Silicon solidification near a well-characterized grain boundary: comparison between experiment and analytical model

Abstact: A model based on Ben Amar-Pomeau (BAP) equation for faceted solid-liquid interfaces is proposed, in order to interpret experimental results obtained in silicon solidification experiments. We focus here on the case of a Σ27a grain boundary. The dynamics of the grain boundary groove displays pinning of the groove bottom, steady increase of the facets that bound the groove, and, at regular time intervals, rapid solidification of the liquid trapped inside the groove. The proposed model produces a time evolution of the solid-liquid interface that compares very quantitatively with the experiments.

Grain boundaries usually have detrimental effects on the conduction properties of silicon. These effects can result from local breaking of the crystalline translational order and/or breaking of the chemical purity. Understanding the role of grain boundaries is thus crucial to help controlling the quality of silicon produced through a solidification process for applications such as solar energy conversion.

During my visit at IMR Sendai, one year ago, I worked in Pr. Fujiwara's group, specifically discussing one of their experiments where the time evolution of a grain boundary of the Σ27a type was observed [1]. Near the grain boundary, the solid-liquid (S-L) interface forms a wedge groove limited by two (111) facets. The deepest point of the groove appears to be pinned at a fixed location. As time flows, the two facets that bound the groove increase in size. At regular time intervals, rapid solidification of the liquid trapped inside the groove occurs (see Fig.1) and the groove recovers its initial small size. This evolution has a period of a few tens of seconds.

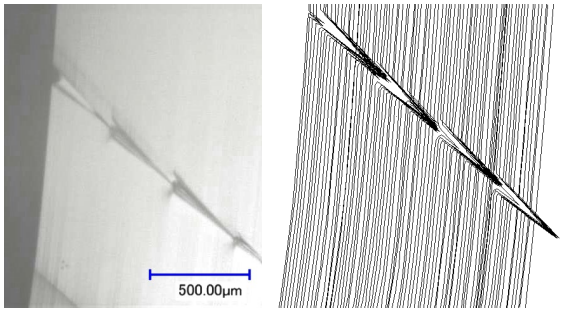

Fig. 1 S-L front evolution in the experiment

In order to interpret this experiment, I proposed a simple model based on the following assumptions [2]:

1. BAP interface equation holds any time
2. Groove bottom is fixed
3. Facet normal velocity is zero
4. Global front velocity *V* is constant
5. Temperature gradient *G* in the groove reduces in time, due to thermal effects

A simple code based on this model was implemented with the experimental values *V*=15.7 µm/s and *G*=3.7 K/cm that correspond to Fig.1. Time evolution of the front over a period of 30 s is represented in Fig.2.

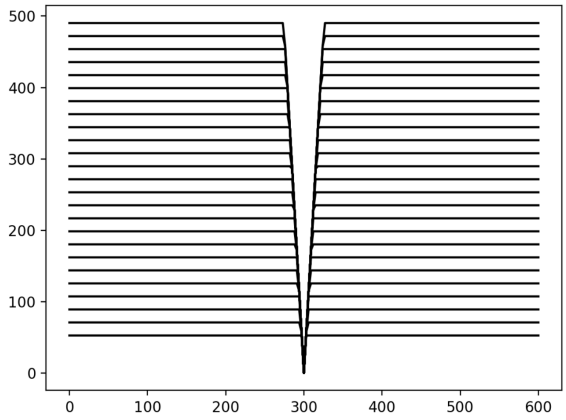

Fig. 2 S-L front evolution in the model (scales in µm)

The proposed model produces a time evolution of the solid-liquid interface that compares very quantitatively with the experiments. Possible improvements of the model would consist in relaxing some of the assumptions made (1 to 5). For instance, assumption 4 may be made less stringent to mimic the experimental observation that the outer front velocity is not perfectly constant (see Fig.1).

References

[1] Lu-Chung Chuang and K. Fujiwara, unpublished results.
[2] Jean-Marc Debierre, unpublished results.

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