Global Simulation of CZ and FZ Bulk Crystal Growth: from Quasi-Dynamic and Dynamic Modelling to Process Control and Crystal Quality Optimization

F. Dupret[a,b], R. Rolinsky[b], L. Wu[b], F. Loix[b],
A. de Potter[b], N. Van den Bogaert[b], and V. Regnier[b]

[a] CESAME Research Center, Université catholique de Louvain,
B-1348 Louvain-la-Neuve, Belgium
[b] FEMAG*Soft* S.A. Company, B-1435 Mont-Saint-Guibert, Belgium

When Silicon ingots are grown for IC or PV applications, the crystal diameter has to conform to current market requirements while the crystal defects and composition have to be perfectly controlled. The present paper is devoted to illustrate CZ and FZ process optimization by use of the time-dependent FEMAG.2 software. First, the "off-line control" technique is devoted to determine the heater power and pull rate histories required to obtain a crystal of constant diameter and optimal quality by means of fully transient simulations. Other command parameters such as crystal and crucible rotation rates, magnetic field intensity, etc., can be optimized as well. Secondly, the use of quasi-dynamic numerical simulations shows very efficient to study the transient effects experienced by the system during bulk crystal growth, without necessitating a fully dynamic simulation. A main application of this technique is to improve the design of an automatic controller of the growth process.

Introduction

The growth of Silicon (Si) crystals by the Czochralski (Cz) or Floating Zone (FZ) technique for electronic (IC) applications has been governed for more than 50 years by two technological objectives. First, the crystal diameter has to be nearly constant and the largest possible according to market requirements. Secondly, the product quality has to be perfectly controlled in terms of crystal defects and composition. On the other hand, growing Cz Si crystals for photo-voltaic (PV) applications requires to minimize both the energy consumption and the growth duration without, however, generating a too large content of micro-voids in the crystal. Achieving these somewhat contradictory goals is by no means easy since increasing the crystal diameter requires a larger melt volume and hence results in a much more complex melt flow regime with complicated heat, momentum and species transport effects, a very sensitive solid-liquid interface shape (with a less uniform thermal gradient), and in general an enhanced dynamic system behavior. A similar enhancement of the system dynamic behavior can result from the use of a high pull rate to increase the growth speed. Therefore, in general, designing the furnace hot zone requires to introduce appropriate heat shields in order to well-control the radiation heat transfer while in Cz growth a satisfactory melt flow pattern can only be obtained for large diameter crystals by the action of transverse or configured magnetic fields. Moreover the selection of optimal process parameters (heater power or inductor voltage, crystal pulling rate, crystal and crucible or feed-rod rotation rates, magnetic field intensity if any, ambient gas flow rate, etc.) becomes much more difficult in view of the

increased system nonlinearity and time-dependency, especially during the critical process stages (necking, shouldering, tail-end stage, crystal detachment, …).

Nonetheless, in front of these technological difficulties, huge progress has been achieved in the last decades in different scientific domains. First, the physics of radiation and convection, on the one hand, and of defect formation and transport in Si crystals, on the other hand, is much better known, and hence the mathematical models governing Si growth are better and better established. Whereas important improvements remain necessary in the modeling of turbulence in the melt and the ambient gas (including the modeling of melt turbulence under the effect of a magnetic field) while the material parameters governing point- and micro-defect evolution in Si single crystals still are insufficiently known, an almost complete picture of the physics of Si growth today is available. Secondly, numerical methods and computers have also quickly progressed since the development of the first models of Cz and FZ growth achieved in the 1980's. Nowadays the quasi-steady or time-dependent simulation of these processes has become possible in an acceptable computing time, with sufficiently refined meshes to resolve the key details of the problem, and with appropriate numerical techniques to handle the system deforming geometry (which comprises several moving components together with free boundaries such as the melt-crystal and melt-gas, and possibly the melt-feed rod, interfaces).

Having at one's disposal the appropriate physical models, numerical tools and computer hardware directly opens the route to Cz or FZ process optimization by means of numerical simulation. The objective of the present paper is to illustrate how this straightforward strategy can be applied by use of the FEMAG-CZ or FEMAG-FZ software (collectively called FEMAG) as today co-developed by FEMAG*Soft* S.A. Company and the CESAME research center of the Université de Louvain (Belgium).

The global and time-dependent FEMAG-CZ and FEMAG-FZ models

FEMAG software products are currently used by major Si growers in the world. The numerical model is both global and dynamic, and takes the effect of melt convection into account. Diffuse surface radiation is considered, while frequency-dependent material properties are modeled by means of the band-energy technique. Radiation calculations are performed by accurate integration of the surface view factors around the furnace axis. The global model of FEMAG-CZ takes all important physical phenomena of the growth process into account, i.e. heat transfer by conduction in every furnace constituent and by convection in the melt and gas phases, together with solidification at the solid/liquid interface, surface tension, etc. Geometrical unknowns are dynamically coupled to the other unknowns, i.e. temperature field, velocity field, electrical potential (in the presence of a magnetic field), 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 the FEMAG.1 software family already performed global quasi-steady or time-dependent simulations, the 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 (axial, cusp or rotating) magnetic fields. The objective of launching the FEMAG.2 software generation has been

to provide a fully automatic dynamic simulator predicting the entire growth process, without any manual user's intervention during simulation, while handling correctly the switches between the growth stages (poly-crystal melting, seeding, conical growth, shouldering, body growth, tail-end stage and after growth cooling), together with coupling the dynamic calculations with accurate melt flow prediction.

However 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 in Cz growth, the volume of the molten region decreases continually and can take a complex shape during tail-end stage. Similar geometrical difficulties are encountered in the modeling of FZ growth. The solution adopted in FEMAG.2 combines several approaches based on a representation of the furnace by means of deforming unstructured meshes together with automatic mesh generation. New geometrical methods have been designed to allow easy calculation of the different system free surfaces (solidification front, melt/gas interface including crystal/melt and crucible/melt or feed rod/melt menisci, and crystal/gas surface) through a single mathematical formulation, valid for all possible configurations. These methods allow the user to perform easy time-dependent simulations even for those stages of the process where important geometrical changes occur.

Another important issue to address in the development of FEMAG.2 was related to the complexity of dynamic melt flow modeling. In fact, in Cz Si growth, two time scales have to be considered. The short scale, typically of the order of tens of seconds, governs the basic transients associated with melt flow oscillations at the different process stages – noting that the flow exhibits weak turbulence superposed to 3D azimuthal and temporal structured oscillations. The long time scale, typically of the order of tens of minutes, is associated with the flow and heat transfer transients caused by the long term system evolution – since melt and crystal shapes continually change and can be very complex during some growth stages (especially during the beginning and the end of the growth process), while the heat transfer is strongly affected by melt-crystal interface deformation and by the heater power evolution required to grow a crystal of the prescribed shape. Although the melt flow in FZ Si growth is normally laminar, its behavior is also oscillatory and rather complex.

Therefore the basic problem to address in order to couple flow predictions with global dynamic simulations was to develop a model able to average the effect of the flow oscillations above the steady laminar regime. To this end, two models (viz. the "Mixing Length" and k-l models) were investigated, as based on the Boussinesq approach with use of an additional eddy viscosity and thermal conductivity to account for the enhancing effect of the flow oscillations on heat and momentum transfer in the melt or the ambient gas. In the former case the additional viscosity and thermal conductivity are functions of the mixing length l only, while they are functions of the mixing length and the additional kinetic energy k in the latter case. In both cases, the mixing length represents a key parameter whose accurate modeling allows the user to fit the numerical predictions to experimental measurements, by means of an appropriate tuning of the boundary layer thicknesses along the melt or gas interfaces with the surroundings.

A typical time-dependent inverse global result obtained by means of FEMAG-CZ.2 is shown in Fig. 1.

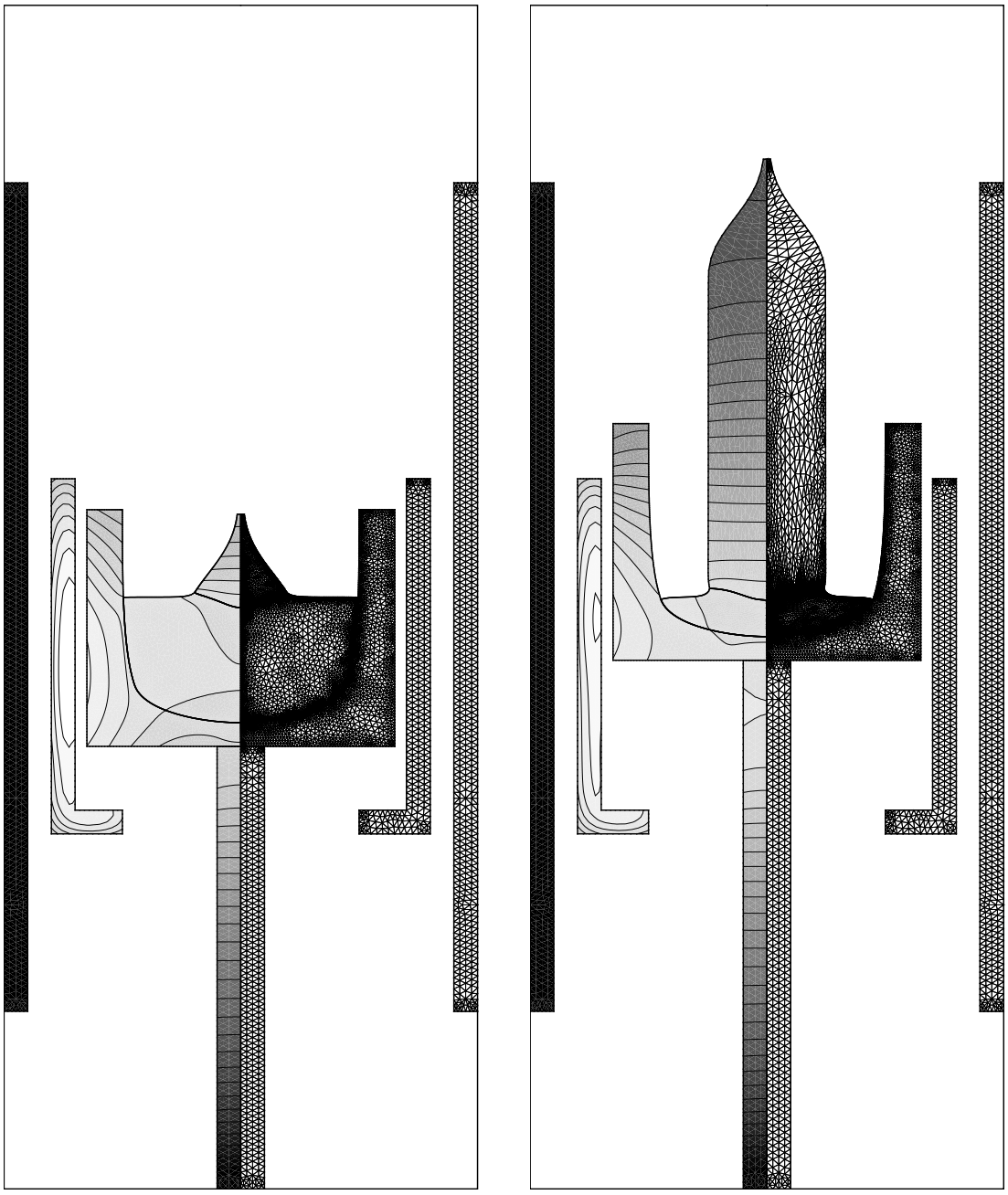

Figure 1. Growth of a 100 mm Si crystal (pulling rate: 0.5 mm/min; crystal rotation rate: 10 rpm; crucible rotation rate: -5 rpm). Temperature field by steps of 50 K and deforming mesh calculated at 2 growth stages by means of a transient FEMAG-CZ.2 simulation.

Prediction of defects and species distribution in the solid phase

A key issue in Cz or FZ Si growth is to reduce defect density to the lowest possible level. Therefore the effort paid for several years to understand the mechanisms governing the

formation and evolution of vacancies, self-interstitials, micro-voids, clusters, dislocation loops, etc., in the growing crystal has brought reasonably good models on the basis of Voronkov's theory. However numerical experiments reveal a high sensitivity of the defect distribution both to the material parameters governing defect diffusion, recombination and agglomeration, and to the thermal gradient prevailing in the crystal (especially along the solidification front). Therefore accurate numerical models are needed when the objective is to improve the growth process.

Using the FEMAG.2 software, we here present a fully time-dependent model devoted to predict the global heat transfer in the furnace, the solid-liquid interface shape, and the resulting distributions of point- and micro-defects in the crystal as calculated from the Sinno-Dornberger (S-D) model together with an extension of the lumped model of Voronkov and Kulkarni. All the transients are considered including the effects of crystal and crucible lift, of the heat capacities of the furnace constituents, of the thermal inertia of the solidification front, and of the dynamic defect governing laws. In addition to the classical point-defect evolution mechanisms, a new lumped model is introduced to calculate the formation and growth of micro-defects in order to predict their densities and size distributions anywhere in the crystal.

We also show that dynamic effects deeply affect the defect distribution in the crystal. Indeed, the interface deformation caused by any change of the operating conditions directly affects the temperature gradient above the interface and the resulting defect densities through the V/G ratio. Moreover, as point- and micro-defects are transported while diffusing and reacting, the defect distribution in the crystal is a picture of the past history of defect generation and can only be predicted by means of a dynamic model.

Another key issue in Si growth is to control the density of oxygen (in Cz growth) and any other species (including dopants and impurities) inside the crystal. To address this problem several important difficulties have to be solved. First, the transport of any species in the melt is governed by complex mechanisms where the flow oscillations play a major role with respect to the very low molecular diffusivity. Here again an additional diffusivity has to be introduced in order to account for the enhancing effect of the flow oscillations on mass transfer in the melt (or the ambient gas), and the Mixing Length or *k-l* model can readily be used for this purpose. The second and more important difficulty to overcome in order to simulate species transport in the melt and the gas in Cz or FZ Si growth is to well-model the boundary conditions along the different interfaces separating the flows from their surroundings. In particular the way oxygen escapes from the melt to the gas in Cz growth strongly affects its distribution in the crystal and therefore the boundary layers along both sides of the melt-gas interface have to be accurately modeled. On the other hand segregation can deeply affect the distribution of some dopants in Si crystals. Here again addressing this problem requires to appropriately model the melt boundary layer located along the solidification interface.

The ultimate goal of these investigations is to get a complete and reliable picture of the entire set of mechanisms governing the quality of Cz- or FZ-grown Si crystals.

Off-line and on-line process control

The main interest of a time-dependent simulator such as FEMAG.2 is to help the crystal grower in the design of a new furnace (including the design of the furnace hot zone) and the optimization of the growth process. This latter objective can be achieved in two ways. On the one hand, the "off-line" control technique is devoted to optimize the selection of the crystal growth processing conditions. In other words, off-line control provides master (or profile) curves that have to be followed by the processing conditions in order to grow a crystal of the highest quality. On the other hand, various kinds of time-dependent simulations can be very efficiently used to improve the design of a Cz or FZ "on-line" (or off-line) controller.

Off-line control

In general 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 or inductor voltage, …) are calculated to satisfy these constraints. Typically, in inverse 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; pulling rate; crystal, crucible or feed rod 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 in order to optimize crystal quality.

Typically, in Si 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 or feed rod 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.

On-line control

The other significant interest of time-dependent simulations is to provide various attractive techniques to improve the process control. High quality controller design can be achieved by means of quasi-dynamic and direct dynamic simulations.

Quasi-dynamic simulations. For a given crystal shape and vertical position, a quasi-steady global model of the pulling process is defined by making the assumption that all operating conditions are kept constant and that the solid-liquid interface shape is kept fixed while the solidification heat is released from the solid-liquid interface in proportion to the pull rate. The resulting equations do not contain transient terms anymore. This

model is inverse, because it is necessary to let one of the process parameters (typically the heater power) become an unknown whose value is calculated in order to get the prescribed crystal diameter.

The *quasi-dynamic* simulation technique is an extension of the quasi-steady model where the crystal position is again frozen together with the geometry (including the crucible height), while the melt-crystal interface is allowed to dynamically deform and the other process parameters are allowed to change with time. In other words, the geometrical modifications resulting from the upward motion of the crystal, the crucible, the pedestal, etc., are not considered, while the sole effect of the crystal vertical motion is to release solidification heat along the melt-crystal interface. However, this interface itself (and only this interface) is allowed to deform, hence releasing some extra-solidification heat, and the transients of the melt and all other components are taken into account together with any possible change of the operating conditions (pulling rate, rotation rates, etc.). In this way the simulation is able to capture the short time scales governing the melt flow dynamics and their effect on the melt-crystal interface deformation and the heat transfer in the crystal just above this interface. Obviously the quasi-dynamic simulation model represents a key tool to improve the design of an off-line or an on-line controller of the growth process.

As an example, Figs. 2-5 depict the results obtained by designing a controller on the basis of quasi-dynamic simulations. The objective is to optimize the quality of an Si crystal as measured either by the axial interface deflection z_{ax} (defined as the difference between the vertical positions of the melt-crystal interface at the tri-junction and on the axis) or by the well-known v/G ratio. The control variable is the pulling rate v_{pul}. The short time constants governing the system have been identified by performing a quasi-dynamic simulation of the system response to a 5% stepwise decrease of the pulling rate. A simple PI controller was subsequently designed from these results and inverse, off-line controlled, dynamic simulations were performed to analyze the effect of this controller on the resulting crystal quality.

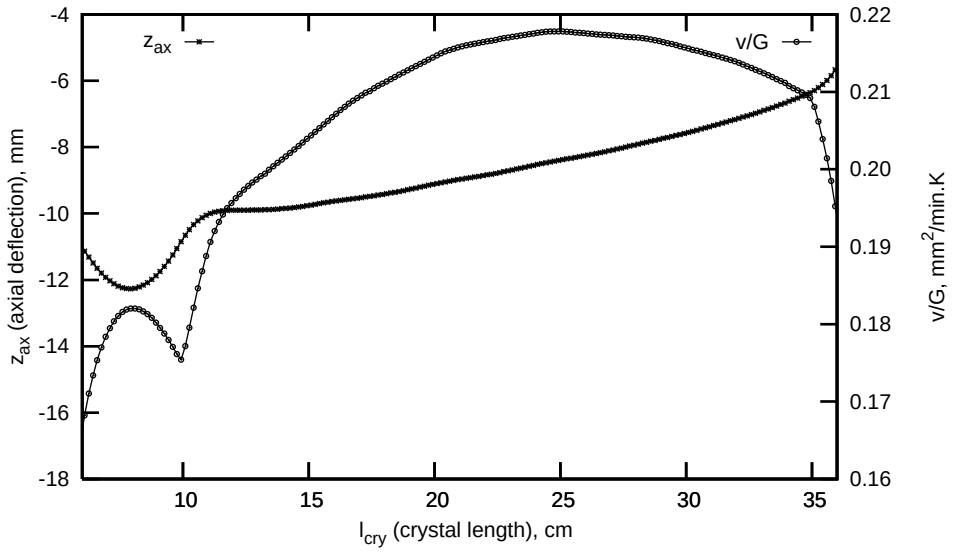

Figure 2. Uncontrolled simulation of the problem of Fig. 1. Evolution of the axial interface deflection z_{ax} and the v/G ratio as a function of the grown crystal length l_{cry}.

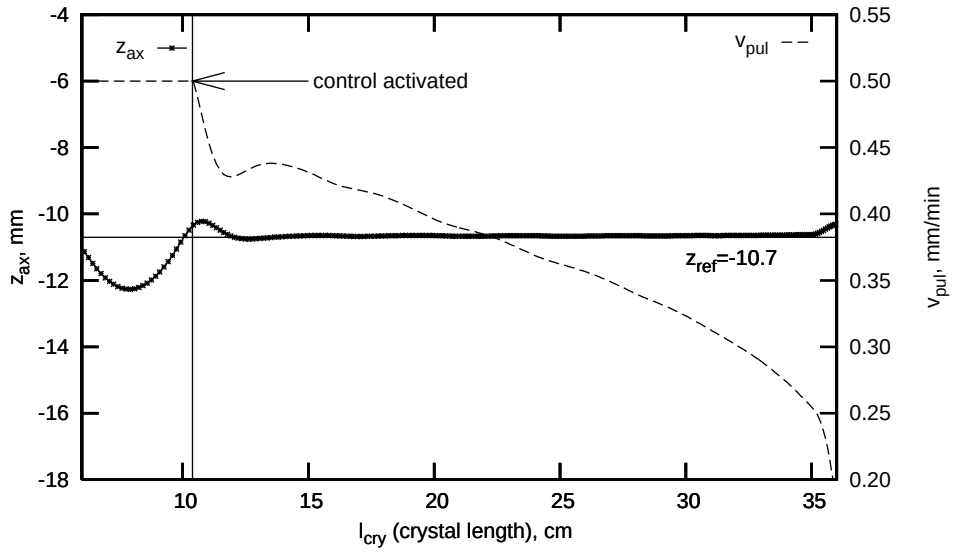

Figure 3. First transient simulation, with an off-line controlled axial interface deflection z_{ax} while the pulling rate v_{pul} is the control variable.

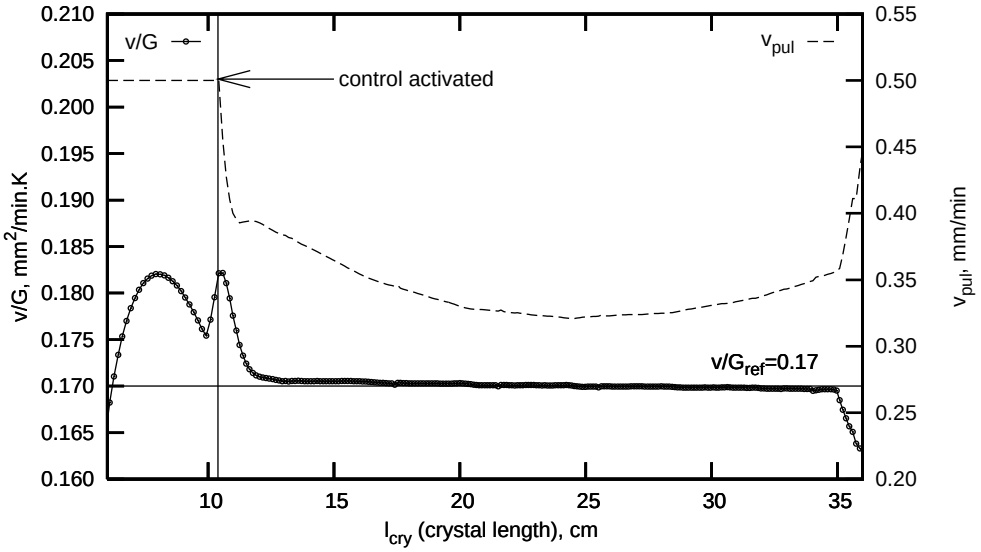

Figure 4. Second transient simulation, with an off-line controlled v/G ratio while the pulling rate v_{pul} is the control variable.

The results clearly show that our procedure was quite successful. The quality of the identified controller can immediately be observed from Figs. 3 and 4, where the system quickly stabilizes to the prescribed z_{ax} or v/G by appropriate action on the pulling rate. Moreover, Fig. 5 indicates in addition that well-controlling either of these variables should result in an improved crystal quality as long as the calculated difference between the interstitial and vacancy densities C_I and C_V represents a good indicator of this quality (it is worth recalling here that growing Si crystals with a low C_I - C_V is a requirement for several IC components).

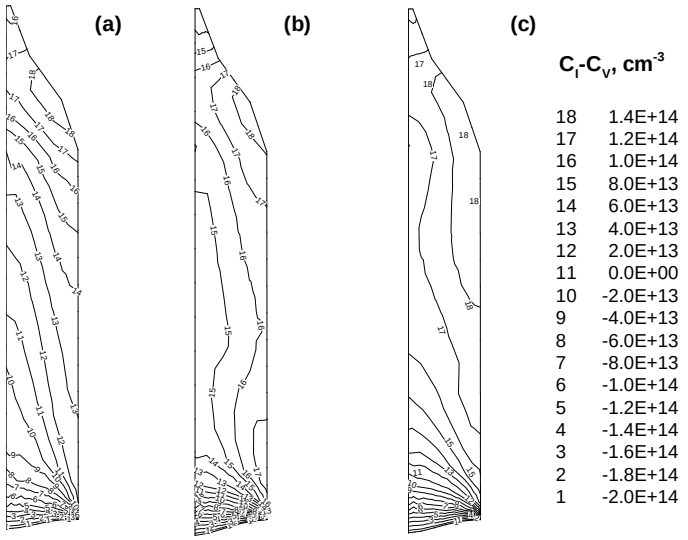

Figure 5. Isovalues of C_I - C_V in the crystal for the three considered transient simulations of the problem of Fig. 1. (a) uncontrolled simulation; (b) off-line controlled axial interface deflection z_{ax}; (c) off-line controlled v/G ratio.

Direct dynamic simulations. Finally, the *direct dynamic* simulation technique is defined by first performing an inverse dynamic reference simulation (where the pull rate profile and the crystal shape are imposed while the heater power history is calculated to obtain the imposed crystal shape), and then by perturbing this reference simulation by slightly modifying the heater power or the pull rate history and calculating the resulting crystal shape. Typically, stepwise decreases of the heater power or the pulling rate profiles can be applied and, in this way, the direct dynamic simulations are able to capture the longer time scales of the growth furnace dynamics and their delayed effect on the crystal diameter. Obviously this technique represents a valuable complementary tool for the design of a crystal growth controller with respect to quasi-dynamic simulations.

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