



The Software for
Bulk Crystal Growth Simulation



Center for Systems Engineering
and Applied Mechanics of UCL

QUALITY OPTIMIZATION OF CZOCHRALSKI-GROWN SILICON CRYSTALS BY MEANS OF THE OFF-LINE CONTROL TECHNIQUE

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The objective of developing simulation tools is to help the crystal growers in the design of new furnaces and the selection of optimal growth conditions. The FEMAG software is currently developed by FEMAGSoft S.A. Company together with the CESAME center of the University of Louvain. FEMAG's global model takes all important phenomena of the crystal growth process into account. Diffuse surface radiation is considered, while frequency-dependent material properties are modeled by the band-energy technique. Laminar and non-laminar flow models are considered, including or not the effect of axisymmetric magnetic fields. The objective of launching a new FEMAG generation has been to provide a fully automatic dynamic simulator predicting the entire growth process, while coupling the calculations with accurate melt and gas flow predictions.

Dynamic simulations can be direct or inverse. In this latter case, some constraints are introduced (such as prescribing the crystal shape) and an equal number of natural inputs (heater power, pull rate...) are calculated to satisfy these constraints. Typically, in inverse Czochralski (Cz) simulations, the heater power history is calculated to constrain the crystal to grow with the prescribed shape. "Off-line control" consists in extending the inverse simulation technique in order to optimize the growth process.

Precisely, off-line control aims at determining an appropriate evolution of the processing parameters (heater power, pull rate, crystal/crucible rotation rates, magnetic field intensity...) in order to optimize crystal shape and quality. Here, the simulation is managed by a controller, which retroacts by searching optimal command parameters to satisfy selected quality criteria. Therefore the simulator plays the role of the real process, while the off-line controller supervises the simulation. At each time step the retroaction loop transmits information about the system state to the controller, which in turn evaluates the required evolution of the processing parameters to optimize crystal quality.

Typically, in Cz Silicon growth, the objective is to determine the heater power and pull rate histories required to obtain a constant diameter crystal of optimal quality. Additional command parameters such as crystal and crucible rotation rates, magnetic field intensity if any, etc., can be optimized as well. Crystal quality is measured by simulated results such as the defect density above the crystal-melt interface, or the deflection of this interface, etc. Examples will be shown where the defect density in the crystal is controlled by appropriate action on the crystal rotation rate and/or the design and intensity of a cusp magnetic field.