Project C9

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

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Mathematics for key technologies

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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\(_2\)C, ... 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:

\[ \Omega_g \quad \Gamma_r \quad \Gamma_0 \quad \Omega_s \]

Optimization of the gradient temperature \( \nabla y \) in the gas phase \( \Omega_g \) by controlling the heat source \( u \) in the solid phase \( \Omega_s \):

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

The temperature distribution \( y \) is given by the solution of the stationary heat equation:

\[
(SL) \quad \begin{cases} 
-\text{div}(\kappa_s \nabla y) = u & \text{in } \Omega_s \\
-\text{div}(\kappa_g \nabla y) = 0 & \text{in } \Omega_g \\
\kappa_g \left( \frac{\partial y}{\partial n_r} \right)_g - \kappa_s \left( \frac{\partial y}{\partial n_r} \right)_s = G\sigma |y|^3 y & \text{on } \Gamma_r \\
\kappa_s \frac{\partial y}{\partial n_0} + \varepsilon\sigma |y|^3 y = \varepsilon\sigma y_0^4 & \text{on } \Gamma_0.
\end{cases}
\]
We impose inequality state constraints to avoid melting in $\Omega_s$ and to ensure sublimation in $\Omega_g$:

$$y(x) \leq y_m(x) \quad \text{a.e. in } \Omega_s,$$

$$y_a(x) \leq y(x) \leq y_b(x) \quad \text{a.e. in } \Omega_g.$$

Additionally, we consider the following control-constraints:

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

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

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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

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

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

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

Let $\tilde{u}$ 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 $(P_{\gamma})$ converging strongly in $L^2(\Omega_s)$ to $\tilde{u}$ as $\gamma \to \infty$. 
Numerical result

**Figure:** Control $u_h$

**Figure:** State $y_h$

**Figure:** Lagrange multiplier $\mu_h^a$

**Figure:** Lagrange multiplier $\mu_h^b$
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.


Selected Publications


