The Software for
Bulk Crystal Growth Simulation

Center for Systems Engineering
and Applied Mechanics of UCL

PREDICTION OF DEFECT FORMATION IN CZOCHRALSKI SILICON GROWTH

F. Dupret[1,2], N. Van Goethem[1], N. Van den Bogaert[2], A. de Potter[2], R. Rolinsky[2]
[1]*CESAME, Université catholique de Louvain, Louvain-la-Neuve, Belgium*
[2]*FEMAGSoft S.A. Company, 4 av. A. Einstein, B-1348 Louvain-la-Neuve, Belgium*

A major issue in Czochralski silicon 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 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 software, we present a fully time-dependent model in order to predict the global heat transfer in the furnace, the solid-liquid interface shape, and the 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 furnace constituent heat capacities, of the solidification front thermal inertia, 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.

It is also shown 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 thermal gradient above the interface and the resulting defect densities through the V/G ratio. Moreover, since point defects are transported while diffusing and reacting, the defect distribution inside the crystal is a picture of the past history of defect generation and can only be predicted by means of a dynamic model.

Finally, a major drawback of the S-D model and its variants and extensions comes from the strong discrepancy between the model diffusion coefficients and their experimental counterparts as proposed by several authors (experimental values are between 1 and 2 orders of magnitude higher than in S-D model). To reconcile both approaches, an attempt is made to adapt the model parameters in order to better agree with available measurements of self-interstitial and vacancy diffusions while respecting the V/G criterion. It is shown that introducing a thermal drift effect can facilitate the construction of a relevant model.

Correspond. author: F. Dupret, phone +32-(0)10-47-2350, fax +32-(0)10-47-2180 fd@mema.ucl.ac.be