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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:

- 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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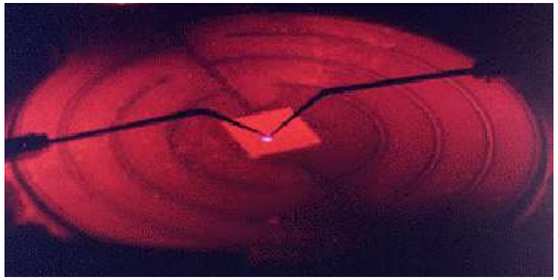
Applications of SiC bulk single crystals

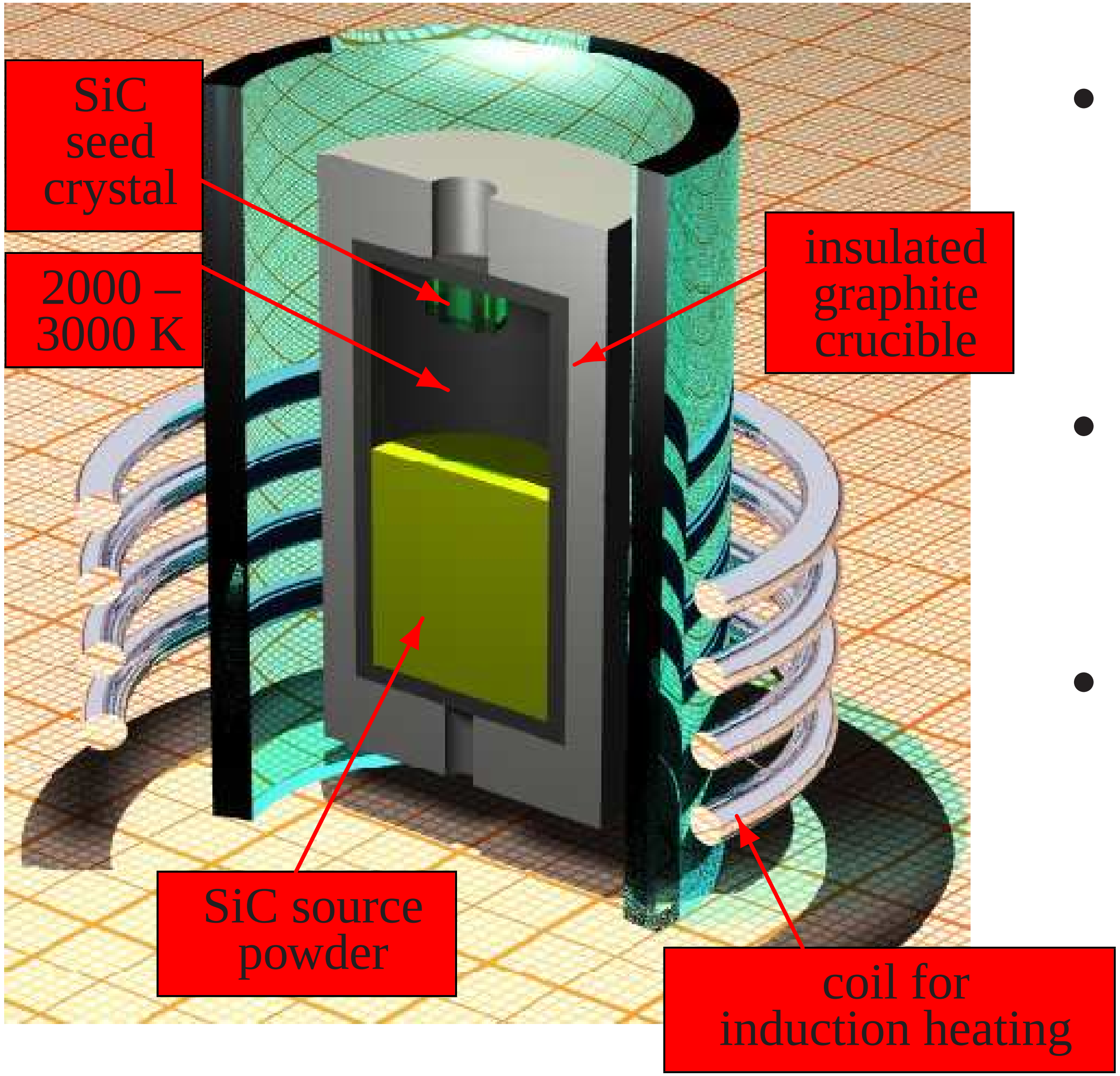
Light-emitting diodes:
Lifetime: $\approx$ 10 years
Light extraction efficiency $>$ 32 %
(light bulb: $\approx$ 10 %)

Blue laser:
Its application in the DVD player admits up to 10-fold capacity of disc

SiC-based electronics still works at 600 deg. Celsius,
SiC sensors placed close to car engines can save resources and costs



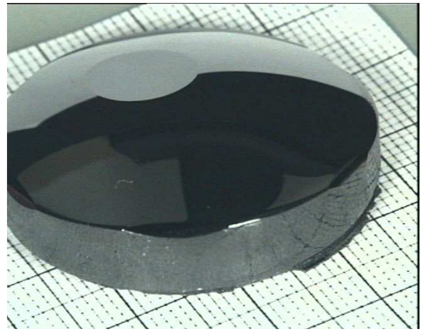
SiC growth by physical vapor transport (PVT)



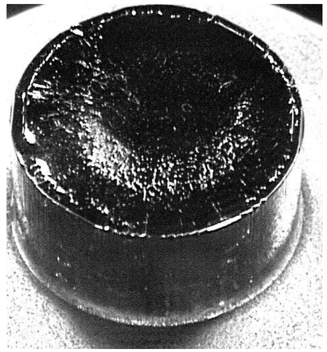
- polycrystalline SiC powder sublimates inside induction-heated graphite crucible at 2000 – 3000 K and ≈ 20 hPa
- a gas mixture consisting of Ar (inert gas), Si, SiC_2, Si_2C, . . . is created
- an SiC single crystal grows on a cooled seed

Problems:

- Needed: Perfect single crystals as large and as quick as possible (currently: $\varnothing$ 5 – 10 cm, one growth run: 2 – 3 days)



- High energy costs, high costs for apparatus replacement (every 10 runs)
- Wrong control parameters (setup, position of induction coil, heating power) $\Rightarrow$ (costly !) failure of growth run



- High temperatures prevent measurements inside growth apparatus $\Rightarrow$ experimental optimization of process is difficult and costly

Goal:

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

Model includes

1. Heat conduction in gas, graphite, powder, crystal
2. Radiative heat transfer between cavity surfaces (nonlocal integral operators)
3. Semi-transparency of crystal (band model)
4. Induction heating (Maxwell's equations)
5. Mass transport in gas, powder, graphite (Euler equations, porous media equations, . . .)
6. Chemical reactions in gas (reaction-diffusion equations)
7. Crystal growth, sublimation of source powder, decomposition of graphite walls (multiple free boundaries)

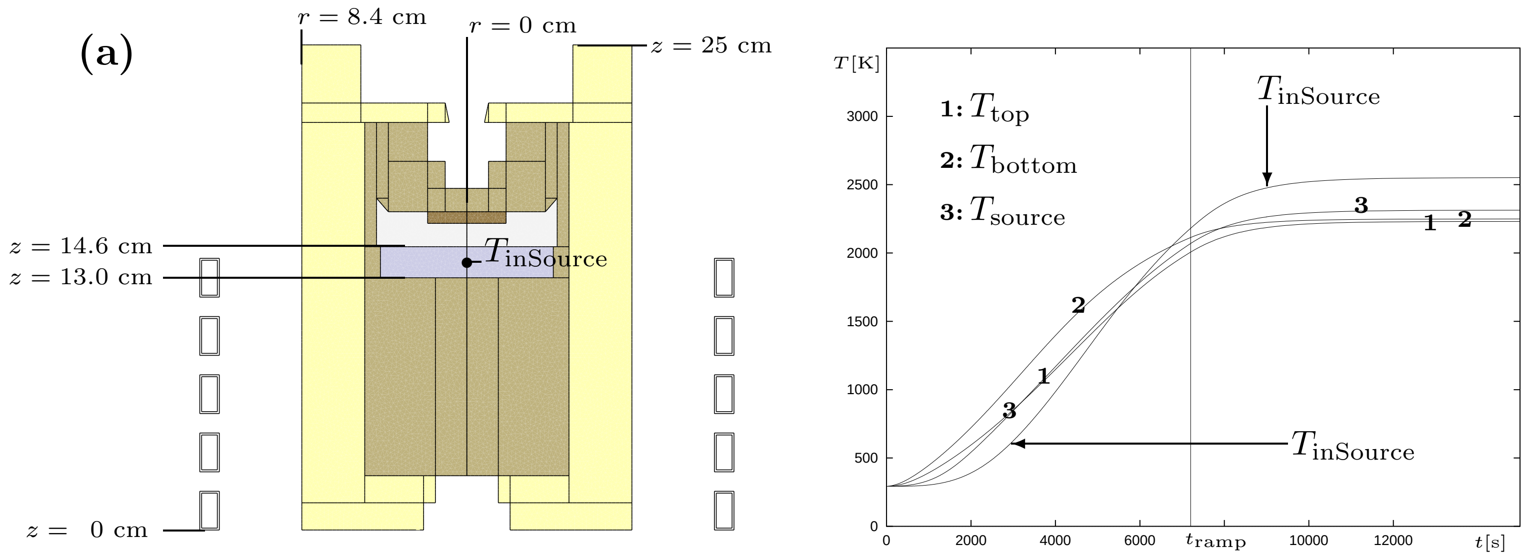
Mathematical results

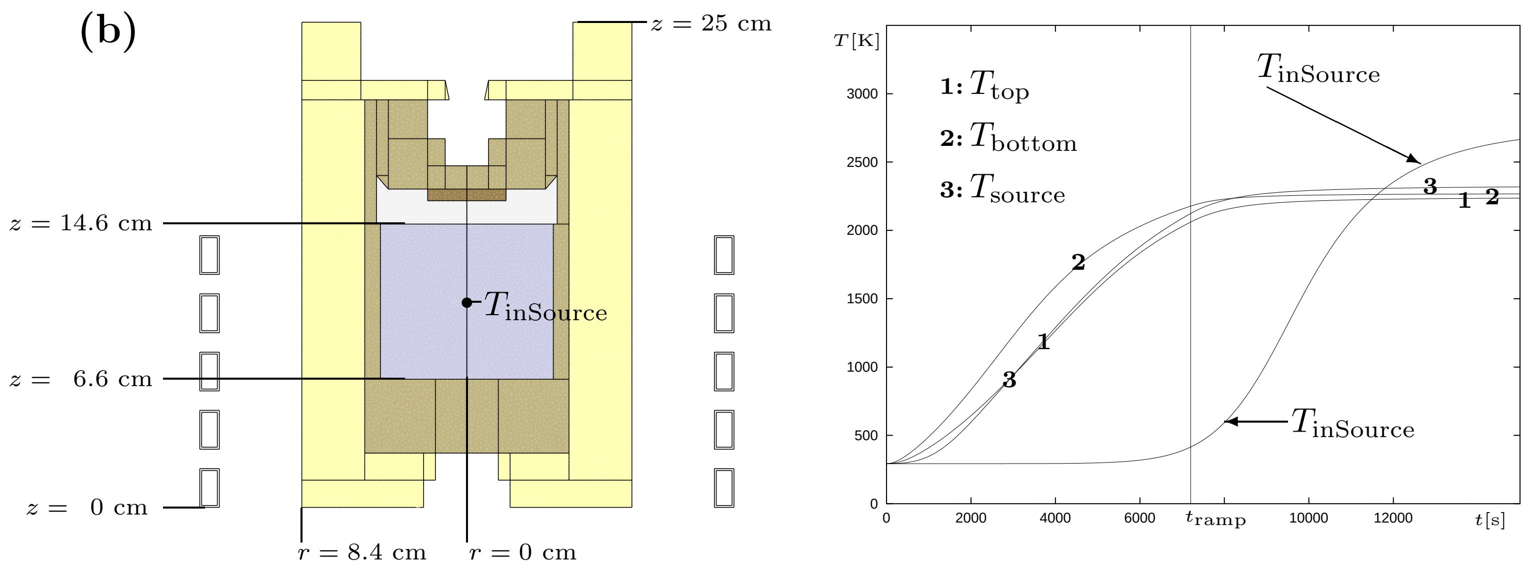
- Discrete existence and uniqueness of a solution to a finite volumes scheme for the nonlinear (quasilinear), nonlocal heat transfer with mixed boundary conditions. Discrete L^∞-L^1 a priori estimates.

- Discrete L^∞-L^∞ a priori estimates, discrete maximum principle in the semilinear, nonlocal case.

- Existence of a (continuous) optimal control in the nonlocal, semilinear case (approximate a prescribed gradient field in the gas phase by controling the heat sources). Necessary optimality conditions were established.

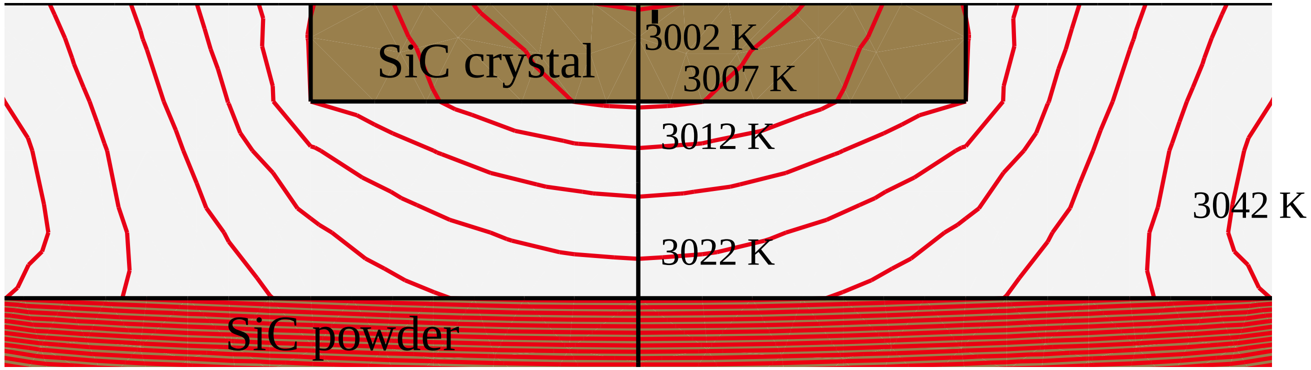
Numerical results: Temperature evolution of the powder charge: $P_{\max} = 7$ kW



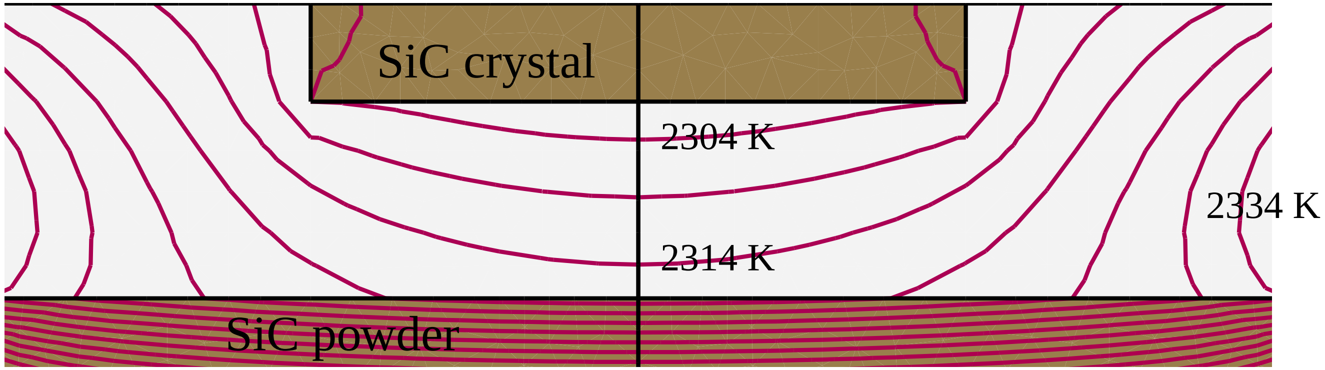


Numerical results: Optimization of temperature field

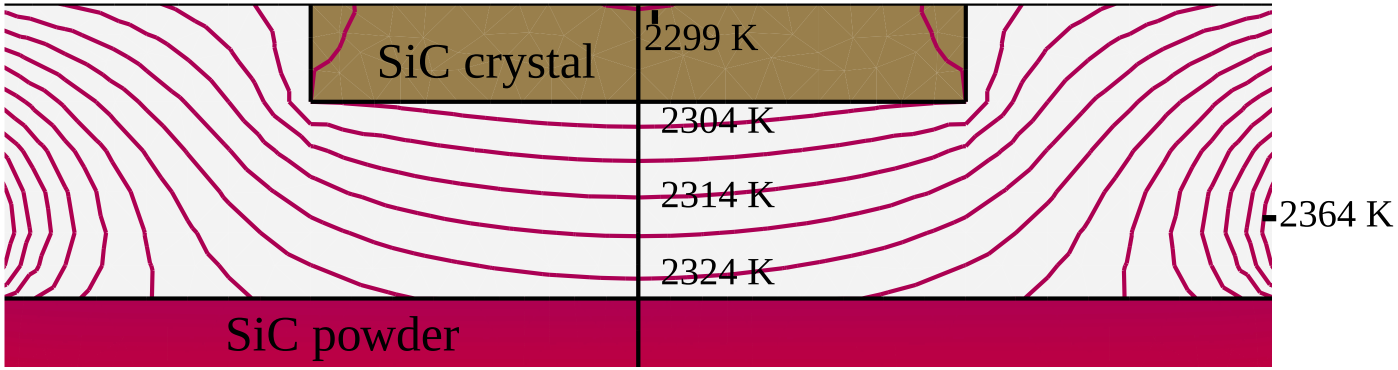
(a): $T(P = 10.0\ \mathrm{kW}, z_{\mathrm{rim}} = 24.0\ \mathrm{cm}, f = 10.0\ \mathrm{kHz})$



(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 $\frac{\mathcal{F}_{r,2}(T) - \mathcal{F}_{z,2}(T)}{2}$



Thank You for Your Attention !

Publications / More Information:

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

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