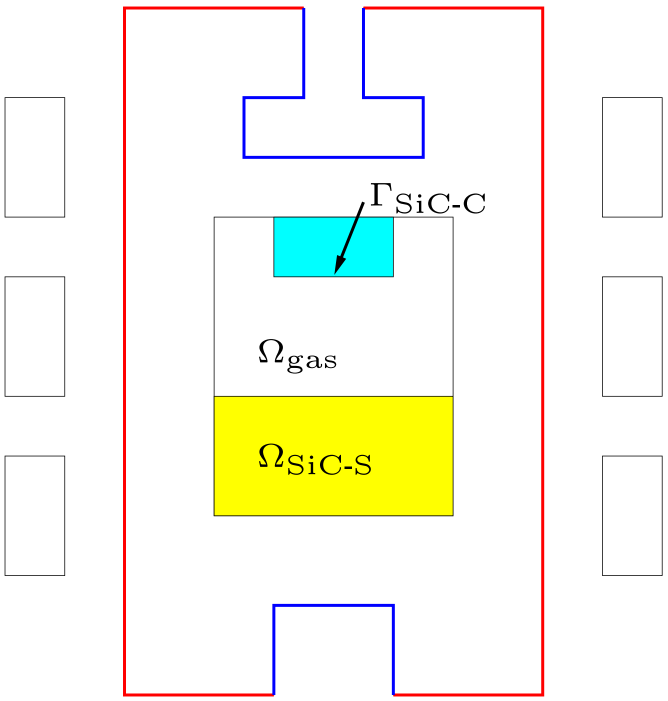
Discrete Existence Result:

Assume that:

- $b_j \geq 0, \quad b_j(\cdot, x, t) \nearrow, \quad b_j(0, x, \cdot) \searrow;$
  $\exists\, L > 0: \quad |b_j(u, x, t) - b_j(\tilde{u}, x, t)| \geq L|u - \tilde{u}| \quad \forall j.$
- $f_j(\cdot, x, t)$ locally Lipschitz; $f_j(0, x, t) \geq 0.$
- $k_j(\cdot, x, t)$ locally Lipschitz; $k_j \geq 0.$
- Functions in interface and boundary conditions are locally Lipschitz and have the "right" monotonicity properties (valid for heat conduction).
- $\mathbf{v}(u, x, t) = v_1(u, x, t) \cdot \mathbf{v}_2(x, t)$, where $v_1(0, x, t) = 0, \quad v_1(\cdot, x, t) \nearrow, \quad v_1$ is locally Lipschitz and bounded from below.
- The discretization of nonlocal operators satisfies a technical condition (satisfied for suitable discretization of radiation operators).

Then the finite volume discretization has a unique solution in $[0, M]^n$, provided that the time step is sufficiently small (n: number of discrete unknowns, M: independent of time discretization).

Stationary optimal control problem for the temperature field



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

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

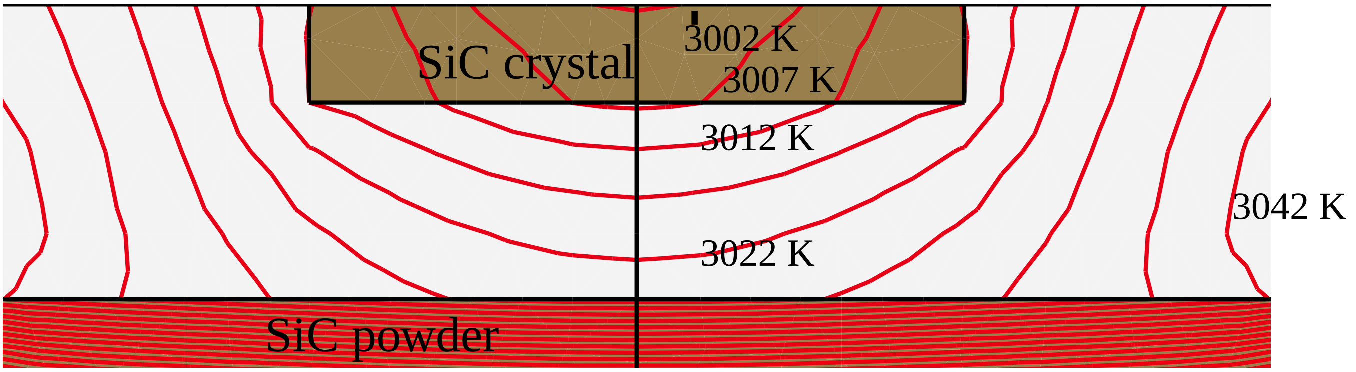
$$-\operatorname{div}\left(\kappa(x,T)\,\nabla T\right) = f(x,P) \quad \text{in } \Omega \setminus \Omega_{\text{gas}}.$$

Constraints:

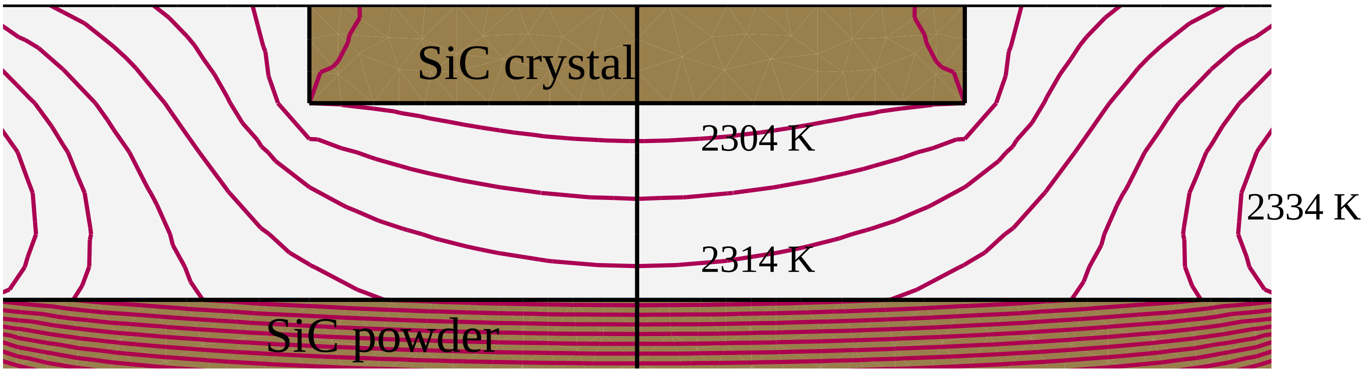
- $T_{\text{room}} \le T \le T_{\max}$ in Ω,
- $T_{\min,\text{SiC-C}} \le T \le T_{\max,\text{SiC-C}}$ on $\Gamma_{\text{SiC-C}}$ (need right polytype),
- $T{\restriction}_{\Omega_{\text{SiC-S}}} \ge T{\restriction}_{\Gamma_{\text{SiC-C}}} + \delta, \quad \delta > 0$ (source temp. $\ge$ seed temp. $+\delta$),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

Numerical results: Optimization of temperature field

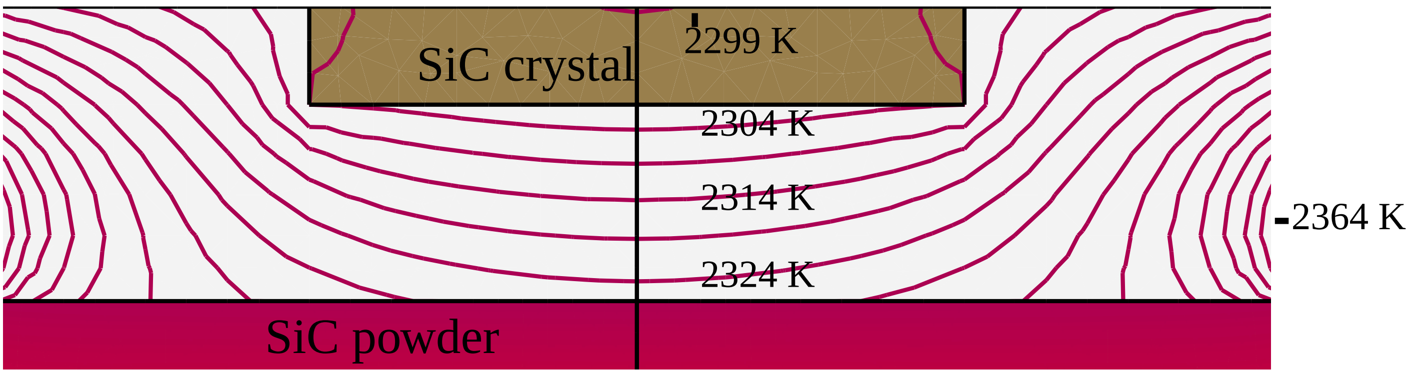
(a): $T(P = 10.0\ \mathrm{kW}, z_{\mathrm{rim}} = 24.0\ \mathrm{cm}, f = 10.0\ \mathrm{kHz})$



(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

- O. KLEIN, P. PHILIP: *Transient conductive-radiative heat transfer: Discrete existence and uniqueness for a finite volume scheme*, accepted for publication in Mathematical Models and Methods in Applied Sciences.

- 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.

- P. PHILIP: *Transient Numerical Simulation of Sublimation Growth of SiC Bulk Single Crystals. Modeling, Finite Volume Method, Results.* Humboldt University of Berlin, 2003. Report No. 22, Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin.

More Publications / Information:

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

`http://www.ima.umn.edu/˜philip/sic/`

- Extended 1-hour talk tomorrow,
  Applied Mathematics and Numerical Analysis
  Seminar, School of Mathematics
  Thu, Sep 16, 11:15 a.m., Vincent Hall 570.