Project C9

Numerical simulation and control of sublimation growth of semiconductor bulk single crystals

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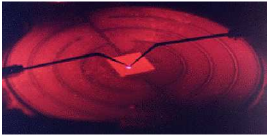
Mathematics for key technologies

Applications of Semiconductor Crystals

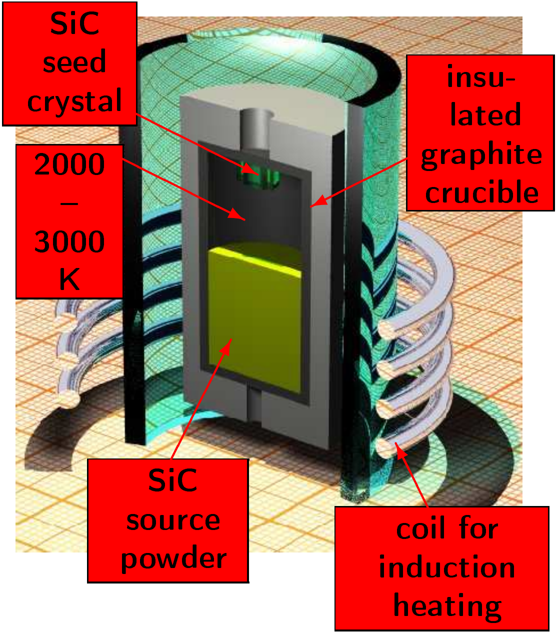
Light-emitting diodes:
Lifetime: $\approx$ 10 years
Light extraction efficiency $>$ 32 %
(light bulb: $\approx$ 10 %)

Blue laser:
Its use in DVD players admits up to 10-fold capacity of disc

SiC-based electronics still works at 600 C; SiC sensors placed close to car engines save resources and costs



Physical Vapor Transport Method



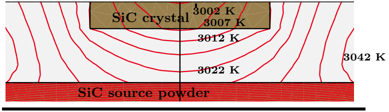
- polycrystalline SiC powder sublimates inside induction-heated graphite crucible at 2000 – 3000 K and $\approx$ 20 hPa
- a gas mixture consisting of Ar (inert gas), Si, SiC_2, Si_2C, … is created
- an SiC single crystal grows on a cooled seed

Computes and optimizes temperature and magnetic fields in axisymmetric apparatus.

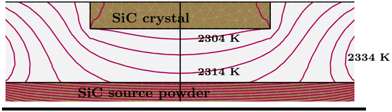
- Computation of temp T accounts for anisotropic conduction [Geiser, Klein, Philip, 2006/7], radiation, and electromagnetic heating.
- Numerical optimization of T field in growth apparatus:
  - Small radial T gradient on crystal surface avoids defects.
  - Large vertical T gradient between source and crystal increases growth rate.
  - State constraints: Need prescribed T range on seed, source, and apparatus.

Numerical Results:
Optimization of Temperature Field

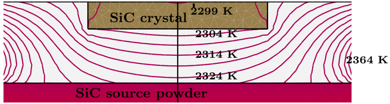
(a): Generic (Unoptimized) Temperature Field



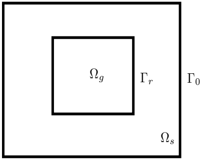
(b): Minimized Radial Gradient on Crystal Surface



(c): Minimized Radial Gradient on Crystal Surface & Maximized Vertical Gradient Between Source and Seed



- A fairly simplified model for the seeded sublimation growth geometry:



- Optimization of the gradient temperature ∇y in the gas phase Ω_g by controlling the heat source u in the solid phase Ω_s:

$$(P) \qquad \text{minimize } J(u,y) := \frac{1}{2}\int_{\Omega_g} |\nabla y - y_d|^2 \; dx + \frac{\beta}{2}\int_{\Omega_s} u^2 \; dx.$$

- The temperature distribution y is given by the solution of the stationary heat equation:

$$(SL) \quad \begin{cases} -\mathrm{div}(\kappa_s \nabla y) = u & \text{in } \Omega_s \\ -\mathrm{div}(\kappa_g \nabla y) = 0 & \text{in } \Omega_g \\ \kappa_g (\frac{\partial y}{\partial n_r})_g - \kappa_s (\frac{\partial y}{\partial n_r})_s = G\sigma\, |y|^3 y & \text{on } \Gamma_r \\ \kappa_s \frac{\partial y}{\partial n_0} + \varepsilon\sigma\, |y|^3 y = \varepsilon\sigma\, y_0^4 & \text{on } \Gamma_0. \end{cases}$$

- We impose inequality state constraints to avoid melting in Ω_s and to ensure sublimation in Ω_g:

$$\begin{array}{rcccll} & & y(x) & \leq & y_m(x) & \text{a.e. in } \Omega_s, \\ y_a(x) & \leq & y(x) & \leq & y_b(x) & \text{a.e. in } \Omega_g. \end{array}$$

- Additionally, we consider the following control-constraints:

$$u_a(x) \leq u(x) \leq u_b(x) \text{ a.e. in } \Omega_s$$

where u_a and u_b reflect the minimum and maximum heating power.

Theorem (C. Meyer, J. Rehberg and I. Yousept, 2007)

For every $u \in L^2(\Omega_s)$, the state equation (SL) admits a unique solution $y = y(u) \in H^1(\Omega) \cap C(\overline{\Omega})$ and there exists a constant $c > 0$ independent of u such that

$$\|y\|_{H^1(\Omega)} + \|y\|_{C(\overline{\Omega})} \leq c\,\left(1 + \|u\|_{L^2(\Omega_s)} + \|u\|^4_{L^2(\Omega_s)}\right).$$

- Based on the continuity of y, we established first-order necessary and second-order sufficient conditions for (P).
- Lagrange multipliers associated to the pointwise state constraints of (P) are in general Borel measures $\Rightarrow$ Regularization is necessary.
- Utilizing a "Moreau-Yosida" type regularization to the optimal control problem (P):

$$(P_\gamma)\begin{cases} \min\limits_{u\in L^2(\Omega_s)} f(u) := J(u,y(u)) + \frac{\gamma}{2}(\|\max(0,y(u)-y_b)\|^2_{L^2(\Omega_g)} \\ \qquad\qquad\qquad + \|\max(0,y_a-y(u))\|^2_{L^2(\Omega_g)} + \|\max(0,y(u)-y_m)\|^2_{L^2(\Omega_s)}), \\ \text{subject to} \qquad u_a(x)\le u(x)\le u_b(x) \text{ a.e. in } \Omega_s. \end{cases}$$

Theorem (C. Meyer and I. Yousept, 2007)

Let $\bar{u}$ be a local solution of (P) satisfying the second-order optimality conditions. Then, there exists a sequence $(u_\gamma)_{\gamma>0}$ of local solutions to (P_γ) converging strongly in $L^2(\Omega_s)$to $\bar{u}$ as $\gamma\to\infty$.

Numerical result

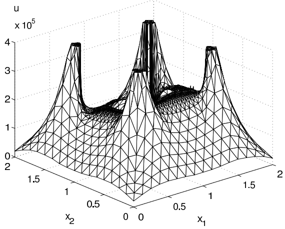


Figure: Control u_h

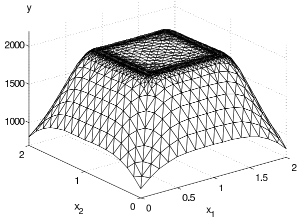


Figure: State y_h

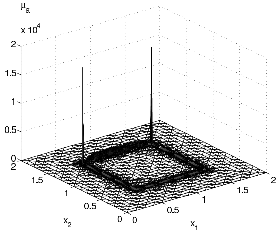


Figure: Lagrange multiplier μ_h^a

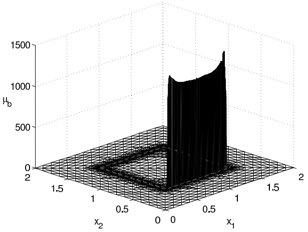


Figure: Lagrange multiplier μ_h^b

Further research

- Including Maxwell's equations in the model analysis.
- Study of optimal control of induction heating based on the Maxwell's equations: First- and second-order optimality conditions, numerical analysis and numerical simulation.

- M. Hintermüller, F. Tröltzsch, I. Yousept: *Mesh-independence of semismooth Newton methods for Lavrentiev-regularized state constrained nonlinear optimal control problems*, submitted.
- F. Tröltzsch, I. Yousept: *Lavrentiev type regularization for optimal boundary control problems with pointwise state constraints*, submitted.
- 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*, submitted.
- J. Rehberg, C. Meyer, I. Yousept: *State-constrained optimal control of semilinear elliptic equations with nonlocal radiation interface conditions*, submitted.
- J. Geiser, O. Klein, P. Philip: *Transient numerical study of temperature gradients during sublimation growth of SiC: Dependence on apparatus design*, J. Crystal Growth 297 (2006), 20 – 32.

- J. Geiser, O. Klein, P. Philip: *Numerical simulation of temperature fields during the sublimation growth of SiC single crystals, using WIAS-HiTNIHS*, J. Crystal Growth 303 (2007), 352 – 356.
- C. Meyer, I. Yousept: *Optimal control of temperature distribution in seeded sublimation growth processes of semiconductor single crystal*, submitted.
- F. Tröltzsch, I. Yousept: *A regularization method for the numerical solution of elliptic boundary control problems with pointwise state constraints*, Comp. Opt. Appl. 2007 (in press).
- 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*, Crystal Growth & Design 6 (2006), 2021 – 2028.
- C. Meyer, P. Philip, F. Tröltzsch: *Optimal Control of a Semilinear PDE with Nonlocal Radiation Interface Conditions*, SICON 45 (2006), 699 – 721.
- C. Meyer, P. Philip: *Optimizing the temperature profile during sublimation growth of SiC single crystals: Control of heating power, frequency, and coil position*, Crystal Growth & Design 5 (2005), 1145 – 1156.