XIII International Autunmn Meeting
"Gettering and defect engineering in Semi-conductor Technology", GADEST 2009
September 26 – October 02, 2009, Döllnsee-Schorfheide, Germany

Optimization of Silicon Ingot Quality by the Numerical Prediction of Bulk Crystal Defects

F. Loix[2*], F. Dupret[1,2*], A. de Potter[2], R. Rolinsky[2], N. Van den Bogaert[2], V. Regnier[2]

[1]*CESAME Research Center, Université catholique de Louvain, Bâtiment EULER, 4 av. Georges Lemaître, B-1348 Louvain-la-Neuve, Belgium*
[2]*FEMAGSoft S.A. Company, 7 Rue André Dumont, Axis Parc, B-1435 Mont-Saint-Guibert, Belgium*

Responsible author : loix@femagsoft.com – 0032-10.226.452

The growth of Silicon (Si) ingots by the Czochralski (Cz) technique for electronic (IC) applications has been governed for more than 50 years by two, somewhat contradictory, technological objectives. First, the crystal diameter has to be nearly constant and the largest possible according to current market requirements. Second, 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 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 will require to introduce appropriate heat shields in order to well-control the radiation heat transfer while 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, crystal pulling rate, crystal and crucible 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, compared to the high difficulty to address these different technological issues, it is worth observing that huge progress has been achieved in the last decades in several scientific domains. First, the physics of radiation and convection in Cz furnaces, and of defect formation and transport in growing Si crystals, is much better known, and hence the mathematical models governing Cz Si crystal growth are better and better established. In spite of the important improvements that 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) and of the still insufficient knowledge of the material parameters governing point- and micro-defect evolution in Si single crystals, 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 growth achieved in the 1980's. Nowadays the quasi-steady or time-dependent simulation of the Cz process 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 interfaces).

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

We will here focus on the Si ingot quality prediction and its optimization. We 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 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. We hence show that dynamic effects deeply affect the defect distribution in the crystal (fig 1.). In addition to the classical point-defect evolution mechanisms, a new lumped model is developed to calculate the formation and growth of micro-defects in order to predict their densities and size distributions anywhere in the crystal.

Another key issue in Cz Si growth is to control the density of oxygen and any other species (including dopants and impurities) inside the crystal. Modeling issues will be here again detailed.

Finally, off-line process control principles will be addressed. Results will illustrate how this tool can help in optimizing crystal shape and quality.

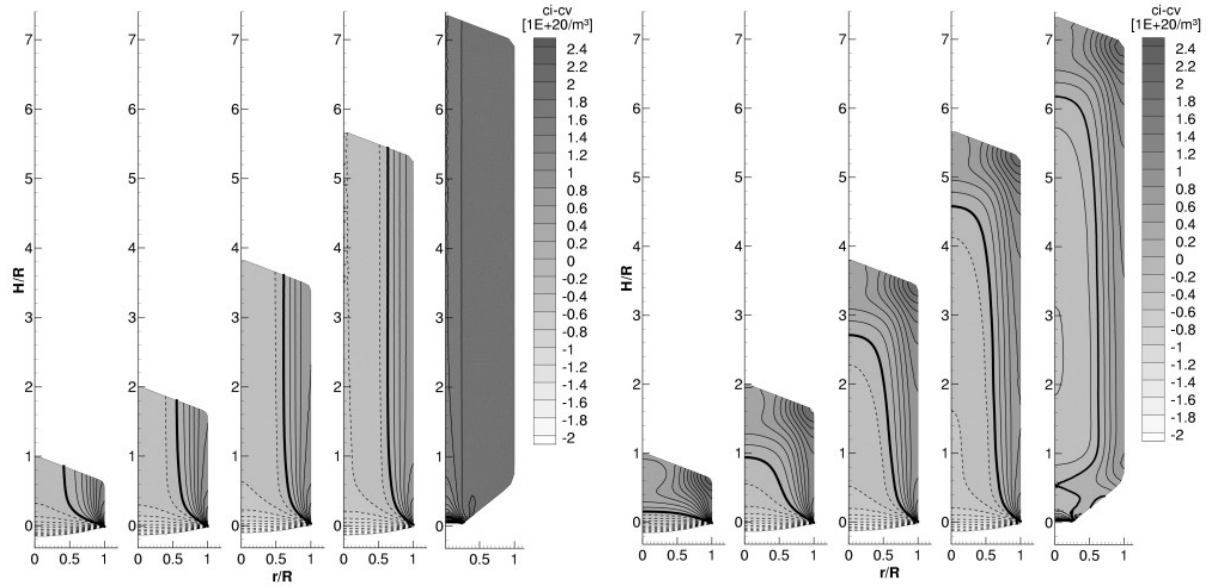

Fig. 1. Predicted defect delta C_i-C_v distribution (C_i, C_v being the concentration of interstitials , vacancies respectively) with a quasi-steady (a) and a time-dependent (b) simulation. The OSF ring is located at the position where delta ~= 0. This picture highlights the strong impact on the point defect of the transient effects in the growing crystal.