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Micropipe formation and its driving force issues in SiC growth

This application note reports our understanding of micropipe formation mechanism and its driving force issue existing in SiC material development. Superscrew dislocations, which include open-core (also called micropipe) and closed core screw dislocations, have been the subject of long-standing scientific controversy. One key question still remains unanswered: how the growing crystal does manage to bring together the equivalent number of lattice dislocations closely enough to form open-core micropipes with large Burgers vectors.

It has been experimentally demonstrated that micropipes nucleated from the crystalline regions that incorporate defects such as inclusions, polytype disturbances, thermally induced stress, low-angle grain boundaries, partial dislocations, voids, etc and were mostly formed at the very initial stage of growth. There are many theories or mechanisms that have been proposed to explain the formation of micropipes in SiC. However, while these proposed theories may be partially successful in explaining the micropipe formation, they are certainly not the only possible models and there is a question as to their total applicability to a wide variety of experimental observations of micropipe formation. The famous Frank’s model has successfully predicted the existence of open-core dislocations in the crystals with large unit cells and its derived correlation between the radius and Burgers vector values of micropipes has basically been validated, but it is difficult to use this model to explain the origin and formation of micropipes with large Burgers vectors. Frank’s theory cannot be used to explain how micropipes with large Burgers vectors converge into a single structure; the theory does not explain how the forces of repellence are overcome. Several mechanisms depicting the coalescence/mergence of elementary dislocations or micropipes with the same-sign Burgers vectors have been proposed to understand the formation of the dislocations with large Burgers vectors. However, these mechanisms are in direct opposition to the mechanics of repellence properties of the dislocations with same-sign Burgers vector, and do not explain the ramification of micropipes simultaneously occurring during crystal growth. In fact, most micropipes with large Burgers vector values are only formed at the very initial stage of growth and many of these were dissociated, merged and annihilated (between opposite-sign dislocation) at the later stage of crystal growth.

Using our newly developed quantitative defect study method (see reference 1), the characteristics of superscrew dislocations in SiC has been systematically investigated. From this investigation, the properties of superscrew dislocations in SiC can be summarized (reference 2-3) as follows:

(1) The relationship between diameters and the Burgers vector values of micropipes statistically follows Frank’s prediction.

(2) The surface energy of the micropipes in 6H SiC is estimated to be about 2.0 J/cm-2.

(3) For both 4H and 6H SiC, the histogram of Burgers vector values associated with micropipes follows a Gauss distribution with most possible absolute Burgers vector value of about 100 Å. This result implies that the formation and transformation of micropipes are governed by a fundamental mechanism.
(4) A unique repellence and aggregation behavior was found for both clustered micropipes and elementary screw dislocations with same sign Burgers vectors. On one side, the clustered or aggregated superscrew dislocations with the same sign of Burgers vectors repel each other in a micrometric range, thus they do not merge into one with a bigger Burgers vector (a giant Burgers vector micropipe); on the other side, these superscrew dislocations remain together within a short distance (several microns).
(5) The transformations of superscrew dislocations, such as dissociation, coalescence and aggregation, follow the principle of Burgers vector conservation and energetically favored behavior. This result does not support the micropipe formation theories which are based on the coalescence of elementary dislocations or micropipes with same sign Burgers vectors.

Based on above results, a mechanism of mismatched-coalescence between multiple nucleation sites is proposed to understand the formation of micropipes with large Burgers vectors at the early stage of SiC bulk growth. The belief has been that the growth of SiC starts from multiple nucleation sites. Figure 1a schematically shows a SiC growth from two nucleation sites. The initial growth of each nucleation site could be in any formats, such as Lely growth, dislocation-, terrace- or impurity- assisted, etc. They will continue to grow in c-axis direction [0001] (SiC crystal growth direction) and lateral directions (basal plane growth). Ideally the lateral growths will lead to coalesce at the equivalent basal planes (marked with the same numbers in Fig. 1a) between two sites and would form into a large single crystal. In a real growth, the imperfection or disturbances such as surface quality, localized uniformity and impurity would occur at the initial growth stage, and some of coalescences between nucleation sites could be mismatched. Figure 1b schematically illustrates a mismatched coalescence in which the equivalent basal plane 3 in the left nucleation site is merged with the equivalent basal plane 4 in the right nucleation site and they would lead to $1c$ mismatch coalescence. In real situations, the value of mismatched lattice layers is determined by the relative orientation and position between nucleation sites, and it could be any nc.

The proposed micropipe formation mechanism is based on the above mismatched coalescence between multiple nucleation sites. Figure2 shows a $4c$ micropipe formation originated from four $1c$ mismatched coalescence occurred among 5 nucleation sites S_1-S_5. For simplicity, let us assume that each nucleation site has already grown 4 layers of SiC basal planes (Fig. 2a) and will just keep expending these 4 basal plane layers in the rest of the growth. Due to some disturbances, there are four $1c$ mismatched coalescences occurred between S_1 and S_2, S_1 and S_5, S_5 and S_4, S_4 and S_3 (4c in total), and no mismatched coalescence between S_2 and S_3. These mismatched coalescences will lead to a $4c$ dislocated basal plane layer around the center C (Fig. 2b) after the corresponding layers (highlighted with gray in Fig. 2a) in all nucleation sites fully coalesce. As the growth continues, the subsequent growth will follow this pattern and a $4c$ micropipe will inevitably be formed after all four basal planes fully coalesce (Fig. 2c).

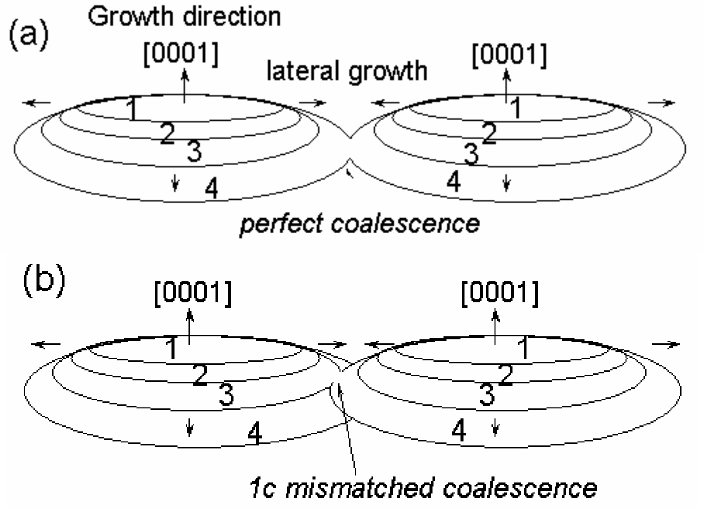

Figure 1, Illustration of coalescence between two nucleation sites (a) perfect coalescence, (b) 1c mismatched coalescence

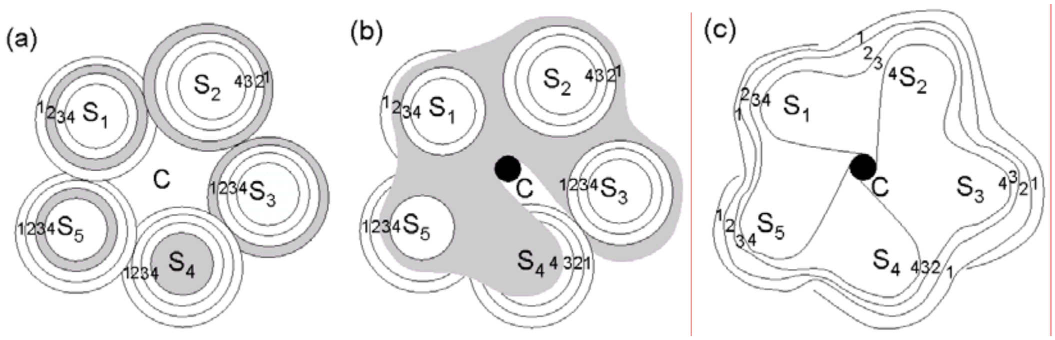

Figure 2, Schematic diagram of 4c micropipe formation originated from four 1c mismatched coalescence among five nucleation sites: (a) four 1c mismatched coalescences occurred between nucleation sites S1 and S2, S1 and S5, S5 and S4, S4 and S3, (b) Illustration of 4c mismatched basal plane after the layers (highlighted with gray in (a)) fully coalesce, and (c) A 4c micropipe will be formed after all four basal planes fully coalesce.

After the initial coalescences enclose the center C as shown in Figure 2a, the further coalescences are likely to occur in a same manner which would induce a large stress around the center point C. This stress would push the above mismatched coalescences into the center to form a micropipe. We believe that this stress is the driving force for the micropipe formation at the early stage of growth as well as for superscrew dislocation aggregation in the later stage.

The involved nucleation sites could be as low as 3 and with no upper limit. If the total mismatch is 1c, an elementary screw dislocation will be formed. It is understandable that the most possible superscrew dislocation formation would be three nucleation sites with total mismatched-coalescence of 1$\boldsymbol{c}$ or -1$\boldsymbol{c}$**.** This could explain the majority of superscrew dislocations in SiC observed to be elementary screw dislocations.

The disturbances in the proposed mechanism could be caused by different factors which can be used to explain various previously identified various micropipe formation phenomena. In modified Lely growth, any poor seed surface quality, localized uniformity, void, or growth process instability could lead to a mismatched coalescence between nucleation sites and formation of micropipe with large Burgers vectors. The inclusions or impurities would be another main source for the disturbance since nucleation from them usually have different orientations and inevitably lead to mismatched coalescence. It is worthwhile to point out that the mismatched coalescence does not necessarily cause a grain boundary between nucleation sites if the further coalescence continues in the same layers. However, under poor growth condition, if the coalescence mismatch is large and the induced stress is of sufficient magnitude, further coalescence in the same equivalent layers could be interrupted and a grain boundary would be created between nucleation sites. The formation of grain boundary could be used to explain the previously reported formation of mosaic structures in SiC. The stress caused by large-value mismatched-coalescences could also be used to explain the generation of stacking fault clusters and partial dislocations at the beginning of micropipe formation. According to the proposed micropipe formation mechanism, both micropipes and stacking fault clusters/partial dislocations are the products of the mismatched coalescence procedure, other than that the stacking fault clusters and partial dislocations would lead to micropipe formation.

This research also indicates that high-c superscrew dislocations in SiC are quasi-stable, and it is possible to develop micropipe-free SiC.

Reference:

[1] MaxMile Technologies, LLC, application note: “A method to determine the Burgers vector value of superscrew dislocations in SiC at the wafer level”.
[2] “Superscrew Dislocation in Silicon Carbide: Dissociation, Aggregation and Formation”, to be published.
[3] “A Method to Determine Superscrew Dislocation Structure in Silicon Carbide,” to be published.