IDENTIFICATION OF DEFECT-SUPPRESSING GRAIN BOUNDARIES IN MULTICRYSTALLINE SILICON BASED ON MEASUREMENTS OF AS-CUT WAFERS USING ADVANCED IMAGE PROCESSING

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ABSTRACT: The mobility and multiplication of dislocation clusters in cast Silicon depend on many factors, especially grain competition and grain boundary types. The great success of High-Performance (HP) mc-Si material in the last years is mainly based on a high occurrence of stress-absorbing grain boundaries. Where the growth of a dislocation cluster is confined by a grain boundary, the cluster displays distinct margins. Therefore cluster and grain show a mutual boundary and a corresponding vertical development. We present an image processing tool that extracts those regions with corresponding and possibly correlated development of dislocation clusters and grain structure in multicrystalline silicon (mc-Si), based on photoluminescence (PL) and optical measurements on wafers with a vertical distance in the brick of 4-8 mm. The vertical development of grain structure and PL signal is reconstructed layer by layer through the complete brick height and thus allows an insight into the whole crystal development of the whole brick and a spatially resolved macroscopic 3D-analysis on industrial scale. Grain orientations and grain boundary types were investigated within regions with corresponding development in and around dislocation clusters. Exemplary results quantitatively support the general assumption that among the dislocation-suppressing grain boundaries, random grain boundaries have the largest share with 42%.

Keywords: dislocation clusters, grain boundaries, deformation field, stress absorption

1 INTRODUCTION

Silicon wafer material quality is crucial for increasing solar cell efficiency and reducing costs per watt peak and defect development has a large impact on bulk lifetime. In previous research, theories and models have been developed with regard to the interaction between grain and defect development [3–5]. Yet, up to now, the connection between grain and defect development has not been investigated quantitatively on a statistically relevant basis due to the lack of suitable methods. Within the frame of this work, we have developed a method to identify regions automatically with specific defects (such as dislocation clusters) within the analysed wafers and to quantify the effect of grain boundaries on dislocation development as well as their development. With these means, theories and models based on few empirical data can be investigated on a statistical basis and thus a deeper insight into crystal defect development can be gained. Moreover, our method allows a complete reconstruction of the macroscopic development process of grain structure and defect development and will provide valuable feedback for crystal growth.

To investigate and quantify the effect of grain boundaries in detail, the grain boundary types and grain orientations serve as important input parameters for our evaluation. They can be determined with Laue measurements [1]. Although this method is non-destructive and faster than electron back scattering diffraction (EBSD), it is still a detailed single-wafer measurement and takes time according to the number of grains to be measured. The identification of the critical regions in the wafer, which is part of our method, makes it possible to reduce the necessary measuring coordinates considerably, thereby ensuring more relevant data in a shorter time. Moreover, our method tracks the development of dislocation clusters through brick height by fast measurements – Photoluminescence (PL) and optical measurements – on as-cut wafers and thus extends the impact of the detailed information vertically through brick height, for as far as the dislocation cluster extends and the grain relation remains the same.

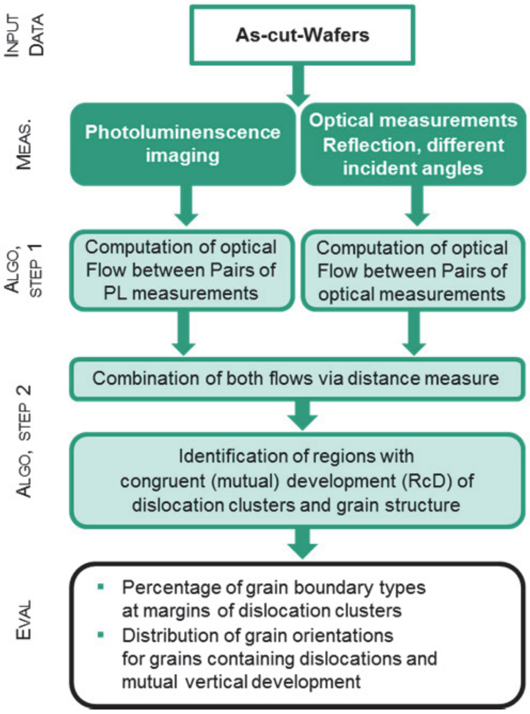


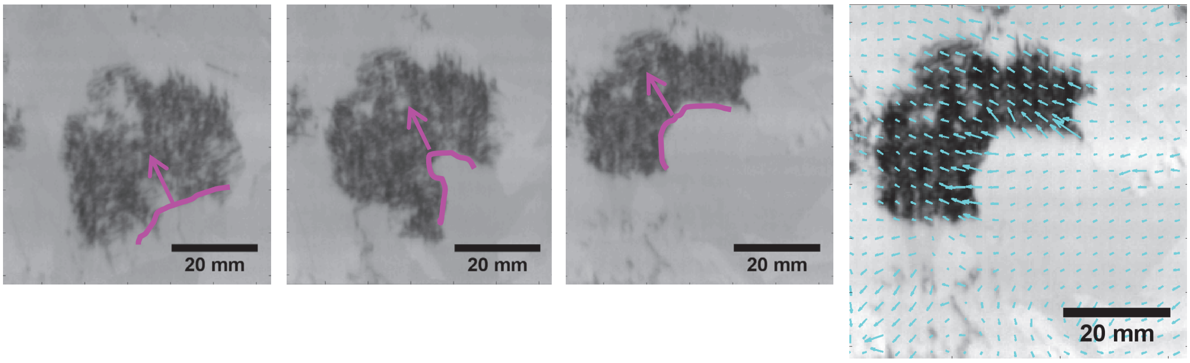
Figure 1: Outline of the method and included algorithm and evaluation steps.

2 MEASUREMENTS AND ANALYSIS

2.1 Algorithm for image registration

The outline of our method and algorithm is shown in Figure 1. Aligned PL images and optical image stacks (different illumination angles) serve as input for the so-called image registration. We track the vertical development of defect objects via vector fields that characterize the development of grain structure or PL signal from wafer to wafer (vertical distance between 4 and 8 mm). In particular, the optical flow is computed following the method of Bruhn et al. and Liu et al. [2,3]. This type of image registration methods can be based on

a) Height position 667 **b) Height position 717** **c) Height position 767** **d) Optical flow betw. pos. 767-777**



e) Cross correlation pos. 767-777 **f) Relative vector length difference** **g)Dislocation margins**

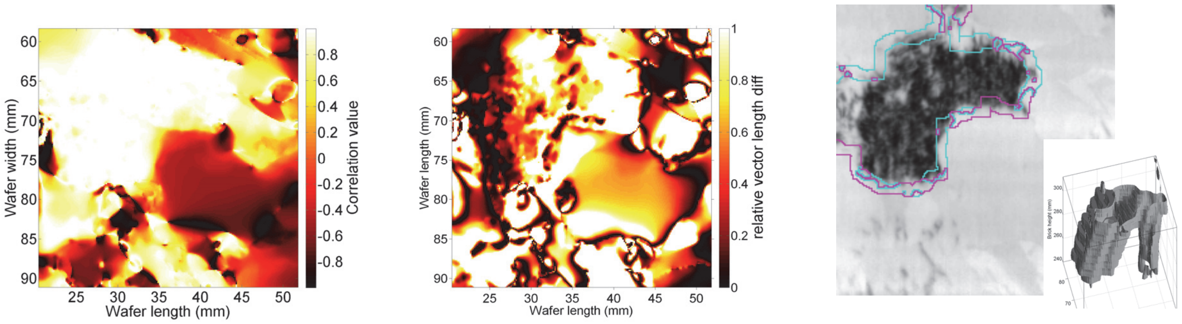


Figure 2: a)-c) Sequence of PL image sections showing the development of the same dislocation cluster over a vertical distance of 19 mm between subsequent wafers. The boundary to the overgrowing grain and its movement are marked magenta. **d)** Flow field corresponding to PL-image in c), plotted as cyan overlay arrows. **e)** Angular and **f)** length distance as intermediate results within the algorithm for flow comparison between PL and optical image. **g)** Regions at cluster margins, marked cyan for mutual flow fields and magenta otherwise. In the corner, part of the corresponding reconstructed 3D object is shown.

different image properties and criteria. In our case, the vector field is computed so that the image intensity and gradient, i.e., PL intensity or the vector of reflection values under different illumination angles remain constant along the flow. To ensure that the problem is well-defined and reflects the physical reality, other conditions (e.g. a certain flow homogeneity, called regularity) must be included in the function [4,5]. With the solver used for the optical flow calculation, it is possible to reconstruct the flow in regions with homogeneous intensity (like high-quality parts in PL images), using the parts surrounding this region that contain more information. Especially if several of the surrounding grains show a similar development, this information completion is reliable.

2.2 Evaluation and possible error sources

The vector fields resulting from the respective optical flow computations based on PL and optical measurements provide locally resolved information about grain competition and defect development in vertical direction, see for example Figure 3 a) and b).

By combining the two flow fields for every wafer pair, we identify regions where the respective vertical development of grain structure and dislocation clusters coincide and thus indicate an interaction or correlation between crystal structure and defect development. We will call these regions *regions with congruent development* (RcD). These correlations between the development of grain structure and defect clusters are investigated by computing a similarity measure between the vector fields characterizing the development of the grain structure and the defect clusters, respectively. The normalized cross correlation value, i.e., the cosine of the angle between the flow vectors, serves as measure for the angular distance. Cross correlation values near 1 signify similar flow directions and thus a corresponding vertical development of grain boundaries and dislocation clusters, see Figure 2 e). Relative differences between the flow vector lengths, visualized for the same wafer region in Figure 2 f), serve as additional distance measure. Combining those measures at the grain boundary locations gives us the RcD and thus the means to quantify the impact of the grain structure on the dislocation development. In Figure 2 g), the result can be observed as a cyan marking around dislocation clusters for the RcD, whereas the regions with magenta contours do not belong to the RcD.

The RcD are marked and grain boundaries that confine dislocation clusters are extracted. For this purpose, dislocation lines were first extracted from PL images [6] and then isolated from recombination-active grain boundaries by combining the PL feature image with the grain boundary structure extracted from the segmented optical images [7].

Laue measurements are applied on chosen samples and yield information about grain boundary types in the regions of interest and grain orientations within the dislocation cluster regions. Along with the optical flow fields and the identified regions of interest, all information is available for a quantitative evaluation of the impact of different grain boundary types on dislocation development. Thus, among the grain boundaries that confine dislocation clusters, the percentages of the respective grain boundary types are evaluated. Furthermore, the orientation of grains containing dense dislocation clusters is separated in those within the RcD and those outside. It must be remarked again that in the inner part of the grains, the development flow is completed from the surrounding regions.

As in-situ-measurements are not applicable for measuring grain growth and dislocation cluster development of large-scale bricks during growth, no reference method exists, and, to our best knowledge, no other methods with the same purpose have been published. A useful and necessary criterion to test the correctness of the vector field between a pair of wafers is that, if used as a mapping function, one of the images can be computed by warping the other image with the flow field. One of the main challenges for the computation of the vector fields is the relative lack of information within many image regions. Thus the solution is not unique, i.e., even if the deformation field reproduces the next image from the previous one perfectly, this does not mean that this is indeed the only accurate way how the object can have developed. Via further constraints in the underlying equations, the algorithm can complete missing information, yet it is not possible to prove the correctness of the identified solution unambiguously.

2.3 Material set

A large set of bricks (more than 1000 wafers from 11 bricks of different materials and manufacturers) is investigated in terms of optical flow computation. Fast 2D wafer measurements, namely PL and optical (reflection) measurements, are applied on every tenth or 20th wafer throughout the bricks. PL imaging serves to extract the recombination-active defect structures [6], the optical measurements serve to extract the grain structure [7], different illumination directions highlighting different contrasts between grains. The RcD are marked for all wafers. For three bricks (conventional mc-Si), grain orientations and grain boundary types determined via Laue measurements serve for a detailed analysis.

3 RESULTS AND DISCUSSION

3.1 General results and suitability of the analysis

Optical flow fields give direct feedback concerning relevant crystal growth properties to crystal growers. By proceeding from wafer pair to wafer pair, the whole vertical development is characterized. In the following we name the most important properties that can be recognized directly from the visualized flow vector fields as they can be seen in Figure 3 a) and b):

- Lateral growth direction (via vector angle)
- Relation between flow directions in neighbor grains or near grain boundaries
- Overgrowth angles at grain boundaries (via vector length and knowledge of wafer distance)

The color code for the optical flow fields simplifies the understanding of the growth information because it shows the development in high resolution and makes it possible to compare flows quickly with the naked eye. It can be considered as a 2D mapping which leads to a 3D understanding of the brick if observed for consecutive wafer pairs. Thus, while not directly showing or analyzing 3D objects, we get an impression of every whole brick we analyze.

Our method is suitable to give an insight into crystal growth. It fulfills the necessary criterion that the flow field, used as a mapping function can reproduce the next wafer from the previous except up to a reasonable error threshold. The flow field may be inaccurate especially at grain corners, i.e. sharp direction changes of the grain boundaries because the differential equations are based on differentiable functions.

In comparison with the expectations via naked eye, the flow fields mainly show good results, see for example Figure 2 a)-d). This concerns the developments for PL and optical measurements separately but also, in particular, for the comparison of the developments in and at dense dislocation clusters. However, we also observe inconsistencies in the flow from wafer pair to wafer pair. That means, although the flow vectors in one grain do – normally – not vary much over short vertical distances, general flow directions in a region might differ compared to the next flow. A possible explanation may be that the constraints make the algorithm react more sensitively to small changes like differences in the measurements, noise or saw marks. Yet, this does not yet explain why, in certain regions, the flow directions alternate such that for every second pair they are similar. This requires more thorough investigations.

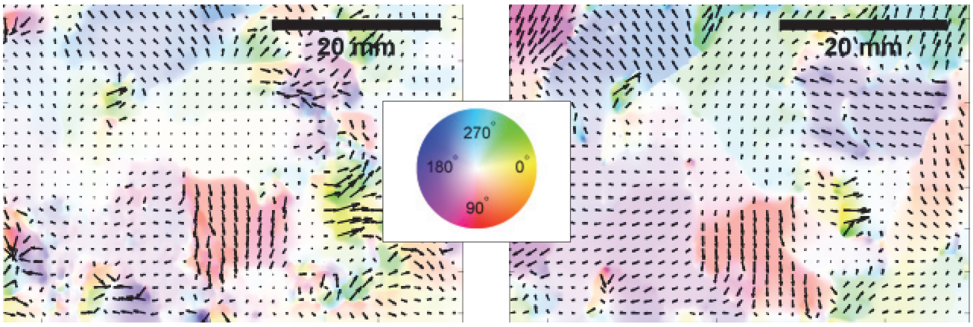
Thus, the method allows the localization of beneficial grain boundaries. Moreover, this is possible without considering dislocation clusters as objects with sharp contours. Scientifically, this is of advantage because dislocation clusters are no compact 3D objects but consist of arranged defect lines.

3.2 Detailed evaluation of flow field correspondence

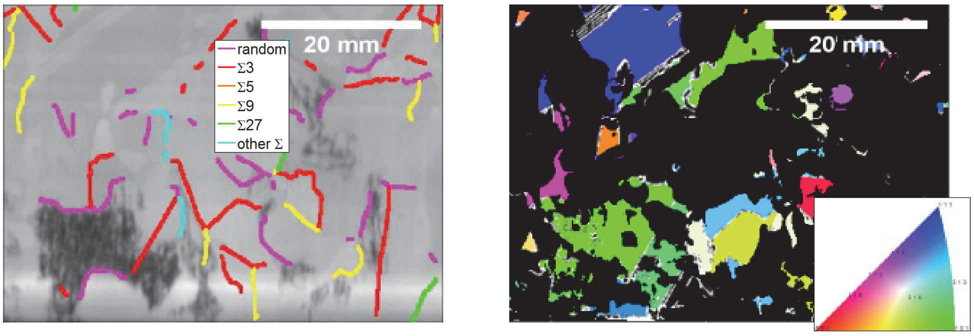
It can be observed that at the margins of dislocation clusters, the percentage of ∑3 and random grain boundaries is very high, see Figure 3 e) as an example.

For random grain boundaries, the high occurrence probability at dislocation margins and in the RcD corresponds to what is expected because they absorb stress. The partly even higher ∑3-percentages probably have other reasons because with the naked eye we do not observe it at sharp dislocation margins and it is known that this grain boundary type does not absorb stress. Usually, for the multiplication and mobility of dislocations, those boundaries do not constitute an impediment. As mentioned before, dislocation clusters are no solid objects. Thus, the term of dislocation margins can be ambiguous. Furthermore, twin grains, which are confined by ∑3 boundaries, often develop mutually with their neighbors and are close to each other. Thus, if by chance they are situated within a RcD, their high spatial density leads to a high percentage.

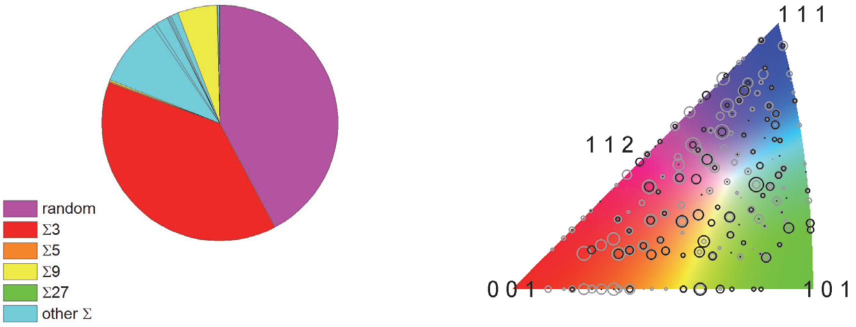
For the results of the grain orientations, we observe that grains with dislocation clusters within RcF are mostly concentrated to few accumulations in the right lower corner of the inverse polefigure, i.e., near to <101>, or central in the figure towards <112> (see for example Figure 3 f), while within the non-congruent flow regions the orientations are rather scattered over the upper regions of the inverse polefigure up to <001> and <111>. As dislocation clusters are most mobile within the gliding planes, some orientations are more often decorated with dislocations. However, our data set is varied but not representative and we will investigate this on a larger data set in the future.


a) Flow field PL

b) Flow field grain structure


c) GB type

d) Grain orientation


e) Percentage of grain boundary types in RcD near dislocation clusters

f) Distribution of grain orientations at dislocation clusters within and outside the RcD

Figure 3: a) and b) Image section of the respective visualized flow fields for a) PL intensity and b) grain structure of an mc-Si wafer. The color in the regions and the direction of the black arrows encode the angle of the development in lateral direction, the saturation (on a relative scale) and length of the black arrows show the length of the vectors, which is related to the vertical overgrowth angle. **c)** Same image section for the PL image with overlayed information on the determined grain boundary types. **d)** Grain orientations in the regions with congruent development. **e)** Percentages of the respective grain boundary types (in terms of line length) in regions with congruent development at the margins of dislocation clusters. **f)** Distribution of grain orientations for those grains within (marked with black circles) and without (marked with grey circles) the RcD containing dislocations.

3.3 Outlook and possible optimization

For the optical flow computation, it has to be kept in mind that the underlying equations for the optical flow contain no physical model for grain growth, which is hardly possible. Still, certain physical properties of the growth make it necessary to find an optimal choice of the underlying model, the image properties used, the solvers, parameters and mathematical constraints. Among these varied degrees of freedom, it will take more time and data evaluation to get closer to the optimum. Especially, achieving consistency between consecutive vector fields will serve to reconstruct the whole grain growth and competition.

Furthermore, decorated dislocation lines evolve relatively fast, so that it is almost impossible to track the exact growth, and thus the crystallographic gliding planes, over the vertical distance of >4 mm. By computing the flow between smaller vertical distances, not only dislocation developments could be tracked with higher accuracy, but also the glide planes could be detected without applying an extra Laue measurement.

The choice of the distance measure between the flow fields will be further optimized since it has a large impact on the results. Moreover, we will discern between sharp (distinct) and ambiguous (indistinct) grain boundaries, which will improve the distinction between the effects of the respective grain boundary types.

4 CONCLUSIONS

We developed a method to analyse locally resolved information about the development of grain structure and larger recombination-active defects like dislocation clusters. This was attained via optical flow computation between wafer pairs. The results consist in vector fields which designate the direction and overgrowth angle within the crystal. By computing the flow for all consecutive wafer pairs through the brick, the whole growth was reconstructed. By comparing and combining the vector fields of grain structure and defects, we gained information where they might be correlated. Those regions with mutual development were extracted and further restricted to the margins of dislocation clusters where grain boundaries may have a beneficial effect. In this way, measurements for the determination of local crystal orientation and grain boundary types can be restricted to fewer data points.

The vector fields displaying the development were in good agreement with the naked eye. They further showed low errors for the comparison between original image and the image calculated using the flow as mapping function. They contain valuable feedback for crystal growers concerning defect growth and grain structure development. With a further optimized algorithm, the flow can be assembled to a complete growth reconstruction.

Within the regions of flow congruency, we investigated the impact of the respective grain boundary types for chosen samples. Our quantitative results support the general assumption that dislocations often occur in certain grain orientations and that random grain boundaries can often suppress dislocation clusters. For a consolidation of those assumptions and a deeper understanding how to suppress defects in the most efficient way, more evaluations and larger data sets with grain orientations and grain boundary types will be carried out.

5 ACKNOWLEDGMENTS

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