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Study of evolution of dislocation clusters in high performance multicrystalline silicon

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ABSTRACT

The evolution of dislocation clusters in High Performance Multicrystalline Silicon was studied by means of photoluminescence imaging, defect etching and Electron Backscatter Diffraction. Cluster height was found to increase as function of lateral size. The largest clusters were found to exist in twinned grains or spanning multiple grains. Dislocation clusters were seen to originate at CSL boundaries and terminate at random angle grain boundaries. It is suggested that termination, as well as generation of dislocation clusters are growth phenomena, which are controlled by the dislocations following the growth front, and that the successful termination of dislocation clusters is a simple function of distance between grain boundaries able to terminate the dislocations at the growth front. It is also suggested that crystal orientation may influence the mechanism through the ability of dislocation clusters to traverse the grain laterally from a generation to a termination site.

1. Introduction

While multicrystalline silicon has been the dominating solar cell technology for many years, the material contains inherent defects such as grain boundaries, dislocations and impurities originating from the crucibles and coating. The interaction between impurities and defects causes severe carrier recombination, particularly in regions where defect clusters are dominating. Such defect clusters tend to follow the columnar grain structure and become increasingly dominating towards the ingot top. This results in reduced lifetime and cell efficiency, and a large scatter in the same parameters from wafers taken from different regions and heights. High efficiency solar cell architectures cannot presently be successfully applied to multicrystalline silicon.

However, recently the influence of nucleation on the properties of defects has been acknowledged. The pioneering work performed at the Tohoku University focusing on nucleation and initial growth showed how grain size and grain orientation preference (texture) could be controlled via the initial supercooling; the growth mode could be varied between nucleation of small grains with a seemingly random orientation and large grains with a preferred vertical orientation of ⟨211⟩ or ⟨110⟩ promoted by lateral dendritic growth in the initial phase [1]. Later it was shown that elements of this mechanism for structure control is likely present in regular industrial production of multicrystalline silicon, and it was suggested that defect density in the bulk material could be related to how well the initial growth had aligned in an horizontal manner [2]. Generation of dislocations at stress concentrations on grain boundaries was proposed to be an important element determining the quality of multicrystalline silicon produced with the proposed dendritic growth method [3], and it has been shown that certain grain boundaries may act as dislocation nucleation centers that may severely affect the crystal quality, i.e. increasing the dislocation density locally in certain grains [4,5]. Although dislocations undergo a series of development and transformation during the thermal cycle of the ingot production, there are good indications that dislocation clusters are originating and achieve their characteristics at high temperature and in close proximity of the solid liquid interface [5–7]. While there are diverging views on this [8] and large focus is also placed on multiplication of existing dislocations due to thermal stress during cooling of the crystal (where differing dislocation density is explained by different conditions for multiplication in different grains), the premise that dislocation clusters originate close to, and follow the growth front, is important for the discussion in this paper.

Industrial development of the technique for achieving structure control through initial dendritic growth proved difficult, and this was mainly attributed to the difficulty in controlling the thermal conditions over large crucible areas. While the emergence of focus on nucleation conditions is rightly attributed to the work performed at the Tohoku University [1,3], it became clear that the other extreme in grain configuration, i.e. small initial grains of random orientation, was not so disadvantageous considering

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dislocation density, and several producers began implementing nucleation schemes that favored this configuration [9]. Such technology proved easier to control, and producers have improved this product to a degree that it is now commonly known as High Performance Multicrystalline Silicon (HPMCSi). It is important to note that different producers have different approaches to achieve this quality and that the label refers to a product with a certain characteristic rather than resulting from a specific process. The characteristics are: Small grain size, high proportion of random angle grain boundaries, low density of dislocation clusters and a mechanism by which dislocation clusters that do appear during crystallization also disappear again at a higher level in the ingot rather than being allowed to dominate the quality all the way to the top of the ingot. All the major suppliers of multicrystalline silicon have now tuned their production to produce material of such quality.

It is highly interesting to understand why this structure is preferential for lower dislocation density. Governing factors can be:

- Reduced possibility of dislocation generation (fewer generation sites).
- Reduced driving force for dislocation multiplication by plastic deformation.
- Increased probability of elimination of clusters by grain selection, termination at special grain boundaries, twinning etc.

This study takes a macroscopic view on these problems and seeks to investigate the origin and disappearance of dislocation clusters, characterized by: Photoluminescence (PL) imaging on as-cut wafers for identification of cluster regions, Electron Backscatter Diffraction (EBSD) for crystal orientation and grain boundary properties, and defect delineation followed by PVScan [10] for dislocation cluster evolution.

2. Material and methods

Two blocks (A and B) from an industrially produced HPMCSi ingot were investigated. A very thin slab was cut away from the bottom to avoid wire breakage during wafer sawing, the remaining part was wafered. Thus properties almost from the very bottom to the very top could be investigated.

Band-to-band photoluminescence imaging on as-cut, non passivated wafers was used to identify regions of high recombination. The photoluminescence measurements were performed in a BT imaging LIS-R1 with a 5V laser power and a 20 s exposure time. A large selection of wafers was measured: all the wafers in the bottom third of the blocks, and every 10th wafer in the top two thirds. The resolution of the imaging was ~160 μm. Localized regions of increased recombination, which were not linear in appearance (i.e. recombination active grain boundaries) were identified as dislocation clusters. The clusters could be traced upwards and downwards from wafer to wafer, and a bottommost and a topmost point of observation recorded. This was identified as the beginning and end of the dislocation cluster, following the argument that dislocation generation primarily happens very close to the solid liquid interface.

Three heights were selected from each block, wafers 100, 300 and 600, the last one is close to the top of the ingot. In these wafers, a representative selection of dislocation clusters was identified. The clusters were traced to the bottom and top, and the maximum area along the height was measured using Adobe Photoshop measuring tools. The clusters were separated into four different categories according to size, see Table 1. The presence of different clusters as function of height was investigated. It should be noted that identification of generation and termination

Table 1
Cluster size categorization.

Category	1	2	3	4
Size (mm^2)	3–10	10–30	30–100	100–300

of dislocation clusters by this method presents problems of interpretation. If generation of a dislocation cluster appears at an electrically active grain boundary and does not quickly separate significantly from it, the correct starting point cannot be identified. Also, for large clusters, the nature of the dislocation source may change over the height such that multiple sources should be accounted for. For similar reasons the termination of the cluster may be difficult to identify. Especially in wafer 600, several of the clusters grew all the way to the top of the ingot, such that the record of the cluster height does not represent the true height potential of the cluster. Finally, as the parameter measured is the electrical activity of the dislocation cluster, and this is known to depend significantly both on density in the cluster as well as the individual recombination activity of the dislocation [11], the properties of size of the dislocation cluster, both laterally and vertically are somewhat subjectively determined. Cluster properties cannot be compared directly, but since ~10 or more clusters were studied in each wafer, trends were observed that were used to characterize the cluster types and cluster evolution.

In the same set of wafers that had been subject to PL imaging, grain boundary measurements were also applied, using a commercially available grain analysis system from Intego [12], which uses multiple angle illumination to visualize grain boundaries. The resolution is ~80 μm. This technique is not capable of detecting grain boundary properties such as coincidence site lattice (CSL), but since (111) Σ3 CSL boundaries have a proportionally very high fraction in multicrystaline silicon and these grain boundaries normally appear as readily identifiable straight lines, it is possible to use this technique to distinguish this type of grain boundaries from other, higher energy grain boundary types. The combination of PL images and grain boundary analysis was thus used to describe characteristics of the grains in which the dislocation clusters appeared. The clusters were separated into three categories, see Table 2, and the presence of the different types as function of height was investigated.

A selection of wafers was subjected to more rigorous grain boundary and grain orientation studies, as well as dislocation density measurements. Two clusters where both generation and termination were quite clearly observable were selected. Samples of $50 \times 50\ mm^2$ were cut from the same lateral position, representing the evolution of the clusters. Particularly high density (~ every 10th wafer) was chosen around the beginning and termination of the clusters. The samples were mechanically polished and Sopori etched. A small region around the cluster was marked using a laser, which made it possible to position the various measurement methods and overlay them: Electron Backscatter Diffraction (EBSD) was used to identify grain boundaries and grain orientation and PVScan was used to study dislocation density and dislocation cluster properties respectively.

3. Results

Examples of uncalibrated PL images and grain analysis images of wafers from different heights in block A are shown in Fig. 1. A clear grain structure can be seen in wafer 100, indicating that the grain boundaries are electrically active. On the other hand, dislocation clusters are few and small. For the other two wafers, the grain boundaries are not so visible; although some grain