WIAS-HiTNIHS: Software-tool for simulation in crystal growth for SiC single crystal : Application and Methods

The International Congress of Nanotechnology and Nano , November 7-11, 2004

Oakland Convention Center, Oakland, San Francisco.

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Introduction

Multi-dimensional and multi-physical problem in continuum mechanics for crystal growth process.

- Task : Simulation of a apparatus of a complex crystal growth with heat- and temperature processes.
- Model-Problem : For the mathematical model we use coupled diffusion-equations with 2 phases (gas and solid).
- Problems: Interface -Problems and material-parameters (different material behaviors)
- Solution: Adapted material-functions and balance equations for the interfaces.
- Methods: Implicit discretisations for the equations and nonlinear solvers for the complex interface-functions.

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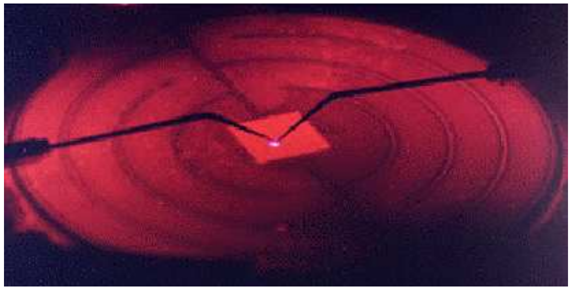
Motivation for the Crystal Growth

The applications are : Light-emitting diodes:
Blue laser: Its application in the DVD player
SiC sensors placed in car and engines



High qualified materials with homogene structures are claimed.

Introduction to the model and the technical apparatus

SiC growth by physical vapor transport (PVT)

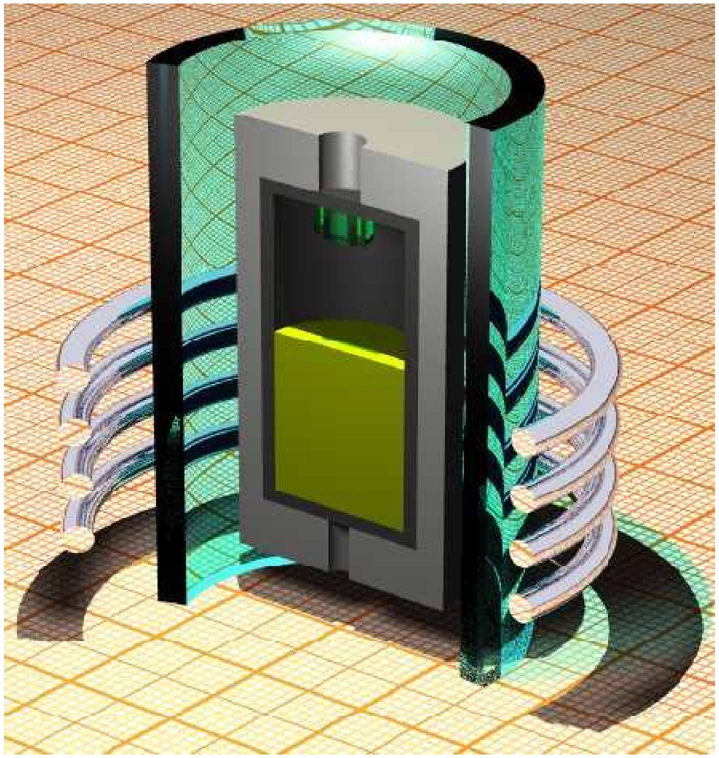
SiC-seed-crystal

Gas : 2000 – 3000 K

SiC-source-powder

insulated-graphite-crucible

coil for induction heating

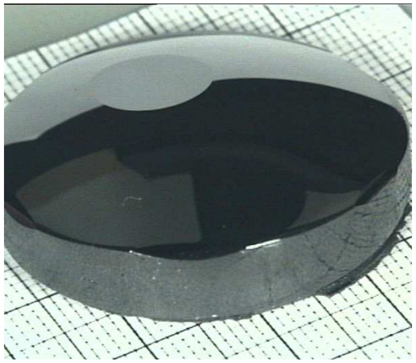


- polycrystalline SiC powder sublimates inside induction-heated graphite crucible at 2000 – 3000 K and ≈ 20 hPa
- a gas mixture consisting of Ar (inert gas), Si, SiC_2, Si_2C, . . . is created
- an SiC single crystal grows on a cooled seed

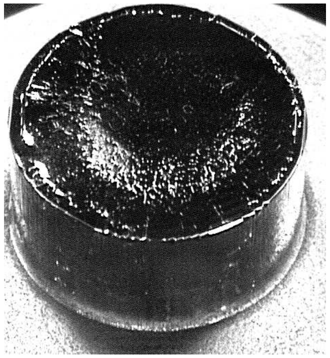
Problems of the technical apparatus

SiC growth by physical vapor transport (PVT)

Good crystal with
a perfect surface
But need of high energy
and apparatus costs



Bad crystal, with
wrong parameters for the heat
and temperature
optimization-problem



Solution : Technical simulation of the process and develop the optimal control of the process-parameters.

Coupling of the simpler models

- Heat conduction in gas, graphite, powder, crystal .
- Radiative heat transfer between cavities .
- Semi-transparent of crystal (band model) .
- Induction heat (Maxwell-equation) .
- Material-functions (complex material library) .

Further coupling with the next models

- Mass transport in gas, powder, graphite (Euler equation, porous media)
- Chemical transport in gas (reaction-diffusion)
- Crystal growth, sublimation of source powder,
  decomposition of graphite (multiple free boundaries)

Nonlinear heat conduction for the solid material (Solid-Phase)

$$\rho^j c_{\mathrm{sp}}^j \partial_t T^j + \nabla \cdot \vec{q}^j = f^j, \quad (1)$$

$$\vec{q}^j = -\kappa^j \nabla T^j, \quad (2)$$

$j \in \{1, \ldots, N\}$ solid materials, N number of solid materials ,

ρ^j: mass density,

c_{sp}^j: specific heat, T^j: absolute temperature,

$\vec{q}^j$: heat flux, κ^j: thermal conductivity,

f^j: power density of heat sources (induction heating).

Nonlinear heat conduction for the gas material (Gas-Phase)

$$\rho^k \frac{z^k R}{M^k} \partial_t T^k + \nabla \cdot \vec{q}^k = 0, \tag{3}$$

$$\vec{q}^k = -\kappa^k \nabla T^k, \tag{4}$$

$k \in \{1, \ldots, M\}$ gas materials, M number of gas materials ,

ρ^k: mass density,

z^k: configuration number, R : universal gas constants,

M^k : molecular mass, T^k: absolute temperature,

$\vec{q}^k$: heat flux, κ^k: thermal conductivity .

Magnetic scalar potential

The complex-valued magnetic scalar potential ϕ :

$$j = \begin{cases} -i\omega\,\sigma\,\phi + \frac{\sigma\,\mathbf{v}_k}{2\pi r} & \text{(inside k-th ring)}, \\ -i\omega\,\sigma\,\phi & \text{(other conductors)}. \end{cases}$$

Elliptic system of PDEs for ϕ:

In insulators: $-\nu \text{div} \cdot \frac{\nabla(r\phi)}{r^2} = 0.$

In the k-th coil ring: $-\nu \text{div} \cdot \frac{\nabla(r\phi)}{r^2} + \frac{i\,\omega\sigma\phi}{r} = \frac{\sigma\,\mathbf{v}_k}{2\pi r^2}.$

In other conductors: $-\nu \text{div} \cdot \frac{\nabla(r\phi)}{r^2} + \frac{i\,\omega\sigma\phi}{r} = 0.$

Magnetic Boundary conditions

Interface condition:

$$\left(\frac{\nu_{\mathrm{material}_1}}{r^2}\nabla(r\phi)_{\mathrm{material}_1}\right)\cdot\vec{n}_{\mathrm{material}_1} \tag{5}$$

$$= \left(\frac{\nu_{\mathrm{material}_2}}{r^2}\nabla(r\phi)_{\mathrm{material}_2}\right)\cdot\vec{n}_{\mathrm{material}_1}\ . \tag{6}$$

Outer boundary condition: $\phi = 0$.

ν: magnetic reluctivity, $\vec{n}_{\mathrm{material}_1}$: outer unit normal of $\mathrm{material}_1$.

Simulated phenomena

Axisymmetric heat source distribution

- Sinusoidal alternating voltage
- Correct voltage distribution to the coil rings
- Temperature-dependent electrical conductivity

Axisymmetric temperature distribution

- Heat conduction through gas phase and solid components of growth apparatus
- Non-local radiative heat transport between surfaces of cavities
- Radiative heat transport through semi-transparent materials
- Convective heat transport

Numerical models and methods

Induction heating:

- Determination of complex scalar magnetic potential from elliptic partial differential equation
- Calculation of heat sources from potential

Temperature field:

- View factor calculation
- Band model of semi-transparency
- Solution of parabolic partial differential equation

Discretization and implementation

Implicit Euler method in time

Finite volume method in space

– Constraint Delaunay triangulation of domain yields Voronoi cells
– Full up-winding for convection terms
– Very complicated nonlinear system of equations
– Solution by Newton's method using Krylow subspace techniques

Implementation tools:

– Program package pdelib
– Grid generator Triangle
– Matrix solver Pardiso

Discretization with finite Volumes and implicit Euler methods

Integral-formulation:

$$\int_{\omega_m} (U(T^{n+1}) - U(T^n))dx - \int_{\partial\omega_m} \kappa_m \nabla T^{n+1} \cdot \mathbf{n} ds = 0 \;, \tag{7}$$

where ω_m is the cell of the node m and we use the following trial- and test-functions :

$$T^n = \sum_{m=1}^{I} T_m^n \phi_m(x) \;, \tag{8}$$

with ϕ_i are the standard globally finite element basis functions. The second expression is for the finite volumes with

$$\hat{T}^n = \sum_{m=1}^{I} T_m^n \varphi_m(x) \;, \tag{9}$$

where φ_ω are piecewise constant discontinuous functions defined by $\varphi_m(x) = 1$ for $x \in \omega_m$ and $\varphi_m(x) = 0$ otherwise. Domain ω is the union of the cells ω_m.

Material Properties

For the gas-phase (Argon) we have the following parameters :
$\sigma_c = 0.0$

$$\kappa = \begin{cases} 1.839\ 10^{-4}\ T^{0.8004} & T \leq 500K\ , \\ -7.12 + 6.61\ 10^{-2}\ T - 2.44\ 10^{-4}\ T^2 + 4.49710^{-7} T^3 & \\ -4.132\ 10^{-10}\ T^4 + 1.514\ 10^{-13}\ T^5 & 500K \leq T \leq 600K\ , \\ 4.194\ 10^{-4}\ T^{0.671} & 600K \geq T\ , \end{cases}$$

For graphite felt insulation we have the functions :
$\sigma_c = 2.45\ 10^2 + 9.82\ 10^{-2}\ T$
$\rho = 170.0$, $\mu = 1.0$, $c_{sp} = 2100.0$

$$\kappa = \begin{cases} 8.175\ 10^{-2} + 2.485\ 10^{-4}\ T & T \leq 1473K\ , \\ -1.19\ 10^2 + 0.346\ T - 3.99\ 10^{-5}\ T^2 + 2.28\ 10^{-8} T^3 & \\ -6.45\ 10^{-11}\ T^4 + 7.25\ 10^{-15}\ T^5 & 1473K \leq T \leq 1873K\ , \\ -0.7447 + 7.5\ 10^{-4}\ T & 1873K \geq T\ , \end{cases}$$

Further Material Properties

For the Graphite we have the following functions :

$\sigma_c = 1\ 10^4$,

$$\epsilon = \begin{cases} 0.67 & T \leq 1200K \ , \\ 3.752 - 7.436\ 10^{-3}\ T + 6.416\ 10^{-6}\ T^2 - 2.33610^{-11} T^3 & \\ -3.08\ 10^{-13}\ T^4 & 500K \leq T \leq 600K \ , \\ 4.194\ 10^{-4}\ T^{0.671} & 600K \geq T \ , \end{cases}$$

$\rho = 1750.0$, $\mu = 1.0$, $c_{sp} = 1/(4.41110^2 T^{-2.306} + 7.9710^{-4} T^{-0.0665})$
$\kappa = 37.715 \exp(-1.96\ 10^{-4}\ T)$

For the SiC-Crystal we have the following functions :

$\sigma_c = 10^5$, $\epsilon = 0.85$, $\rho = 3140.0$, $\mu = 1.0$
$c_{sp} = 1/(3.9110^4\ T^{-3.173} + 1.835\ 10^{-3}\ T^{-0.117})$,
$\kappa = \exp(9.892 + (2.498\ 10^2)/T - 0.844\ \ln(T))$

For the SiC-Powder we have the following functions :

$\sigma_c = 100.0$, $\epsilon = 0.85$, $\rho = 1700.0$, $\mu = 1.0$, $c_{sp} = 1000.0$,
$\kappa = 1.452\ 10^{-2} + 5.47\ 10^{-12}\ T^3$

Numerical experiments

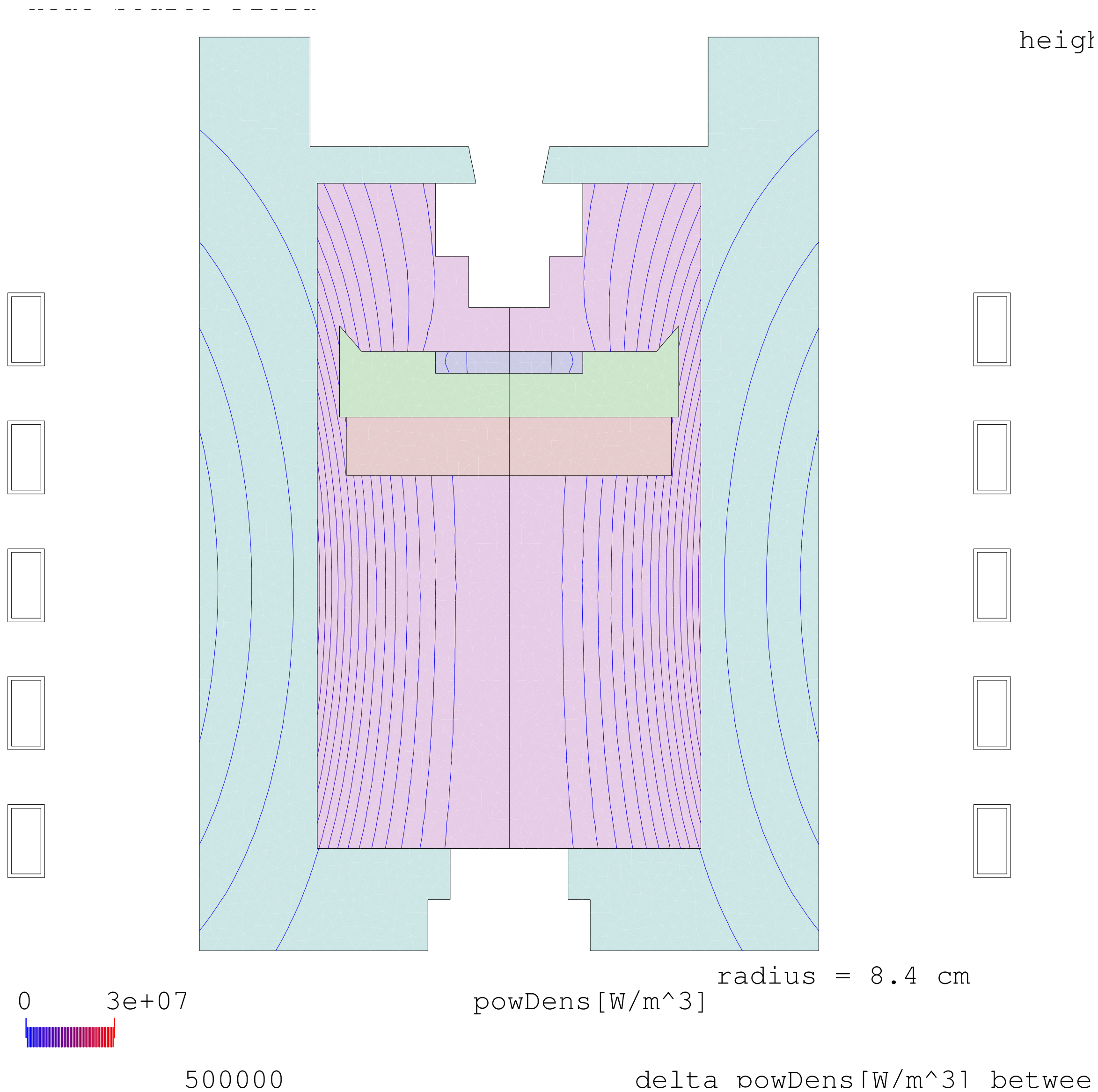
The numerical experiments are done with different material properties on a single computer.

The computational time for the finest case was about 2 h.

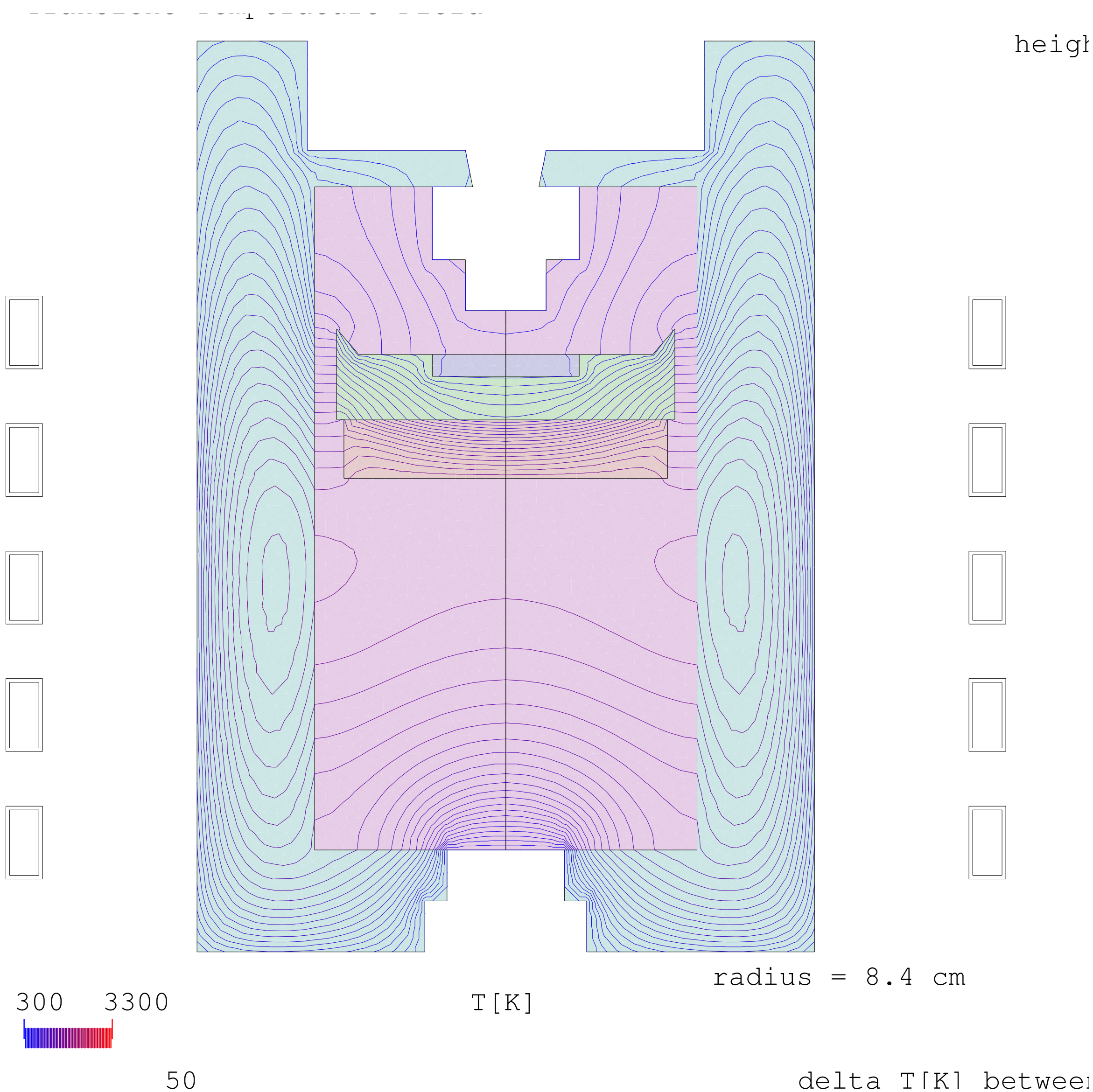
Level	Nodes	Cells	relative L_1-error	Convergence rate
0	1513	2855		
1	5852	11385	$2.1\ 10^{-2}$	
2	23017	45297	$1.25\ 10^{-2}$	0.748
3	91290	181114	$3.86\ 10^{-3}$	1.69
4	363587	724241	$2.087\ 10^{-3}$	0.887

Table 1: The relative L_1-error with the standard finite Volume method.

Nonlinear heat conduction for the gas material (Gas-Phase)



Temperature-source



Conclusions and future works

- Adaptive methods, error estimates.
- Higher order methods.
- Mass transport in gas (Euler equation for the porous media).
- Chemical reaction in gas (diffusion-reaction-equation).
- Crystal growth (multiple free boundaries).