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Modelling of Semiconductor Crystal Growth Processes and its Challenges

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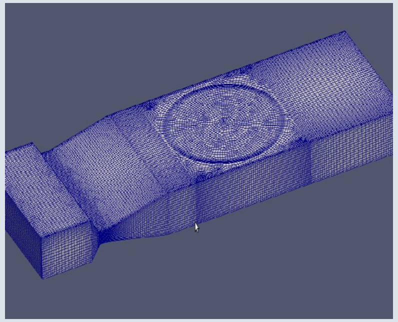
The quality of crystals and the yield in the industrial production
is determined by the presence of

crystal defects

Process-parameters

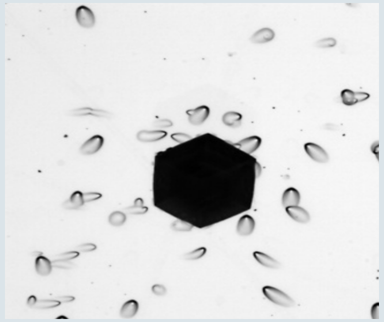
Mass Fluxes, Heater Power, …

Growth Conditions



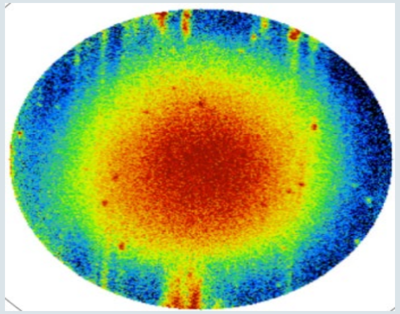
Temperature- T , Flow v, Species C

Defect Formation



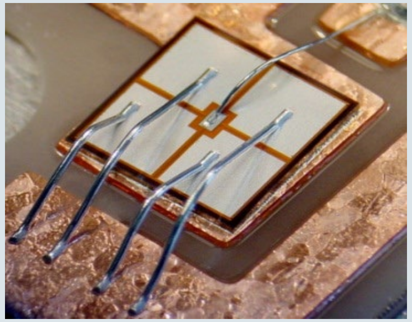
desired or not desired

Material Properties



e.g. Carrier Life Time

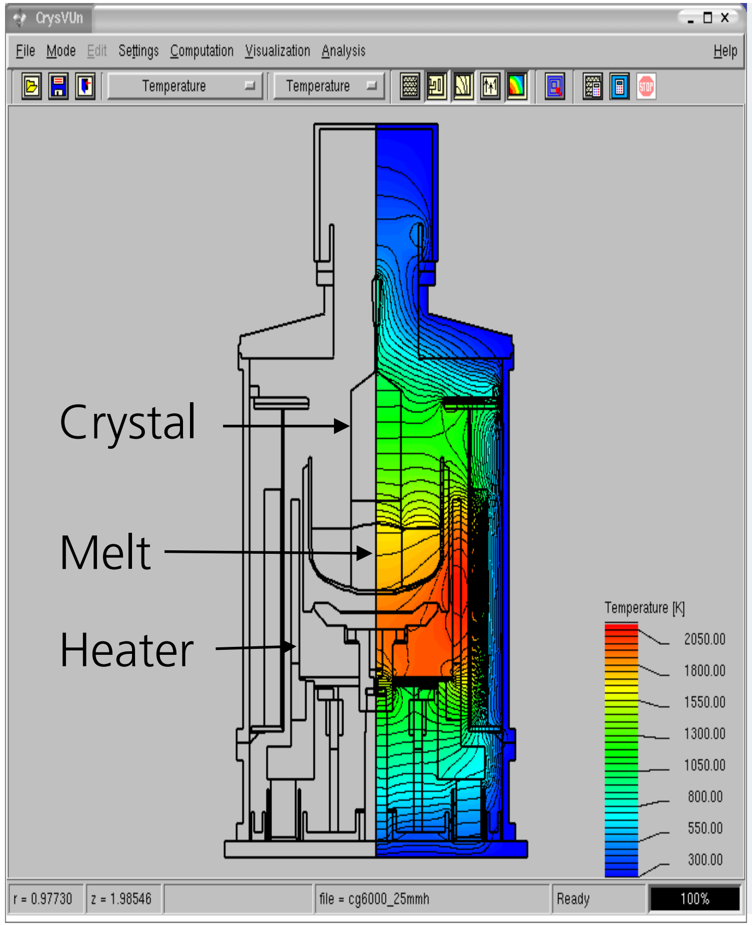
Device Properties



e.g. Reliability

**The formation of crystal defects depends mainly on the heat & mass transport processes occurring during crystal growth!
A quantitative description of the influence of the heat and mass transfer processes on the crystal quality is usually only possible by simulation of the whole crystal growth apparatus.**

Physical phenomena to be considered for modeling of crystal growth processes



Conduction:	an-isotropic material properties
Radiation:	gray emitting surfaces using the view factor method
	more accurate models for other optical media with absorption, scattering, etc.
Convection:	laminar and turbulent convection in gas and melt
	influence of various external forces (rotation, steady or time-dependent magnetic fields)
Heating method:	resistance, inductive, optical heating
Phase transition:	models for treating the growing interface (Stephan problem, facetted growth)
Species Transport:	transport, segregation, reactions
Crystal defects:	von Mises stress, plastic deformation, point defects and their reactions

Requirements on modeling in the field of Silicon Czochralski crystal growth

Dimensions

Puller	diameter: 1500mm, height: > 5000mm
Crystal	diameter: 300mm, height: 3000mm
Crucible	diameter: 900mm, 500mm
Boundary layers (BL)	thickness: 0.1mm
Mesh size in BL	size: 0.01mm

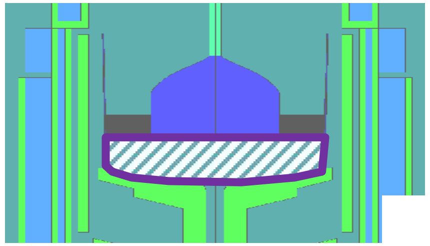
Real Multi Scale Problem: 6 Orders of Magnitude!

Extreme requirements on meshing!
→ A fully 3D, time-dependent model of the whole puller is still impossible!
→ A quasi stationary, 2D-3D coupled model is the standard approach today

Modeling approach using 2D-3D coupling via Reynold’s averaging method[1,2]

Temperature field in the whole puller for given heater power

quasi-stationary 2D

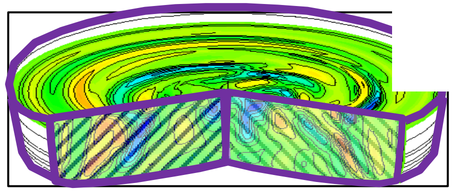


turbulent heat flux

Reynolds averaging

azimuthal averaging (r, z) plane

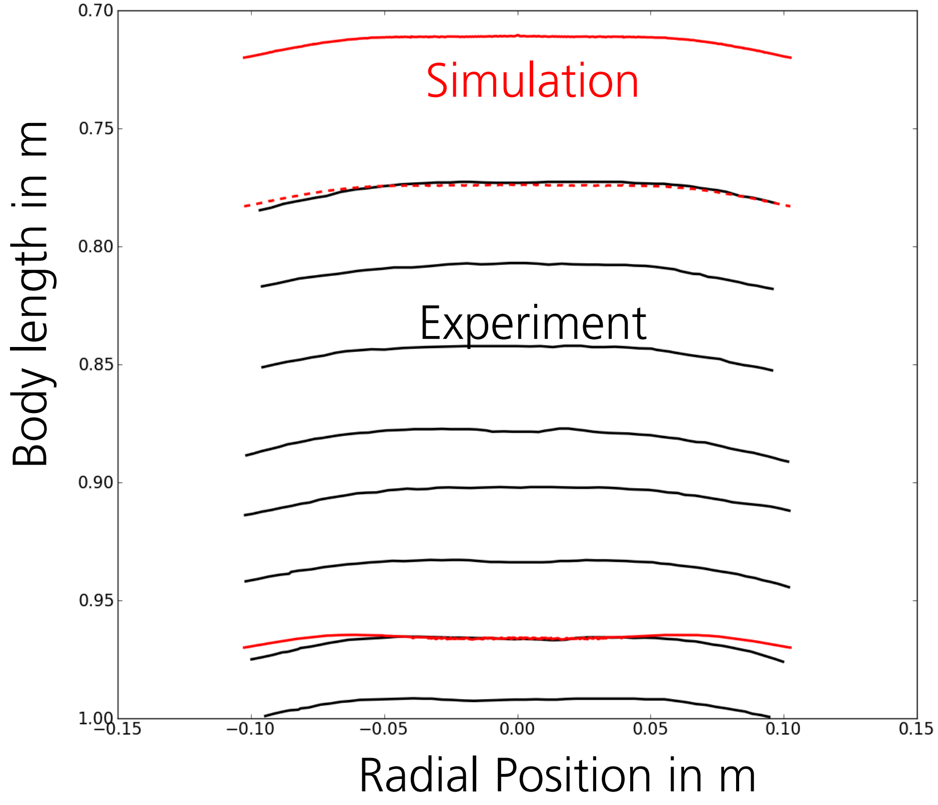
boundary conditions at 3D interface



Transient 3D LES (1000s, 0.025s)

Convective heat & oxygen distribution in the melt

24“/100kg/0.9mm/min/-10rpm/10rpm/



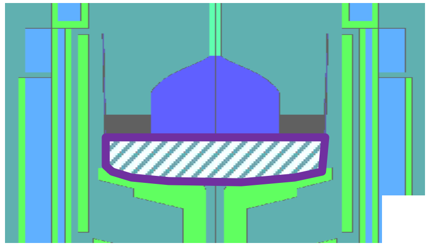
[1] J. Fainberg et al., Journal of Crystal Growth 303 (2007), 124
[2] T. Jung et al., Journal of Crystal Growth 368 (2013), 7

Realistic interface shape and oxygen concentration

Modeling approach using
2D-3D coupling via Reynold's averaging method[1,2]

CrysMAS

quasi-stationary 2D



6-12h

turbulent heat flux

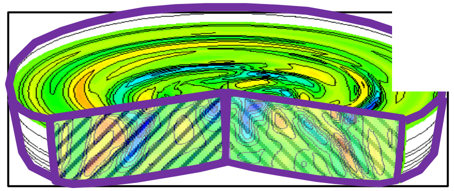
Reynolds averaging

azimuthal averaging

(r, z) plane

boundary conditions at
3D interface

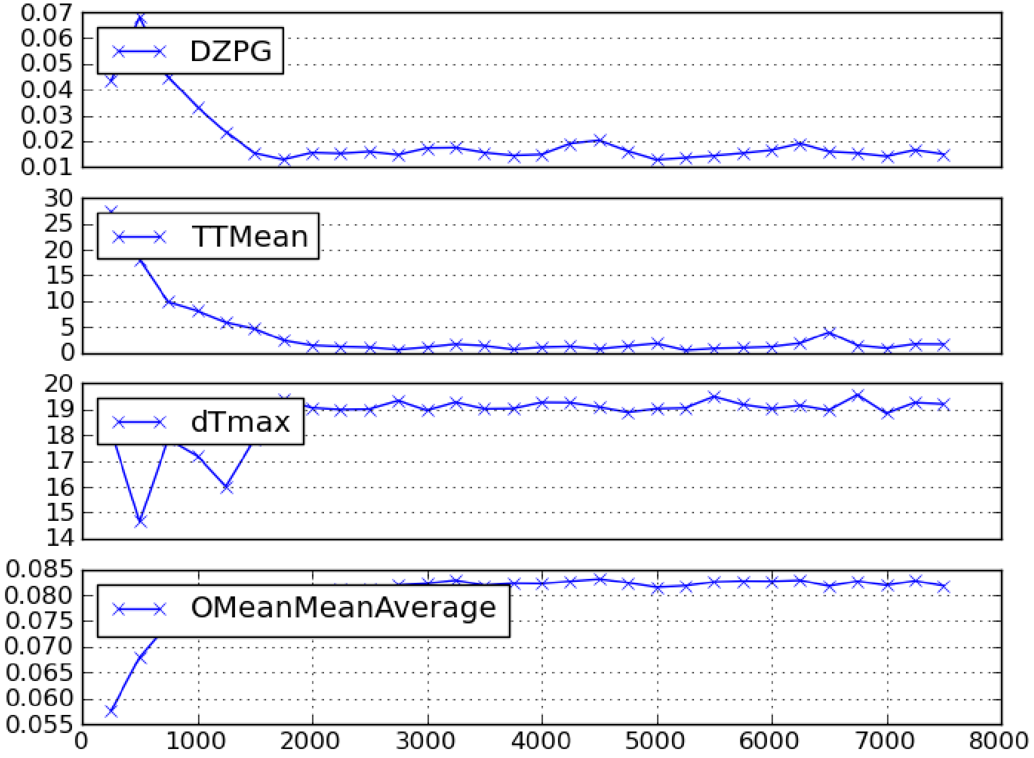
OpenFOAM



Transient 3D
LES (1000s, 0.025s)

40h

Convergence behavior



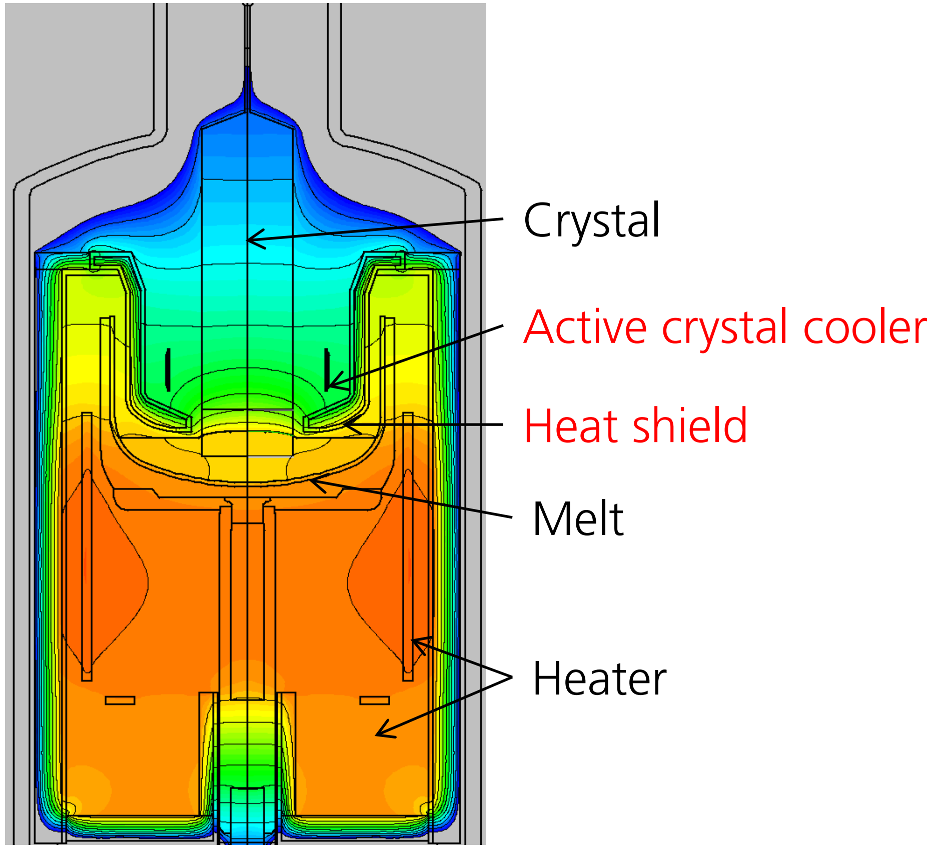
[1] J. Fainberg et al., Journal of Crystal Growth 303 (2007), 124
[2] T. Jung et al., Journal of Crystal Growth 368 (2013), 7

More than 10 2D-3D cycles are typically needed until convergence
→ 30 days total computation time per single data point!

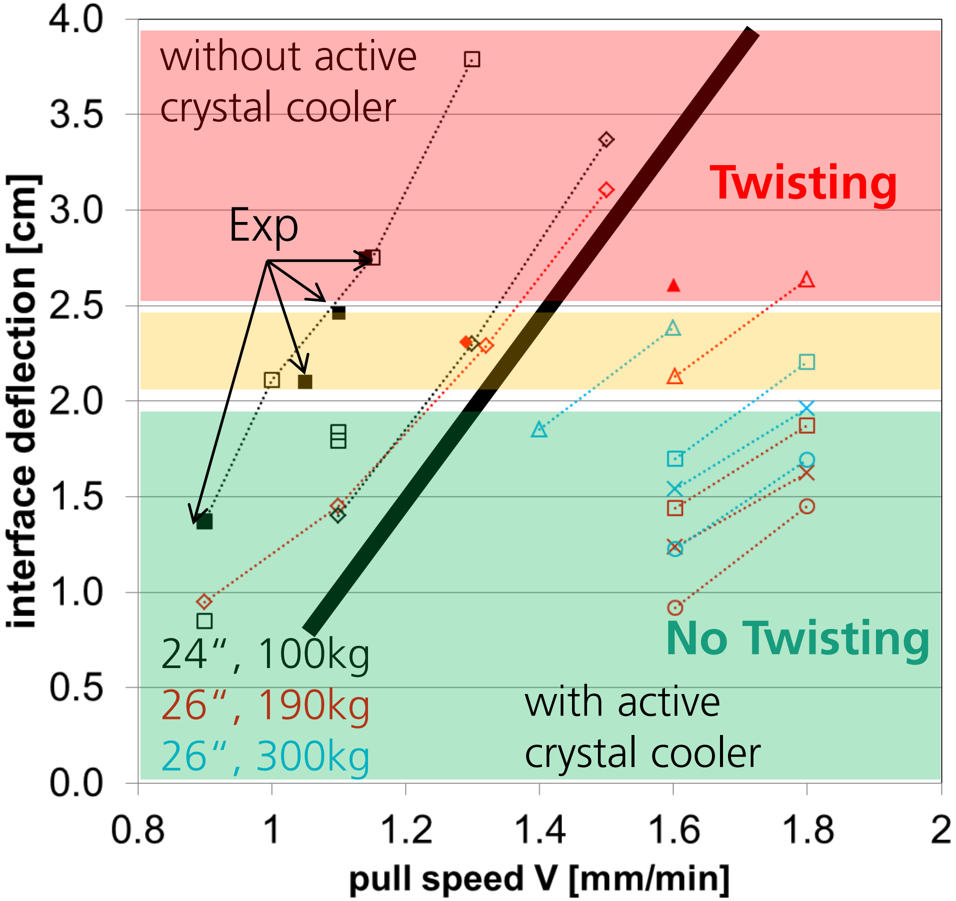
Optimization of hot zone design to achieve maximum possible pull speed

without crystal twisting

Twisted crystal



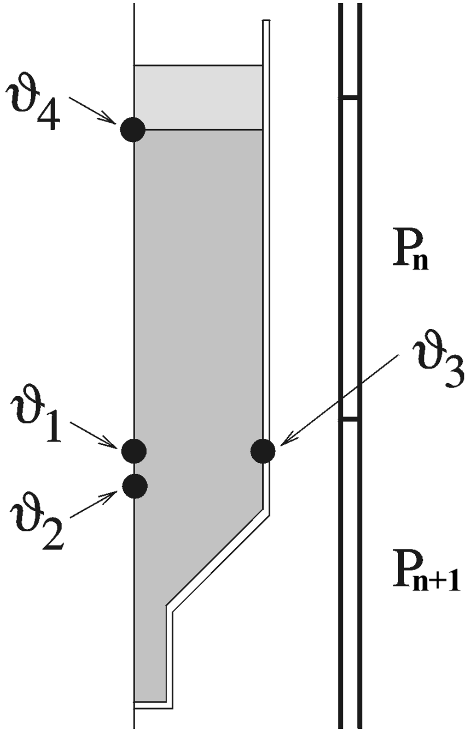
J. Friedrich, T. Jung, M. Trempa, C. Reimann, A. Denisov, A. Muehe, Journal of Crystal Growth 524 (2019) 125168



Increase of charge weight from 100kg to 300kg and pull speed from 1mm/min to 2mm/min and reduction of power demand from 0.6kW/kg to 0.2kW/kg by optimization of hot zone

Machine Learning in Simulation of Crystal Growth Processes

Inverse Problem



forward probem: $\{P_m\} \Rightarrow T(x)$
given M heater powers $P_m \Rightarrow$ compute temperature profile T(x)
problem is well posed (Small changes in BC lead to small effects in solution)

inverse problem: $\{T(x_n)\} \Rightarrow \{P_m\}$
given N temperatures $\{\vartheta_1, \ldots \vartheta_N\}$ at points $\{x_1, \ldots x_N\} \Rightarrow$ find P_m : $T(x_n)=\vartheta_n$, $\forall n \in \{1,..,N\}$
problem is ill-posed (Small changes in BC can lead to big effects in solution)

strategy of solution:
minimize cost function via gradient descent
many evaluations of forward problem
problem specific properties can help
to reduce the computational costs

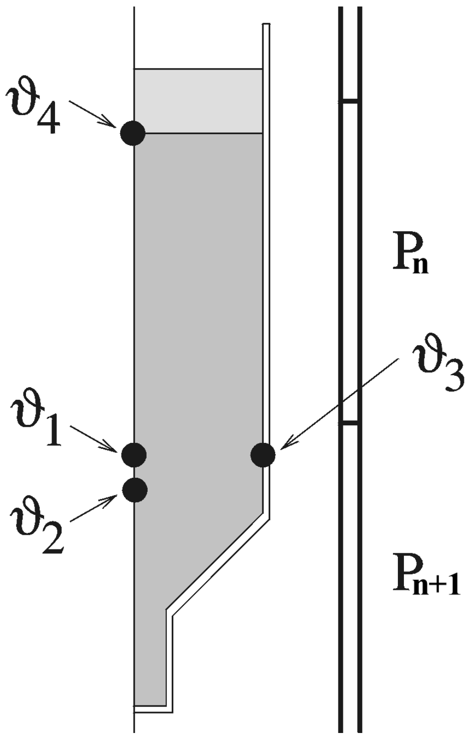
Cost of target deviation | Regularization if N<M

M. Kurz et al, Journal of Crystal Growth 198/199 (1999) 101-106

First time introduced in crystal growth community by Fraunhofer IISB 1999

Machine Learning in Simulation of Crystal Growth Processes

Inverse Problem: Process development with respect to low thermal stress



Grow material with low dislocations densities
under relative high growth and cooling rates, i.e.

- flat interface resp. low thermal stress field in the crystal ($\vartheta_1 - \vartheta_3 = 0$)

under certain constraints, e.g.

- certain axial temperature gradient in the crystal ($\vartheta_1 - \vartheta_2$ = Const. A)
- an upper limit for the overheating in the melt ($\vartheta_4 <$ Const. B)

by

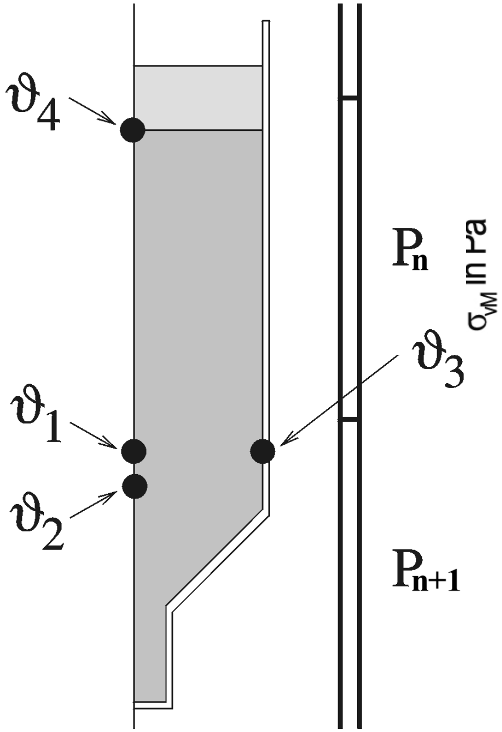
- optimizing geometrical details, e.g. crucible support
- optimizing the heater temperatures (power) versus time using inverse simulation

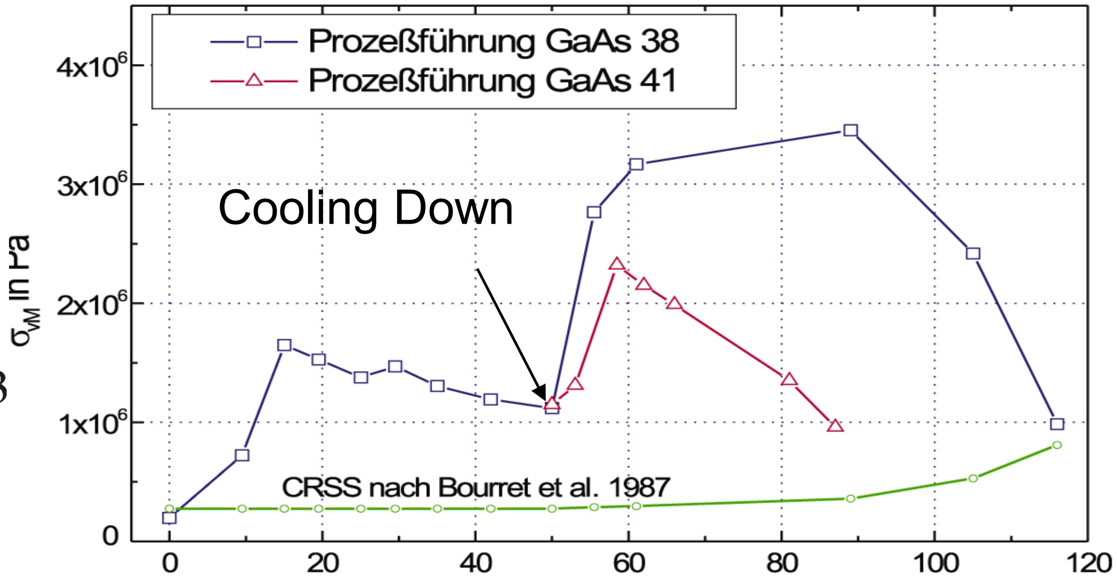
M. Kurz et al, Journal of Crystal Growth 198/199 (1999) 101-106

First time introduced in crystal growth community by Fraunhofer IISB 1999

Machine Learning in Simulation of Crystal Growth Processes

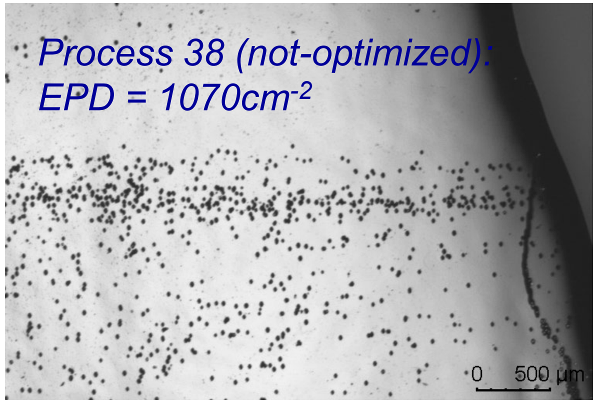
Optimization of heater temperature-time profiles T (x,t) for VGF-growth of GaAs by inverse simulation

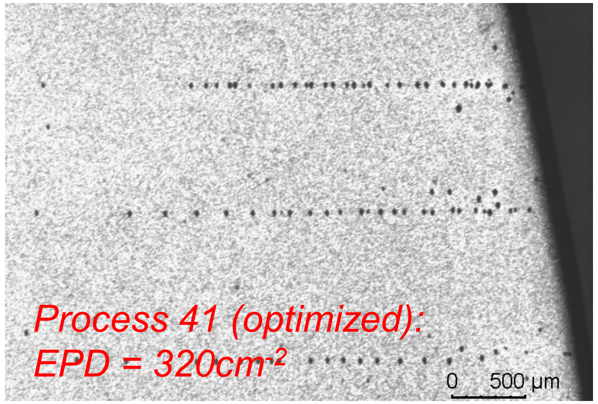




Computed von Mises stress vs. time for two processes

Computed max. von Mises stress in 3"GaAs versus process time for a not-optimized and optimized cooling down process (top). Microscope images of etch GaAs wafers prepared from crystals grown under not-optimized (right top) and optimized (right bottom) cooling down conditions





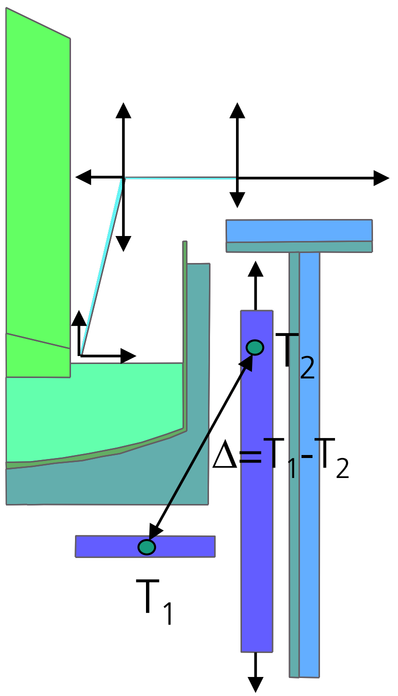
B. Birkmann et al, Journal of Crystal Growth 211 (2000) 157-162

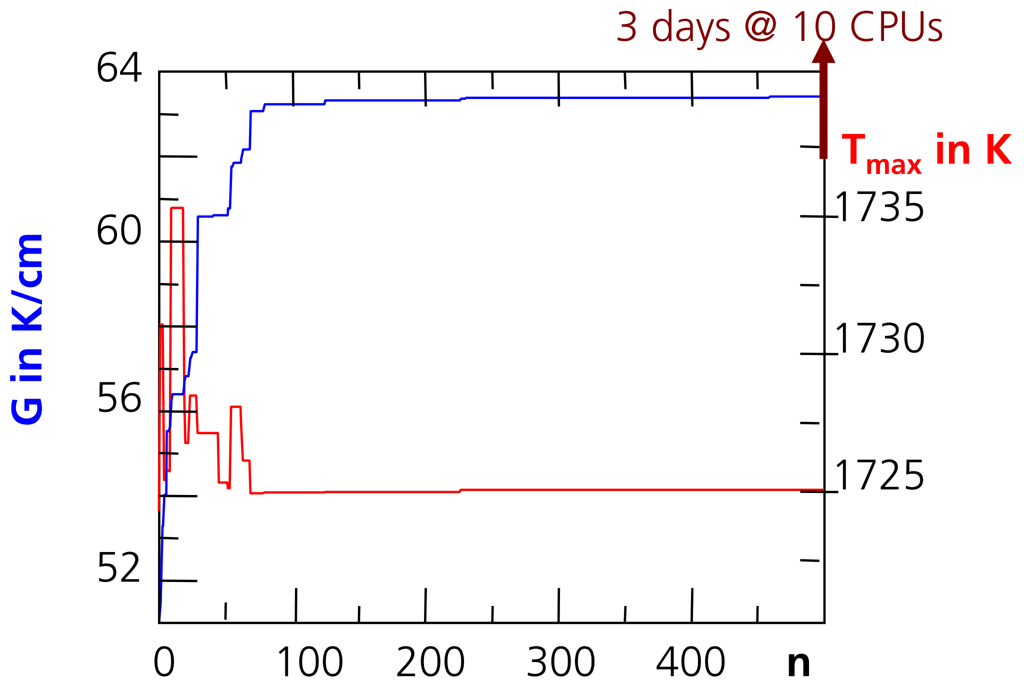
First time introduced in crystal growth community by Fraunhofer IISB 1999

Machine Learning in Simulation of Crystal Growth Processes

Genetic Algorithms: Demonstration of different Use Cases

Use case 1: Automatic optimization of the heat shield design and heater configuration with respect to highest axial temperature gradient G by using a very simplified Cz model





Left: Czochralski set-up for 100mm Si crystals. Right: G and maximum temperature in the melt T_{max} as a function of the number of generations n.

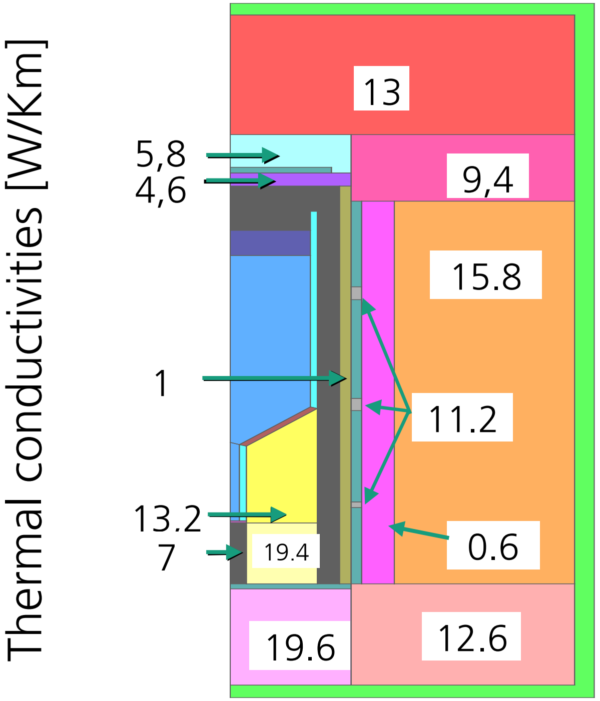
T. Führner et al. J. Crystal Growth 266 (2004) 229

First time introduced in crystal growth community by Fraunhofer IISB 2004

Machine Learning in Simulation of Crystal Growth Processes

Genetic Algorithms: Demonstration of different Use Cases

Use case 2: Optimization of Material Distribution in a very simplified VGF Furnace within 3 days on 14 CPUs (40 000 single thermal simulations).



T. Führer et al. J. Crystal Growth 266 (2004) 229

	T_{top} [K]	T_{max} [K]	Gradient [K/m]	σ_{vMises} [MPa]
Required	1516< T < 1536	<1775	800	
Seed	1537	1775	853	0.4
Cone	1525	1776	785	1.0
Cylinder	1516	1767	795	1.0

Left: optimized material distribution; right: Maximum temperature in the melt T_{top}, in the facility T_{max}, temperature gradient at the interface in the crystal, and max. von Mises stress for the 3 growth stages.

First time introduced in crystal growth community by Fraunhofer IISB 2004

Machine Learning in Simulation of Crystal Growth Processes

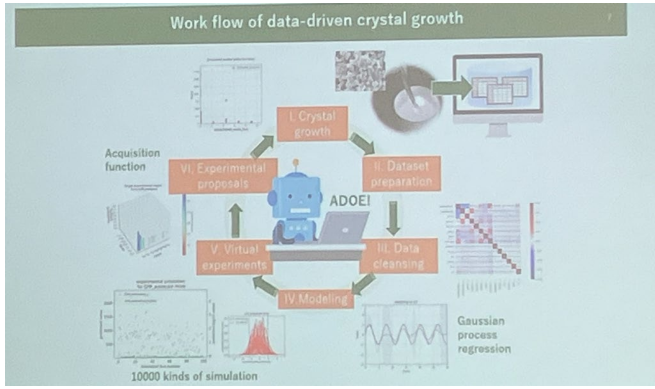
Personal conclusion

The computation time for real problems is usually too long so that ML can become a tool for daily use.

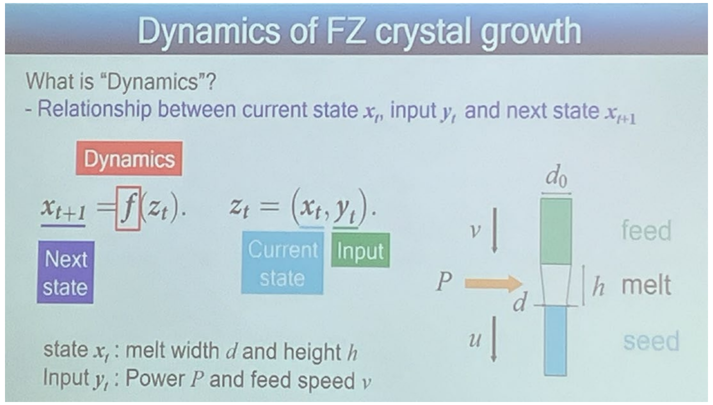
Machine Learning in Simulation of Crystal Growth Processes

Personal conclusion

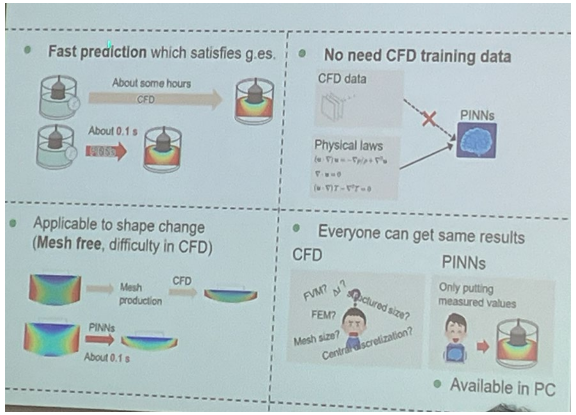
Adadptive Design of Experiments



Intelligent process control



Minimization of CFD simulations



If we will have identified the right use cases,
ML will be definitely helpful!

Summary

- Modeling is an indispensable tool in the field of crystal growth and epitaxy
- Modeling of crystal growth and epitaxy requires a wide range of physical phenomena to be considered
- Modeling of the Cz Si crystal growth process is still a very challenging task
- Machine learning in crystal growth and epitaxy is helpful, but needs the right use cases