DYNAMIC SIMULATION OF THE ENTIRE CRYSTAL GROWTH PROCESS : MULTI-SCALE ANALYSIS OF MELT FLOW TRANSIENTS

V. Regnier, L. Wu, B. Delsaute,
F. Bioul, N. Van den Bogaert, F. Dupret

CESAME, Université catholique de Louvain, E-mail: fd@mema.ucl.ac.be

Abstract

This paper investigates the transient melt flow evolution during a complete Czochralski crystal growth process. Two basic time scales are considered. The short scale concerns the basic transients associated with flow oscillations at different process stages. Accurate understanding of the flow mechanisms at this scale is required to develop an average axisymmetric flow model for complete dynamic simulations. The long time scale is associated with the transients caused by the slower system evolution occurring during the complete growth process. In order to focus on the fundamental effects governing the flow, a model problem is considered where the liquid is placed into a possibly rotating container while a disk of smaller diameter rotates on its top surface. Both the container and the disk are isothermal. Several transient effects are investigated including the effect of disk radius increase or decrease, and abrupt changes of disk or container temperature or rotation rate.

Introduction : dynamic modeling of crystal growth by means of the FEMAG software

There is increasing demand today for robust, reliable and user-friendly software to model bulk growth techniques such as the Czochralski (Cz), Liquid Encapsulated Czochralski (LEC), Floating Zone (FZ) and Vertical Bridgman (VB) processes. The aim is to help predict, design and control the growth processes, and to better understand the factors affecting crystal quality. However, the growth techniques are more and more complex, and optimization can be achieved only by use of suitable numerical modeling that accounts for the severely non-linear physical phenomena involved as well as for the high system thermal inertia. The resulting problem is coupled, global, nonlinear and dynamic. On the other hand, accurate prediction of crystal quality requires both appropriate modeling of the governing physics, and highly accurate dynamic numerical methods for computing the evolution of the solid-liquid interface shape and the temperature field gradient in its vicinity.

The FEMAG simulation software developed in the CESAME center of the University of Louvain is currently used by major crystal growth companies. The numerical model is both global and dynamic, and takes the effect of melt convection into account. Diffuse surface radiation is considered. Geometrical unknowns are dynamically coupled to the other unknowns, i.e. temperature field, velocity field, electrical potential, etc., leading to a complex non-linear system of equations whose solution is found by use of a decoupled scheme at every time step of the simulation. Whereas in its first generation FEMAG already performed global quasi-steady or time-dependent simulations, applications were restricted to top cone, shouldering and body growth stages. Both laminar and non-laminar flow models were considered, including or not the effect of axisymmetric magnetic fields. The objective of launching the FEMAG-2 software generation has been to provide a fully automatic simulator predicting the entire growth process while handling correctly the switches between the growth stages, together with coupling dynamic calculations with accurate melt flow prediction.

A significant difficulty lay in the important evolution of the system geometry during a complete growth process. Indeed, the solidified region is very small during seeding and subsequently becomes larger and larger, while the volume of the molten region decreases continually and can take a complex shape during tail-end stage. The solution adopted combines several approaches based on a representation of the furnace by means of deforming unstructured meshes together with automatic mesh generation. New geometrical methods were designed to allow easy calculation of the different system free surfaces (solidification front, melt/gas interface including crystal/melt and crucible/melt menisci, and crystal/gas surface). These methods allow performing easy time-dependent simulations even for stages of the process where important geometrical changes occur.

Another important difficulty to address in FEMAG-2 development was related to the complexity of dynamic melt flow modeling. Several problems must be solved to accurately couple melt flow predictions with crystal growth process simulation. First, in semi-conductor growth, the melt flow is time-dependent, 3D and weakly turbulent, whereas it can exhibit 3D azimuthal and temporal structured oscillations. The use of an axisymmetric quasi-steady flow model is devoted to average the effect of these oscillations, and the principal issue is to determine reliable average flow models, with the corresponding boundary conditions, above the steady laminar regime. Secondly, due to high nonlinearities, the solution of non-laminar flow problems can be quite difficult while, in most cases, these problems exhibit the numerical stability and convergence issues of transport-dominated systems. To this end, appropriate iterative schemes and stabilization techniques were introduced into the FEMAG-2 flow module. Thirdly, in order to achieve coupling with global thermal calculations, the melt flow problem is solved in FEMAG-2 at several stages of the simulation by using a quasi-steady model, while long term thermal transients are treated by including appropriate source terms into the momentum and energy equations. Interpolation between the collected results provides the flow pattern and the velocity field at each time step of the dynamic simulation.

Crystal quality can be predicted from the melt flow and temperature histories as long as the physical models are known. Therefore, solid phase simulators are currently developed in FEMAG-2 to calculate defect formation, diffusion and recombination, dislocation generation and motion, etc., on the basis of heat transfer and flow simulation results. A related objective is to develop off-line control algorithms, the ultimate goal being to provide an easy way to determine the evolution of the different process parameters (heater power, pull rate, crystal and crucible rotation rates, crucible lift, magnetic field design and intensity…) in order to optimize selected process variables characterizing crystal shape and quality. For all these reasons it is of the utmost importance to develop accurate and reliable flow models for bulk crystal growth dynamic simulation.

Objectives of the paper in terms of melt flow modelling

The present paper is devoted to investigating the evolution of the melt flow regime and pattern during the complete Cz crystal growth process. To this end, two basic time scales must be considered. The short time scale, which is typically of the order of tens of seconds in silicon growth, concerns the basic transients associated with flow oscillations at different stages of the growth process. Accurate understanding of the flow behaviour at this scale is required to develop the average axisymmetric flow model to be used in global dynamic simulations. The long time scale, which is typically of the order of tens of minutes in Cz silicon growth, is associated with the flow and heat transfer transients caused by the long term system evolution. In particular, the melt height is continually decreasing during the complete growth process. In addition, the crystal radius changes significantly during cone growth and tail-end stages, while simultaneously the heat transfer is strongly affected by the heater power modifications required to obtain a crystal of the prescribed shape – it should be recalled that heater power is slowly decreased during conical growth in order to let crystal radius increase, while it experiences a quick peak during shouldering in order to stop conical growth, and it is progressively increased during tail-end stage in order to let crystal radius decrease to terminate the growth process.

As the aim is here to provide better understanding of the crystal growth melt flow transients at these two time scales, a model problem is considered where the liquid is placed into a possibly rotating cylindrical container while a rotating disk of smaller diameter is placed at the top surface of the liquid. The container and the disk are at uniform, but possibly different, temperatures in order to generate buoyancy forces from radial temperature gradient effect. The advantage of this approach is to allow focusing on the fundamental effects governing the flow by reducing the number of system parameters – the latter being the height of the liquid domain, the container and disk diameters and temperatures, and some material properties of the liquid. Additional parameters can be introduced to characterize the imposed magnetic field if any, but any other effect such as radiation transfer, which is not directly affecting the flow, is removed from the model in order to focus on flow issues only. For validation purpose, this system has been the object of isothermal and non-isothermal experimental investigations by means of a simple apparatus.

In order to capture the particular effects related to the flow behaviour at the short time scale (including the detail of its oscillations in a periodic, quasi-periodic or chaotic regime), a particular simulation technique has been developed where the long term effects are frozen while a laminar flow model is used. Very high mesh and time step refinements are required and therefore short time scale simulations, whose understanding represent a first objective of the paper, are limited to rather small periods of time.

On the other hand, long time scale simulations can only be performed provided an appropriate axisymmetric average flow model is introduced. This non-laminar model is developed by fitting the simulations to short time scale results. The second objective of the paper is to investigate by use of this non-laminar model the importance of the long term flow transients resulting from process parameter changes, such as increase or decrease of disk radius, abrupt change of temperature or rotation rate of the disk or the container, etc. To this end, several examples will be completely analyzed and presented at the conference.

References

F. Dupret, P. Nicodème, Y. Ryckmans, P. Wouters, M.J. Crochet, Int. J. Heat Mass Transfer, 33 (1990), 1849.

F. Dupret & N. Van den Bogaert, in *Handbook of Crystal Growth*, Vol. 2B, Ch. 15, Elsevier, Neth. (1994), 875.

R. Assaker, N. Van den Bogaert, F. Dupret, Magnetohydrodynamics, 31 (1995), 254.

N. Van den Bogaert & F. Dupret, J. Crystal Growth, 166 (1996), 446; 171 (1997), 65; 171 (1997), 77.

R. Assaker, N. Van den Bogaert, F. Dupret, J. Crystal Growth, 180 (1997), 450.

F. Dupret, N. Van den Bogaert, R. Assaker, V. Regnier, in Proc. 8th Int. Symp. on Si Mat. Sc. and Tech., 1998 ECS meeting, Proc. Vol. 98-1 of the Electrochem. Soc., Pennington, NJ (1998), 396.

T. Sinno, E. Dornberger, R.A. Brown, W. von Ammon, F. Dupret, Materials Science and Engineering: R Reports, 28 (2000), 149.