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A Computational Investigation of Relationship Between Shear Stress and Multicrystal Structure in Si

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1. Introduction

The solar cells based on Si bulk multicrystals have widely used nowadays due to well-balanced conversion efficiency, production cost and throughput. However, Si bulk multicrystals have contained many crystal defects such as grain boundaries, dislocations, impurities and so on. Therefore, Si bulk multicrystals have room for improvement of crystal quality by controlling multicrystal structure as shown by recent achievement of Fujiwara *et al* [1].

Plentiful researches reported that sub-grain boundary, among other defects, gives harmful impact for solar cell properties [2-5]. Sub-grain boundary consists of aligned dislocations and acts as a recombination site for minority carriers and reduces shunt resistance for majority carriers. Recent study in our group revealed mechanism of generation of sub-grain boundary. We grew Si bulk multicrystals with artificially designed seed crystal and revealed that sub-grain boundaries are generated near grain boundaries. In addition, we disclosed that the density of sub-grain boundaries strongly depends on multicrystal structure such as grain orientation or character of grain boundary. Two-dimensional finite element method indicated that sub-grain boundary is likely to be caused by shear stress on slip surface induced by external isotropic force due to volume expansion at solidification [6].

In this study, we extended computational simulation to three-dimension so that any orientation can be calculated, and one can acquire a guideline for reduction of sub-grain boundary.

2. Computational Procedure

A computational investigation was carried out in following procedures. As shown in Fig. 1, a cylindrical model crystal consisted of two grains, grain 1 and grain 2, was defined. The diameter and the thickness were chosen as 10cm and 1cm, respectively. It is noted that this model corresponds to Si crystal, which grows in a crucible along z direction. The model crystal was meshed into 2665 elements which are given stiffness coefficients as elastic modulus [7]. Change in grain orientation was represented by change in the stiffness coefficients. We systematically varied crystal orientation of both grains and attempted to reveal a relationship between shear stress on slip surface and muticrystal structure. As a boundary condition, 1% displacement toward the center was given to the nodes located at the edge of the crystal by assuming external compressive force owing to volume expansion when Si melt is crystallized. In this calculation, grain boundary is defined by the discontinuous change of elastic modulus between two grains, and no boundary condition such as fixing or shifting at grain boundary is considered. After calculation, the maximum shear stress was adoped among twelve values originating from eight equivalent slip surface of {111} planes and three equivalent <110> directions in diamond structure.

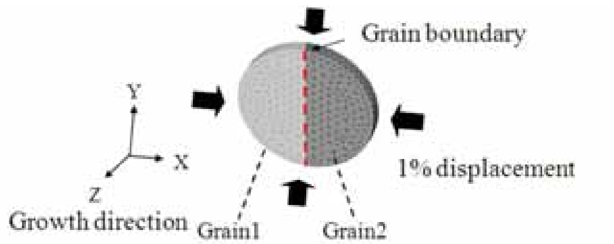

Fig. 1: Geometry of calculation model

3. Results and Discussion

Single Crystal Model

At first, single crystal model is calculated for the purpose of focusing on effect of grain orientation on shear stress. Fig. 2 and Fig. 3 show some examples of shear stress distribution in the model of <001> and <111> in z direction, respectively. As described above, twelve values of shear stress on slip surface must be taken into account, therefore, distinguishing results are shown in Fig. 2 and Fig.3. In the result of growth direction of <001>, the shear stress is acted equally on each slip surface and maximum value results in the same value of 1.48GPa in any slip surfaces. On the other hand, the shear stress is concentrated on a particular slip surface in the result of growth direction of <111> and maximum value becomes larger than that of <001>. Based on our analysis, maximum shear stress becomes small when all {111} planes are evenly subjected to compression forces. In diamond lattice structure, there are 8 equivalent planes of {111} which configure an octahedron. So geometry of the octahedron should be symmetrical for compression forces with respect to reduction of shear stress. The result of single crystal model indicates that growth direction should be controlled to <001> direction in terms of reduction of sub-grain boundary.

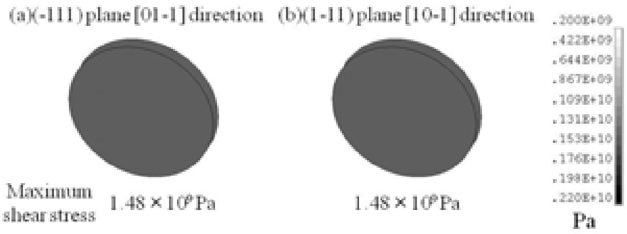

Figure 2: Single crystal model in the case of <100>, <010> and <001> in x, y and z direction respectively; shear stress distribution on (a) (-111) plane toward [01-1] direction (b) (1-11) plane toward [10-1] direction

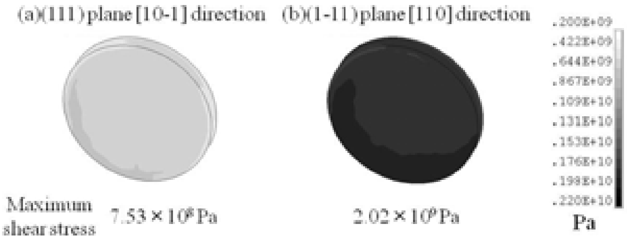

Figure 3: Single crystal model in the case of <11-2>, <-110> and <111> in x, y and z direction respectively; shear stress distribution on (a) (111) plane toward [10-1] direction (b) (1-11) plane toward [110] direction

Multicrystal Model

Fig. 4 shows one of examples of the maximum shear stress distribution in multicrystal model. Grain1 orients <-110>, <-1-12> and <111> in x, y and z direction, respectively. Likewise grain 2 orients <-14-3>, <-413> and <111> in x, y and z direction. The shear stress in grain 1 is larger than that in grain 2. This suggests that shear stress depends on grain orientation as well as single crystal model. In multicrystal model, however, shear stress concentrates near the grain boundary. This result can be caused by discontinuity of elastic modulus between both grains. In this way, shear stress depends on not only grain orientation but also continuity of elastic modulus in multicrystal model.

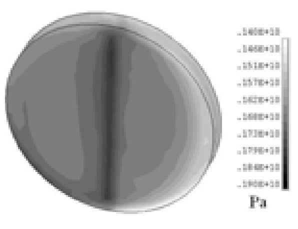

Figure 4: Distribution of shear stress in multicrystal crystal model; grain 1 <-110>, <-1-12> and <111> in x, y and z direction, grain 2 <-143>, <-413> and <111> in x, y and z direction

We carried out the calculation in various multicrystal structure model to pursuit ideal structure in which shear stress can be reduced. Fig. 5 compares calculated results of various structures where the growth orientation is fixed to (a) <001>, (b) <011> and (c) <111>, respectively. The both grains to construct the multicrystals are rotated separately along z-axis of growth direction. Calculations are carried out with 5 degree increment and maximum shear stress in the model is plotted. Shear stress in the case of <001> does not change at any rotation angle, because configuration of the octahedron, which is configured by equivalent planes of {111}, does not change about z-axis rotation. However shear stress in the case of <011> and <111> depends on rotation angle. It is apparent the shear stress in the case of <111> becomes larger than that of <001> and <011> over-all, that is, controlling growth orientation in <001> or <011> has an advantage of suppress of sub-grain boundary occurrence.

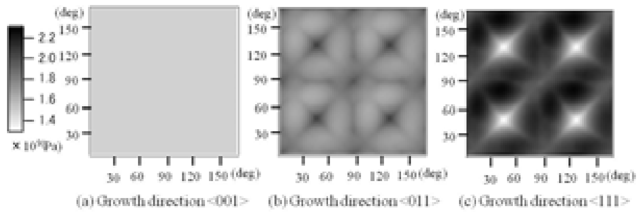

Fig. 5: Maximum shear stress in various grain orientation model is plotted. Growth direction is fixed into (a) <001>, (b) <011>, (c) <111>. X-axis and y-axis represents rotation angle of grain 1 and 2 about growth direction respectively.

4. Summary

In this study, shear stress on slip surface is simulated in various multicrystal structures under external isotropic force by elastic analysis. Shear stress depends on grain orientation caused by geometry of the octahedron configured by {111} planes. In addition, shear stress concentrates near the grain boundary due to discontinuity of elastic modulus. According to our calculation, multicrystal structure should be controlled to <001> direction in growth direction or other structures which result in low shear stress. It is concluded that to control grain orientation and structure of grain boundary in Si multicrystals is a promising route in order to decrease crystal defects by decreasing shear stress.

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