COMPARISON OF THE OXYGEN CONCENTRATION IN CZOCHRALSKI SILICON CRYSTAL OBTAINED BY A SIMPLE LUMPED-PARAMETER MODEL AND SOPHISTICATED 2D-3D SIMULATIONS

J. Friedrich[1*], M. Trempa[1], H. Koch[1], F. Mosel[2], A. Mühe[2]

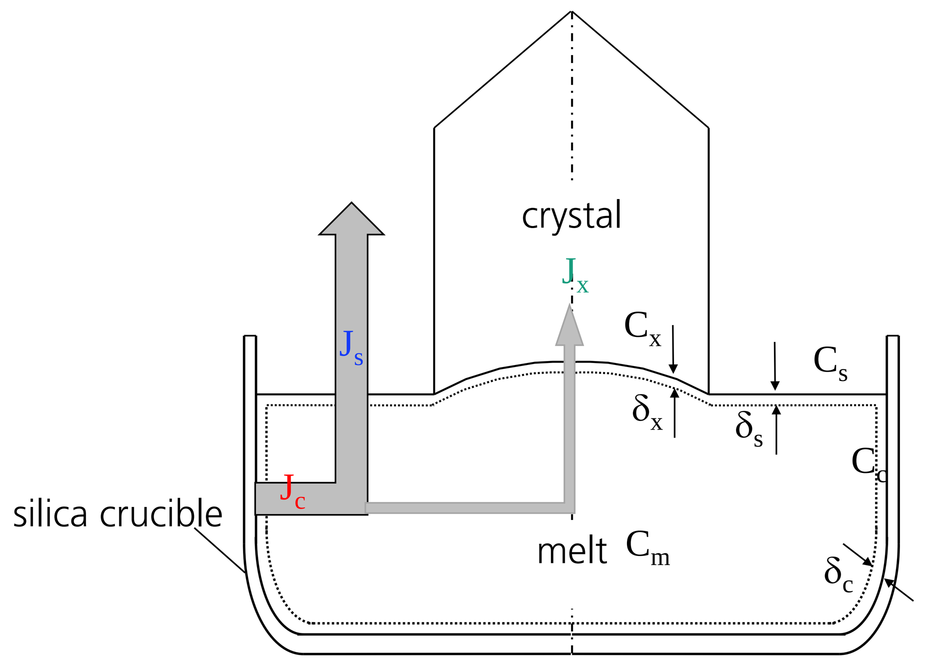
[1] Fraunhofer IISB, Department Materials, Schottkystraße 10, 91058 Erlangen, Germany [2] PVA Crystal Growing Sytems GmbH, Im Westpark 10-12, 35435 Wettenberg, Germany

*email: jochen.friedrich@iisb.fraunhofer.de

Motivation

- Numerical modelling is widely used to improve the Czochralski (Cz) crystal growth technology in order to obtain lower oxygen contents in silicon crystals
- Highly precise numerical simulations, e.g. including calculation of turbulent melt flow, typically take several weeks and need high performance computing clusters
- Our approach is to evaluate which information about oxygen concentration in the silicon crystal can be achieved by a simple, time- and cost saving boundary layer model
- The results of this lumped model are compared to that obtained by a highly sophisticated 2D/3D coupled numerical Cz model for 24″ crucible hot zone ([1],[2])
- Oxygen content was calculated in dependence on the crucible and crystal rotation for different crystal lengths

The boundary layer model



Vari-able	Description
C_c	Equilibrium concentration at crucible wall
C_m	Solute concentration in the melt volume
C_s	Solute concentration at the free melt surface
C_x	Solute concentration at the s/l interface
A_c	Contact area between melt and crucible wall
A_s	Area of free melt surface
A_x	Area of s/l interface
D	Diffusion coefficient
ν	Kinematic viscosity
r_c	Crucible radius
r_x	Crystal radius
δ_i	Solute boundary layer thickness
$\dot{n}_i$	Molar flow rate
J_i	Molar flux
ω_i	Angular velocity
V	Pull speed

Oxygen mass fluxes

- Source:
  Dissolution of the SiO2 crucible $J_c A_c$ $\quad \dot{n}_c = J_c A_c \quad J_c = \frac{D}{\delta_c}(C_c - C_m)$ Eq. 1
- Sinks:
  Evaporation of SiO at free melt surface $J_s A_s$ $\quad \dot{n}_s = J_s A_s \quad J_s = \frac{D}{\delta_s}(C_m - C_s)$ Eq. 2
  Incorporation into the crystal $J_x A_x$ $\quad \dot{n}_x = k_{eff} V C_m A_x$ Eq. 3

Calculation of O concentration

From the balance of the mass fluxes

$$\frac{dn_m}{dt} = 0 = J_c A_c - J_s A_s - J_x A_x \qquad \text{Eq. 4}$$

the pseudo-steady concentration inside the melt volume C_m can be obtained

$$C_m = \frac{1}{1+\frac{A_s\delta_c}{A_c\delta_s}+\frac{A_x\delta_c}{A_c D}V\,k_{eff}}\,C_c \qquad \text{Eq. 5}$$

The equilibrium oxygen concentration at the crucible wall C_c can be assumed to be equal to C_c=2x10^{18}cm^3 and therefore independent from the melt overheating ΔT.

K_{eff} is the effective segregation coefficient according to Burton Prim Slichter.

The diffusion boundary layers δ_i are replaced by the corresponding momentum boundary layers δ_i' using the relation

$$\delta_i = 2.4 * Sc^{-1/3}\delta_i' \text{ with Schmidt number Sc=}\nu/D \qquad \text{Eq. 6}$$

The momentum boundary layers δ_s' at the free melt surface depends on the Marangoni number Ma:

$$\delta_s' = Ma^{-1/3}(r_c - r_x) \text{ with } Ma = \frac{-\left(\frac{\partial\sigma}{\delta T}\right)\Delta T(r_c - r_x)}{\rho\nu^2} \qquad \text{Eq. 7}$$

The momentum boundary layers δ_c' at the crucible wall scales with the Ekman number Ek for the geostrophic flow regime or with the Grashof number Gr for non rotational flows.

$$\delta_c' = 3Ek^{1/2}r_c \text{ with } Ek = \frac{\nu}{2\omega_c r_c^2} \qquad \text{Eq. 8}$$

$$\delta_c' = Gr^{-1/4}r_c \text{ with Gr} = \frac{\beta g\Delta T r_c^3\left(\frac{h}{r_c}\right)}{\nu^2} \qquad \text{Eq. 9}$$

For the calculation of the Ma and Gr numbers a characteristic temperature difference is needed which is assumed to be equal to the maximum melt over heating ΔT. From the 2D/3D simulations for the given 24″ hot zone it was found that ΔT depends mainly on the crucible rotation rate ω_c as follows:

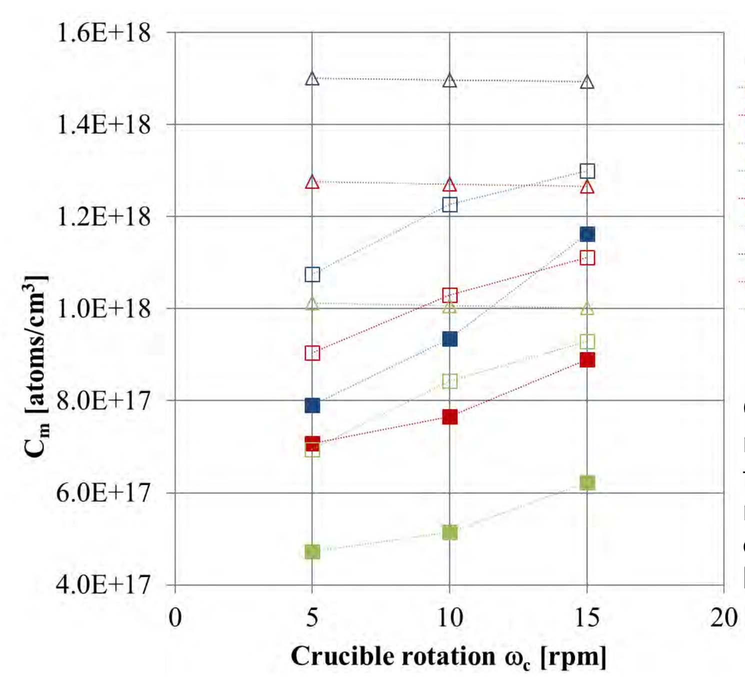
$$\Delta T \approx 27K + 2\omega_c\left[\frac{K}{rpm}\right] \qquad \text{Eq.10}$$

With eqs. 5-10 the oxygen concentration C_m can be calculated as follows

$$C_m = \frac{1}{1+\frac{A_s\delta_c'}{A_c\delta_s'}+\frac{A_x}{A_c(D/V)}\frac{\delta_c'\,2.4\,k_{eff}}{Sc^{1/3}}}\,2\times10^{18} \text{ [atoms/cm}^3\text{]} \qquad \text{Eq. 11}$$

Comparison to 2D/3D simulations

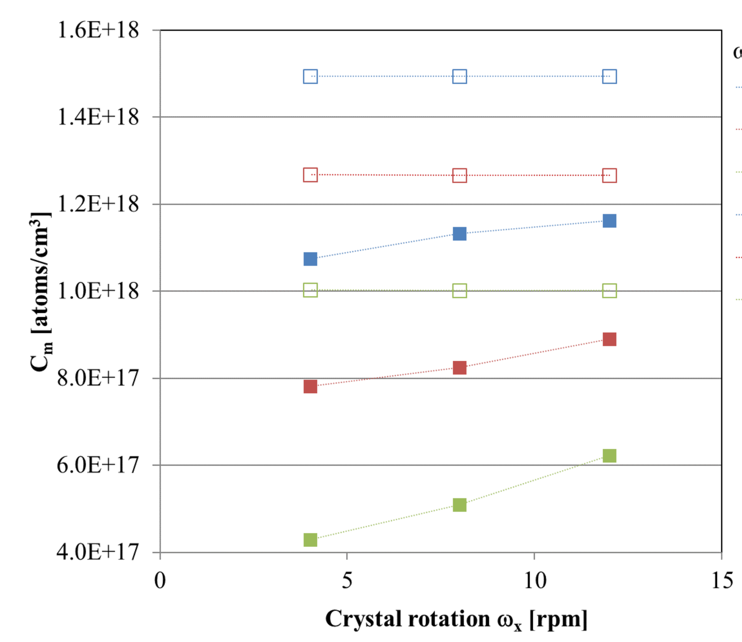
Oxygen concentration in silicon crystal in dependence on crucible rotation ω_c for constant crystal rotation ω_x



Oxygen concentration versus crucible rotation at constant crystal rotation (12rpm) for different body lengths. Full squares represent the results of the simulations, open squares the results of the boundary layer model using eq. 11.

- Qualitative agreement between lumped model and 2D/3D simulations using Ek number (eq.8) in the lump-model:
  The increasing oxygen trend becomes visible (decreasing δ_c at the crucible wall with increasing ω_c, resulting in increasing J_c)
- No matching to 2D/3D model if Gr number is used for calculation of δ_c

Oxygen content in silicon crystal in dependence on crystal rotation ω_x for constant crucible rotation ω_c



Oxygen concentration versus crystal rotation at constant crucible rotation (15rpm) for different body lengths. Full squares represent the results of the simulations, open squares the results of the boundary layer model using eq. 11.

- Slight increase of the oxygen concentration with increasing crystal rotation in the 2D-3D simulation is not reproduced by the boundary layer model
- Complex flow structure itself is contributing much to the real oxygen transport

Conclusion

- The presented simple lumped-model can be used for rough estimation of oxygen concentration in Cz-crystals, e.g. in dependence of ingot length or crucible rotation, which make it interesting for beginners in crystal growth
- However, if high precise analysis of oxygen distribution in crystal and melt is required the lumped model hits the wall and the complex and time consuming 2D/3D simulations are indispensable

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