DYNAMIC PREDICTION OF THE ENTIRE CZOCHRALSKI GROWTH PROCESS AND USE OF THE OFF-LINE CONTROL TECHNIQUE TO OPTIMIZE CRYSTAL SHAPE AND QUALITY

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Proposed session topic: global modeling

The FEMAG software is currently developed by FEMA*Soft* S.A. Company together with the CESAME research center of the University of Louvain. FEMAG's global model takes all important physical 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. Whereas FEMAG-1 already performed global quasi-steady or time-dependent simulations, the applications were restricted to top cone, shouldering and body growth. Laminar and non-laminar flow models were considered, including or not the effect of axisymmetric magnetic fields. The objective of launching FEMAG-2 generation was to provide a fully automatic simulator predicting the entire growth process, while coupling the dynamic calculations with accurate melt and gas flow predictions.
A significant difficulty lay in the important system geometrical evolution during a complete growth process. The method adopted uses unstructured deforming meshes together with automatic mesh generation. Accurate techniques have been designed for the calculation of the system free surfaces. When mesh deformation becomes too large, a new and better behaving mesh is regenerated, while an interpolation technique is applied to recalculate all the fields on this newly generated mesh. In order to achieve coupling with global time-dependent calculations, an appropriate melt flow solution strategy is used.
In general, dynamic simulations can either be direct or inverse – in which case some constraints are introduced (such as prescribing the crystal shape) and an equal number of natural inputs (heater power, pull rate…) are calculated in order 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 the evolution of the processing parameters (heater power, pull rate, crystal/crucible rotation rates, magnetic field design and intensity, power distribution…) in order to optimize selected process variables characterizing crystal shape and quality. In this case, the simulation is managed by a controller, which retroacts by searching optimal command parameters to satisfy selected product quality criteria. Therefore the simulator plays the role of the real process, while the off-line controller supervises the simulation. The retroaction loop transmits at each time step appropriate

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information about the system state to the controller, which in turn evaluates the required evolution of the processing parameters to optimize the crystal quality criteria.
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 in prescribed ranges. Crystal quality is measured by simulated results such as the classical V/G criterion, or the defect density above the crystal-melt interface, or the deflection of this interface, etc. An example is shown in Fig. 1, where the maximum V/G ratio is controlled by appropriate action on the crystal rotation rate.

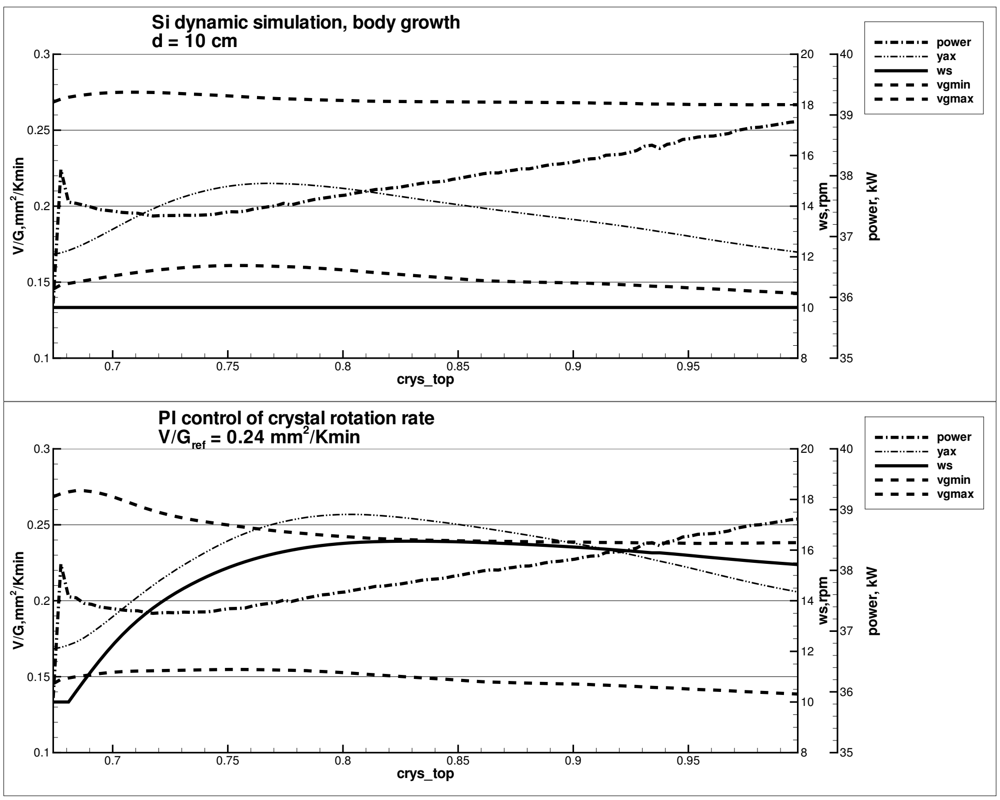

Figure 1. Optimization of maximum V/G ratio on the solidification front by action on the crystal rotation rate. Comparison of non-controlled (top) with PI-controlled (bottom) simulations as a function of grown crystal length. Left axis : max. and min. V/G ratio. First right axis : crystal rotation rate. Second right axis : heater power. Crystal radius : 5 cm. Pulling rate : 3 cm/h.

<u>References:</u>

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