DYNAMIC PREDICTION OF DEFECT FORMATION IN CZOCHRALSKI SILICON GROWTH. ANALYSIS OF THE DISCREPANCY BETWEEN EXPERIMENTAL DEFECT DIFFUSION COEFFICIENTS AND THE V/G CRITERION

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Proposed session topic: defects

A major issue in Czochralski (Cz) silicon (Si) growth is to reduce the defect density to the lowest possible level, especially when the aim is to produce defect-free crystals. Therefore the effort paid for the last years to understand the mechanisms governing the formation and evolution of self-interstitials and vacancies in the growing crystal has brought reasonably good models on the basis of the Voronkov theory. However numerical experiments reveal a very high sensitivity of the defect distribution in the crystal both to the material parameters governing defect diffusion and recombination and to the thermal gradient in the crystal along the solidification front. Therefore very accurate numerical tools are needed when the objective is to improve the crystal growth process on the basis of defect modeling.

Using the FEMAG simulation software, we present a fully time-dependent model for the prediction of the global heat transfer in the furnace, of the solid-liquid interface shape, and of the resulting distribution of self-interstitials and vacancies in the crystal as calculated on the basis of the well-known Sinno-Dornberger (S-D) model [1]. All the system transients are taken into account including the effects of crystal and crucible lift, of the heat capacity of the furnace constituents, of the solidification front thermal inertia, and of the inherently time-dependent defect governing laws. It is shown that dynamic effects deeply influence the defect distribution in Cz Si crystals for two reasons. First, the interface deformation caused by any change of the operating conditions (pull rate, heater power, rotation rates, magnetic field intensity...) and, in particular, the rapid interface shape change experienced during shouldering directly affect the thermal gradient above the interface and the resulting interstitial and vacancy densities through the well-known V/G ratio. Secondly, 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 cannot be correctly predicted by means of a quasi-steady model. Various simulations have been performed to compare time-dependent and quasi-steady predictions and to illustrate the system sensitivity to the above-mentioned dynamic effects. A typical example is shown in Fig. 1.

In spite of these recent progresses, a major drawback of the S-D model and its variants comes from the strong discrepancy between the model diffusion coefficients and their experimental counterparts as proposed in the literature by Stolwijk, Bracht, and other

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authors [2, 3]. In fact these experimental values are between 1 and 2 orders of magnitude higher than in the S-D model. Therefore a major objective should be to reconcile both approaches. To this end, the 2^{nd} objective of the present paper has been to adapt the material parameters governing point defect diffusion and recombination in order to better agree with available measurements of self-interstitial and vacancy diffusion while respecting the V=G criterion. It is shown that introducing a thermal drift effect can facilitate the construction of a relevant model satisfying both conditions.



Figure 1. Comparison of quasi-steady (left) with time-dependent (right) point defect predictions by means of FEMAG simulations. Isolines of the C_{I} - C_{V} distributions. The C_{I} - $C_{V}=0$ isoline is indicated in bold. Crystal radius : R = 7.5 cm. Pulling rate : V = 4.5 cm/h (0.75 mm/min).

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