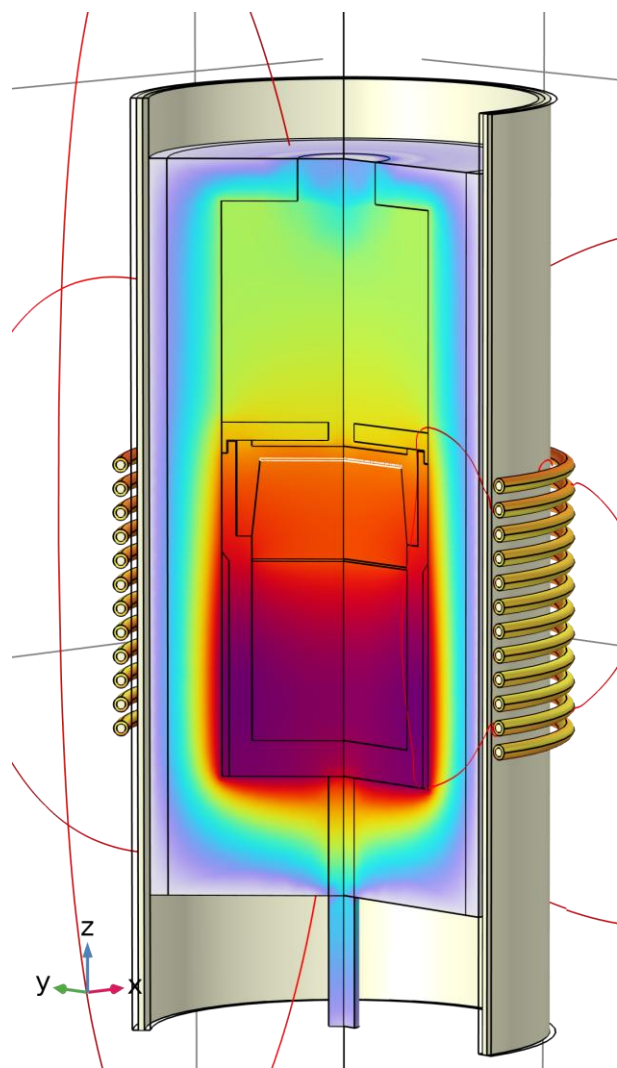
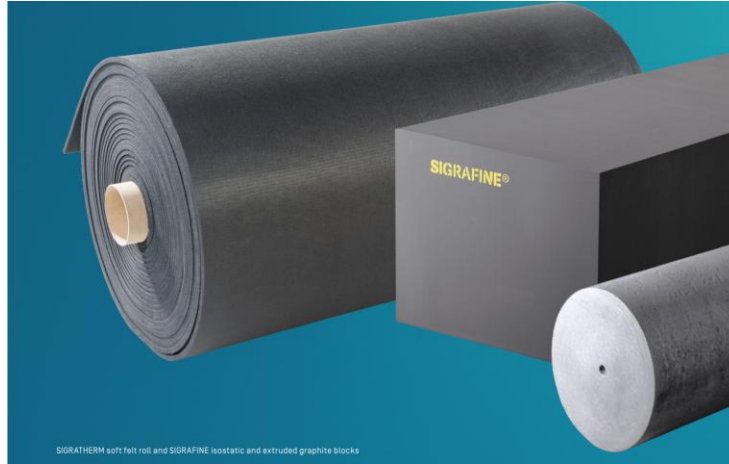
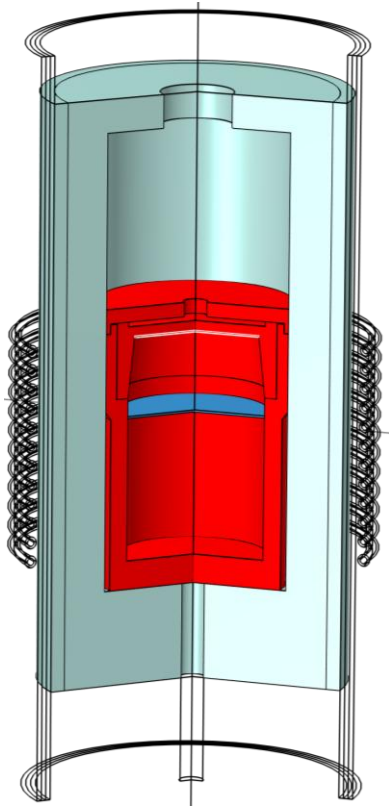


Multiphysics Modeling of PVT Growth of SiC Crystals Coupled with Data-Driven Process Optimization



Industrial context and model scope



Scope:

- 6-inch
- SiC crystal
- graphite crucible and lid
- porous-graphite slab
- carbon-felt insulation
- inductive heating at 10 kHz
- literature-based geometry and operating conditions

The presented geometry and operating conditions are literature-based and do not contain customer data.

Why Model the PVT Growth Process?

Graphite Materials

(Crucibles, Porous Graphite, Felt)

Material Properties

(porosity, thermal conductivity, emissivity, purity, permeability, elec. Resistivity, diffusivity, reactivity)

PVT Process Model

(ind. coupling, temperature, species transport, crystal growth rate, wear)

Material Requirements

(Performance targets for graphite components)

- Detailed process requirements are often proprietary.
- Material-property targets cannot be derived directly from customer feedback.
- Multiphysics simulation provides a virtual application environment for deriving material requirements.

Coupled physics and thermodynamics

MF + HT
Induction heating, conduction,
radiation & temperature control

FP
Porous flow in source, porous
graphite and growth chamber

TCS
Transport of Si(g), SiC₂(g) and Si₂C(g)

PDE
Transient evolution of the SiC source



**Stoichiometric growth at
crystal surface**

Stationary Solution: MF + HT
Induction heating
Heat transfer

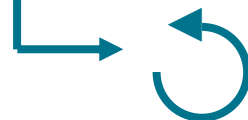


**Transient Solution: FP + TCS
+ PDE**
Surface kinetics
Source evolution

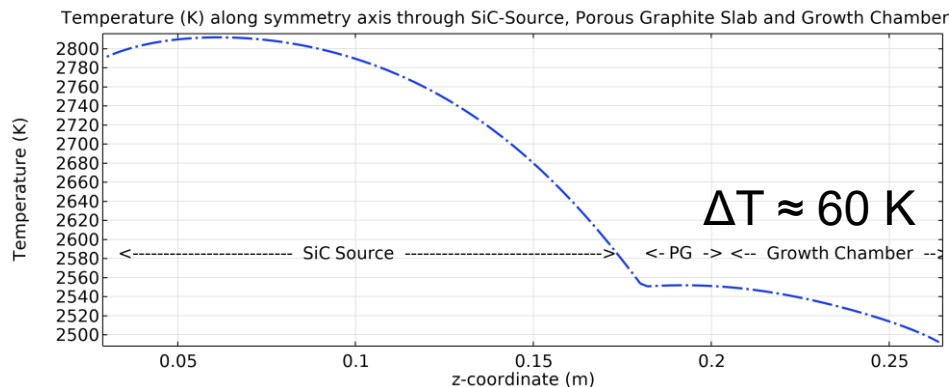
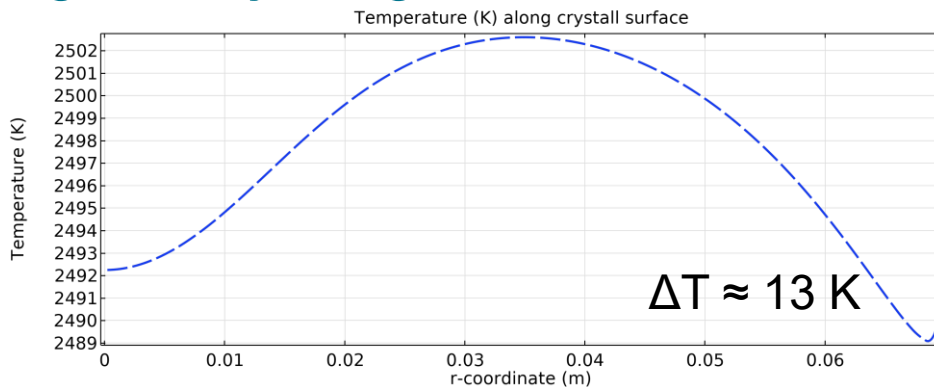
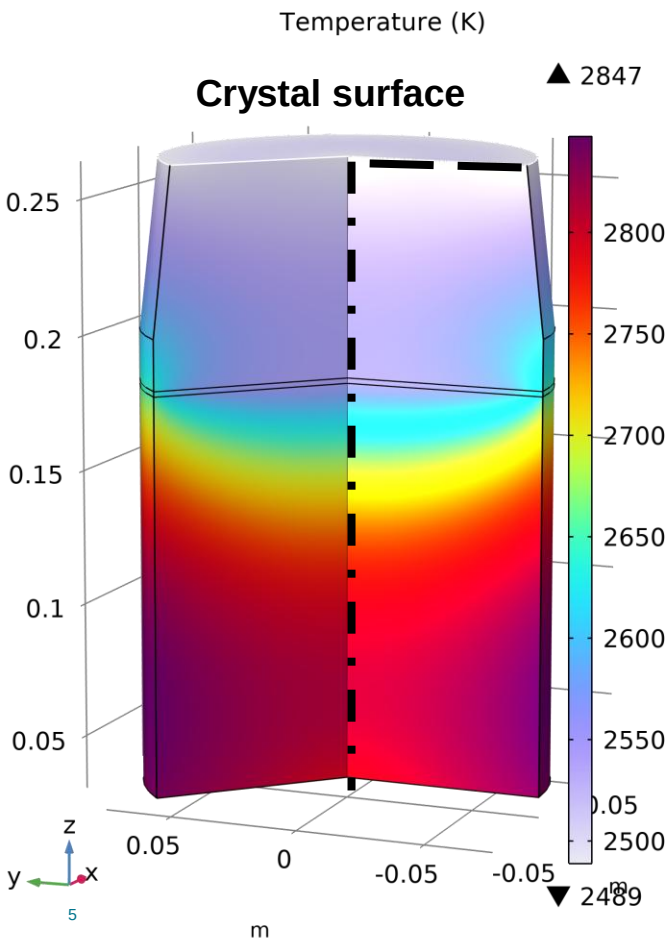


Updated Source Properties:
Porosity
Permeability
Thermal conductivity
SiC content

$\Delta t = 2 \text{ h}$

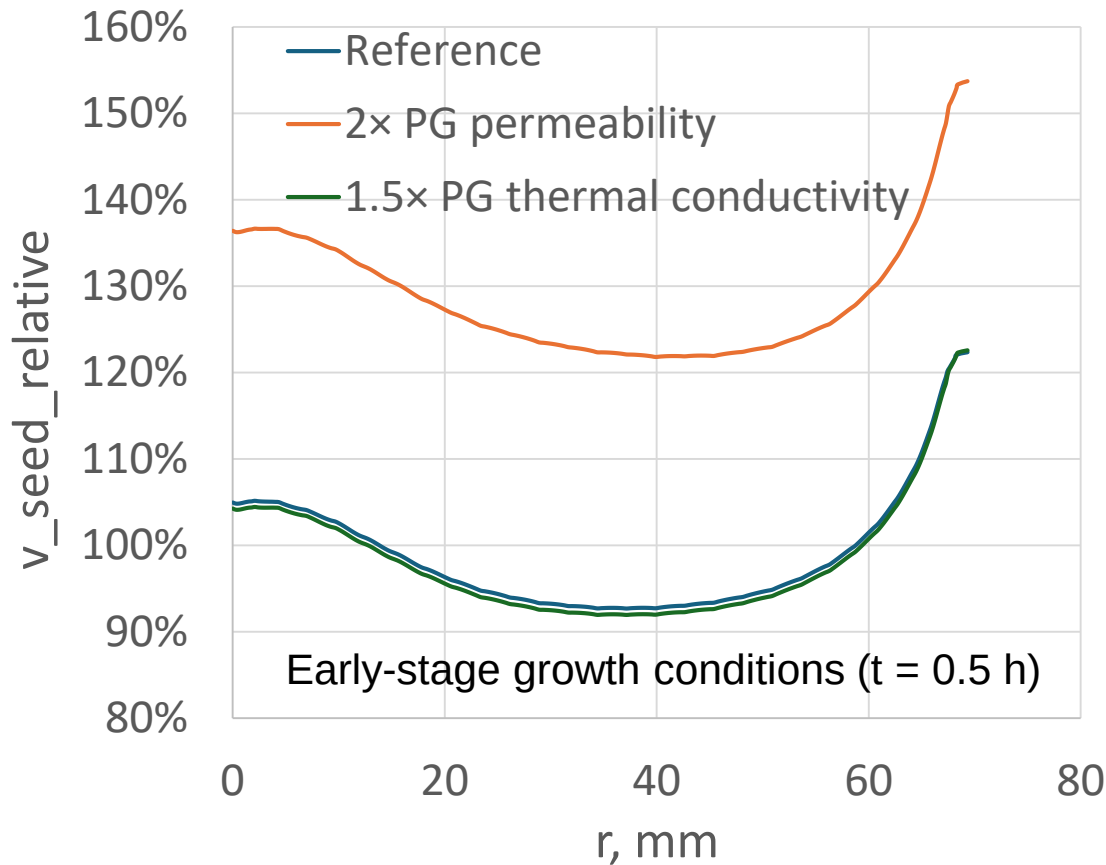


Thermal conditions governing SiC crystal growth



Large axial ΔT drives sublimation and mass transport, while low radial ΔT promotes uniform crystal growth.

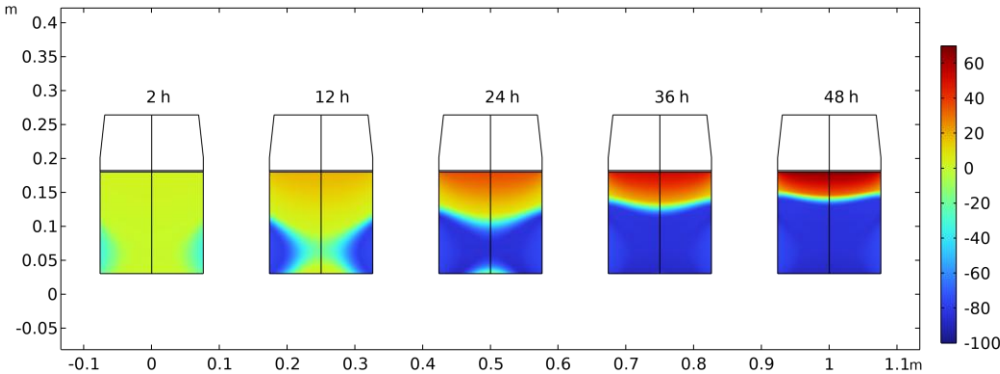
Influence of porous-graphite properties



At the beginning of the process, porous-graphite permeability has a pronounced impact on species supply and the predicted growth rate, whereas the investigated thermal-conductivity change shows a smaller effect under the selected conditions.

Transient source evolution governs long-term growth

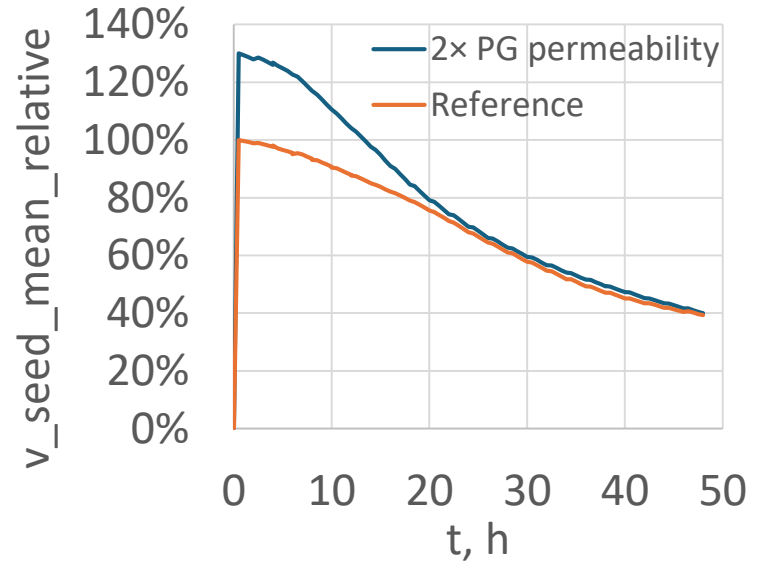
$$\frac{\Theta_{SiC} - \Theta_{SiC,0}}{\Theta_{SiC,0}} \cdot 100 \%$$



Source depletion progressively reduces the predicted growth rate and diminishes the initial advantage of increased PG permeability.

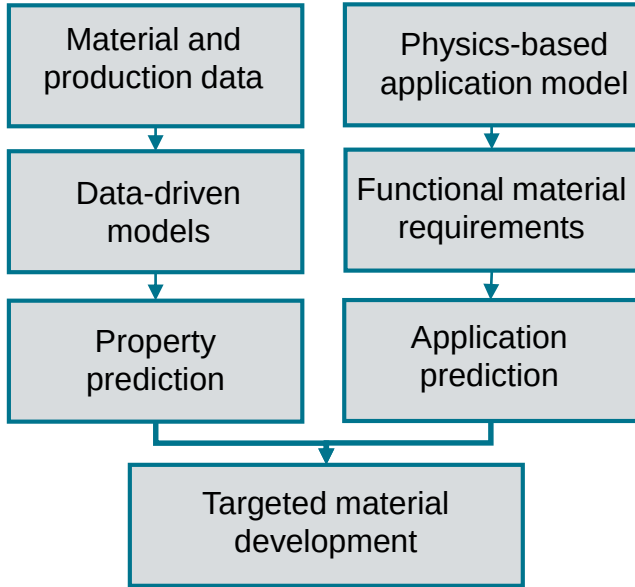
The presented results assume fixed operating conditions. In industrial crystal-growth processes, adjustments of thermal boundary conditions, for example by changing heating conditions or coil position, may partially compensate for these effects.

Predicted long-term growth behaviour is strongly influenced by source evolution.

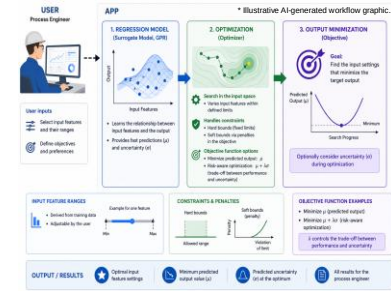
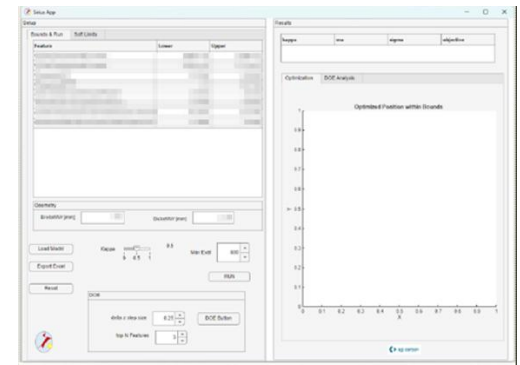
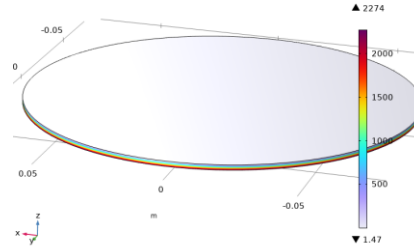
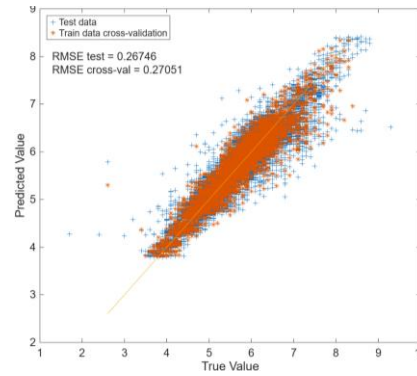


Area-averaged growth rate for the central crystal region ($r < 65$ mm).

Data-Driven Optimization



Physics-based simulation identifies relevant material requirements; data-driven models accelerate material development.



Data-Driven Optimization of Graphite Materials:

- Optimization of porous graphite and carbon-felt materials
- Data-driven models based on production and recipe data
- Robust optimization and user-friendly engineering apps

Conclusions

- **Coupled Multiphysics**

Coupling electromagnetic heating, heat transfer, porous flow, species transport and surface thermodynamics provides an integrated description of SiC PVT growth.

- **Thermal design objective**

A sufficiently large axial temperature difference drives mass transport, while a small radial temperature variation supports uniform crystal-growth conditions.

- **Material properties and time dependence**

Porous-graphite permeability strongly influences the initial growth rate, whereas transient source evolution increasingly governs the long-term process response.

- **Material development**

Physics-based application modeling and data-driven optimization provide complementary tools for deriving material requirements and developing advanced graphite components.

Thank you!