STRATEGIES FOR HANDLING DIFFERENT TIME-SCALES IN CZ SILICON GROWTH

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Proposed session topic: multi-scale

The Czochralski (CZ) crystal growth process has a large spectrum of different time-scales that are important in detailed modeling. The time-scales range from much shorter than one second up to many hours, and they express themselves in the rapid variations of the melt flow to the slow transient behavior of the thermal environment. Unfortunately, it is not possible to completely isolate the different time-scales since the transient flow field affects the global thermal environment in a significant way. Therefore, the modeling of, e.g., the shape of the growth interface requires some multi-scale strategies to account for the different time-scales.

The physical models required for determining the shape of the growth interface include the incompressible Navier-Stokes equations coupled with the global thermal environment. In the Navier-Stokes equations the convection mechanisms due to natural and forced convection as well as due to Marangoni convection need to be accounted for [1]. Thermal modeling includes conduction, convection and radiation. Usually the problem of different time-scales is approached by time-averaging the flow equations directly, i.e. using turbulence modeling [2,3]. The current approach does not require turbulence modeling and may be a good alternative especially if there is no reliable steady-state turbulence model available. Also the method retains most of the true transient behavior that is important when studying the transient features of the growth.

The multi-scale methodology presented here starts with an initial state, which is computed using steady state models of the equations. An increased viscosity is used, as the Navier-Stokes equations do not have a steady-state solution with realistic material parameters. During this initial stage, an active temperature control is used to set the heater power.

After the initial state, transient algorithms are used to approach the real physical system. The material parameters may depend on the time-step size in the transient algorithm, and longer time-steps may be used in the start to speed up the evolution. As there are rapid temperature fluctuations in the real system, the heater control and growth interface algorithms are applied to a suitably time-averaged temperature field. The system does not reach a full convergence. However, the time-averaged quantities should reflect the true measurable quantities of the system in a successful simulation.

The strategies, which are described above, have been implemented in Elmer finite element software [4] and have been applied to an axi-symmetric toy model and to a real CZ growth geometry. We show the time evolution of the growth interface and that of the temperature field. We also demonstrate the effect of the transient heater control. Figure 1 shows an experimental Lateral Photovoltage Scanning (LPS) [5] map of a 150

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mm crystal. This kind of measurement may be used to validate the modeled interface shape as well as the transient growth rate behavior.

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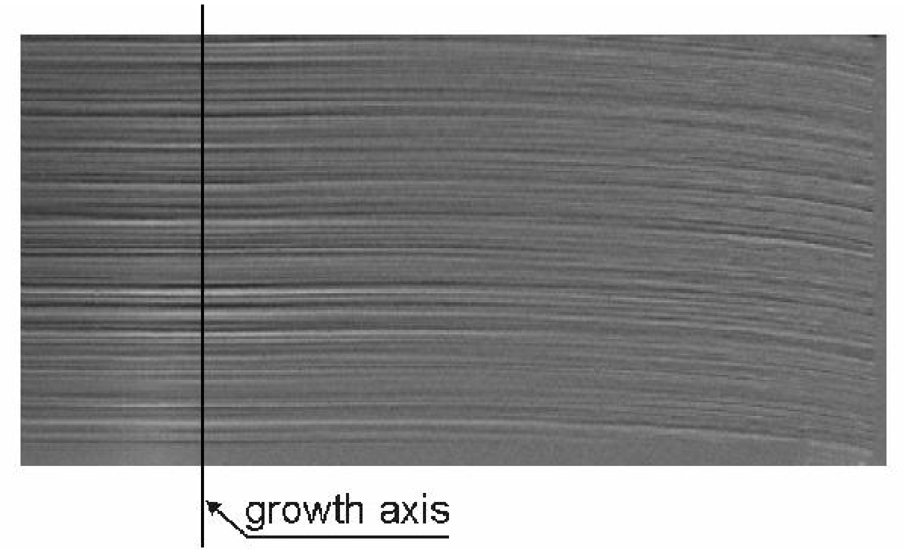

Fig. 1. An LPS map of a 150 mm N(100) crystal. The sample has been cut out of a 50 mm high section of the crystal and etched. The freezing interface shape as well as temporal variations are clearly visible.

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