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

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Show & Tell at IMA
Minneapolis, September 15, 2004
Joint work with:

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  (Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin) (modeling, finite volume method)

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Cooperation with:

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

Supported by:


- German Ministry for Education and Research (BMBF) (1997 – 2002)
SiC growth by physical vapor transport (PVT)

- polycrystalline SiC powder sublimes inside induction-heated graphite crucible at 2000 – 3000 K and \( \approx 20 \text{ hPa} \)

- a gas mixture consisting of Ar (inert gas), Si, SiC\(_2\), Si\(_2\)C, \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 $j$:

$$\frac{\partial \varepsilon_j}{\partial t} + \text{div} \, q_j = f_j, \quad q_j = -\kappa_j \nabla T,$$

$\varepsilon_j$: internal energy, $T$: absolute temperature,
$q_j$: heat flux, $\kappa_j$: thermal conductivity,
$f_j$: power density of heat sources (induction heating).

Interface Conditions

Continuity of the heat flux:

Between solids: $q_{j1} \cdot n_{j1} = q_{j2} \cdot n_{j1}$ on $\gamma_{j1,j2}$.

Between gas and solid $j$:

$$q_{\text{gas}} \cdot n_{\text{gas}} - R + J = q_j \cdot n_{\text{gas}} \text{ on } \gamma_{j,\text{gas}},$$

$n_j, n_{\text{gas}}$: outer unit normal, $R$: radiosity, $J$: irradiation.

Continuity of temperature throughout apparatus.
Outer Boundary Conditions

Emission according to Stefan-Boltzmann law:

\[-(\kappa_j \nabla T) \cdot n_j = \sigma \epsilon_j(T) \left( T^4 - T_{\text{room}}^4 \right),\]

\(\epsilon_j\): emissivity, \(T_{\text{room}} = 293\) K.

On surfaces of open cavities:

\[q_j \cdot n_j - R + J = 0.\]
Finite Volume Scheme

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

$$
\partial_t b_j(u_j, x, t) + \nabla \cdot v_j(u_j, x, t) - \nabla \cdot (k_j(u_j, x, t) \nabla u_j) = f_j(u_j, x, t).
$$

The unknown functions $u_j$ on $\Omega_j$ are connected by interface conditions between adjacent subdomains.

Typical example: $u_j = T_j = \text{temperature on the subdomain } \Omega_j$ (gas, different solid components of the growth apparatus).

Possible interface conditions between $\Omega_{j1}, \Omega_{j2}$:

- $u_{j1} = u_{j2}$ (continuity)
- $-k_{j1}(u_{j1}, x, t) \nabla u_{j1} \cdot n_{pj1} = \xi_{\{j1, j2\}} \cdot (u_{j1} - u_{j2})$, $\xi_{\{j1, j2\}} > 0$ (jump condition)
- $k_{j2}(u_{j2}, x, t) \nabla u_{j2} \cdot n_{pj2} - k_{j1}(u_{j1}, x, t) \nabla u_{j1} \cdot n_{pj1} = A_\gamma(u_1, \ldots, u_N)(x)$ (nonlocal operator; typically: radiation)
Outer boundary conditions (on $\partial \Omega$):

Dirichlet, Neumann, Robin, emission, nonlocal radiation.

Discrete Existence Result:

Assume that:

- $b_j \geq 0$, $b_j(\cdot, x, t) \nearrow$, $b_j(0, x, \cdot) \searrow$;
  $\exists L > 0 : |b_j(u, x, t) - b_j(\tilde{u}, x, t)| \geq L|u - \tilde{u}| \ \forall j$.

- $f_j(\cdot, x, t)$ 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).

- $v(u, x, t) = v_1(u, x, t) \cdot v_2(x, t)$, where $v_1(0, x, t) = 0$, $v_1(\cdot, x, t) \nearrow$, $v_1$ 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:
\[
\int_{\Omega_{\text{gas}}} w(z) \left( \frac{\partial T}{\partial r}(r, z) \right)^2 \, d(r, z) \rightarrow \min.
\]

PDEs \((v_{\text{gas}} = 0, \quad f(x, T, P) = f(x, P))\):
\[
- \text{div} \, \kappa^{(\text{Ar})}(T) \nabla T = 0 \quad \text{in } \Omega_{\text{gas}},
\]
\[
- \text{div} \, \kappa(x, T) \nabla T = f(x, P) \quad \text{in } \Omega \setminus \Omega_{\text{gas}}.
\]

Constraints:
- \(T_{\text{room}} \leq T \leq T_{\text{max}}\) in \(\Omega\),
- \(T_{\text{min, SiC-C}} \leq T \leq T_{\text{max, SiC-C}}\) on \(\Gamma_{\text{SiC-C}}\) (need right polytype),
- \(T|_{\Omega_{\text{SiC-S}}} \geq T|_{\Gamma_{\text{SiC-C}}} + \delta, \quad \delta > 0\) (source temp. \(\geq\) seed temp. \(+\delta\)),
- \(0 \leq P \leq P_{\text{max}}\) (bounds for heating power \(P\) (control parameter)).
Numerical results: Optimization of temperature field

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

(b): $T(P = 7.98 \text{ kW}, z_{\text{rim}} = 22.7 \text{ cm}, f = 165 \text{ kHz})$

Nelder-Mead res. for $\mathcal{F}_{r,2}(T)$

(c): $T(P = 10.3 \text{ kW}, z_{\text{rim}} = 12.9 \text{ cm}, f = 84.9 \text{ kHz})$

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.


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.