Analysis and Control of Structural Defects in Silicon Carbide Epitaxial Layers

Michael Dudley1, *, Ning Zhang1, Yi Chen1 and Edward K. Sanchez2

1Department of Materials Science and Engineering, Stony Brook University, Stony Brook, NY, 11794-2275, USA
2Dow Corning Compound Semiconductor Solutions, Midland, Michigan, 48686-0994, USA

*e-mail: mdudley@notes.cc.sunysb.edu

Abstract

The application of silicon carbide (SiC) based devices continues to face issues relating to defect engineering. Developing nearly-perfect SiC epitaxial layers relies on understanding the behavior of defects at the substrate/epilayer interface. Here we show how threading screw dislocations (TSDs) and basal plane dislocations (BPDs) can be converted into Frank partial dislocations and threading edge dislocations (TEDs), respectively, during epilayer growth. We also demonstrate that scratches on the substrate surface can act as dislocation nucleation centers during chemical vapor deposition (CVD) growth.

1. Introduction

Over the past decade, great advances have been made in the physical vapor transport (PVT) growth of 6H and 4H-SiC substrates. However, full realization of the application potential for these important wide band-gap semiconductors has been hampered by the relatively high densities of defects such as threading screw and edge dislocations which persist in these substrates [1]. Many of these defects are replicated into the subsequently grown homo-epitaxial layers required for device fabrication imposing limitations on their performance [2]. This is particularly true for the case of power devices [3]. The use of substrates off-cut by several degrees from the (0001) basal plane provides opportunities to engineer defect behavior at the substrate/epilayer interface such that defects such as TSDs can be deflected into the basal plane and thus not penetrate into the device active region [4]. However, while this strategy can have a positive effect on the screw dislocation density in the epilayer, it also provides the opportunity for basal plane dislocations to be replicated into the epilayers [5]. For the case of pin devices, this can lead to stacking fault expansion under forward bias leading to device failure [6]. This effect can be mitigated by inducing the replicated basal plane dislocations to deflect towards the growth direction transforming them into TEDs. In this paper we provide a review showing examples of some of the phenomena described above obtained using synchrotron topography. We also explore the nucleation of new defects in the epilayers at scratches on the substrate surface and provide a model for these nucleation processes.

2. Experiment

Commercially available 4H-SiC wafers grown by the PVT technique with an 8° off-cut angle toward the [11-20] direction were used as the substrates for chemical vapor deposition. After CVD growth, monochromatic synchrotron x-ray topographs were recorded from the epilayer. Selected specimens were polished from the substrate side using diamond lapping films and x-ray topographs were recorded from the substrate side. The samples were etched in molten potassium hydroxide (KOH) at 600°C for 10 min. following the x-ray topography. The etch patterns were recorded for further comparison with x-ray topographs. The imaging was carried out at the Stony Brook Synchrotron Topography Station, Beamline X-19C, at the National Synchrotron Light Source at Brookhaven National Laboratory, and Beamline XOR-33BM, at the Advanced Photon Source, Argonne National Laboratory, using Ilford L4 nucleate plates at a specimen-to-film distance between 10 and 15 cm.

3. Results and Discussion

3.1. Deflection of TSDs into Frank partial dislocations

The specimen studied comprised a 100 μm thick epilayer which was thinned down from the substrate side, leaving a substrate of ~30 μm thick and x-ray back-reflection topographs were recorded from both epilayer and substrate sides. Fig. 1(a) is a (0008) back-reflection topograph from the epilayer side and ten linear defects, roughly parallel to [11-20], are visible. These are Frank partial dislocations [7]. A single linear defect magnified from the boxed region in Fig. 1(a) is shown in Fig. 1(b). It appears as dark contrast line at the left end and dagger-shaped white contrast with dark contrast at its bottom edge at the right end. The white circles surrounded by sharp dark contrast rings are topographic images of elementary TSDs [8] and small white or black dots in the grey background correspond to the TEDs, which can be further confirmed by the etch pattern in Fig. 1(c). The large hexagonal pits in the etch pattern correspond to the elementary TSDs, while small hexagonal pits are associated with the intersection of TEDs at the epilayer surface [9].

One can see the one-to-one correspondence between the dislocation images in Fig. 1(b) and the etch pits in Fig. 1(c): the white circles correspond to the large hexagonal etch pits and small white or black dots correspond to the small hexagonal etch pits. Fig. 1(d) is the back-reflection x-ray topograph recorded from the substrate side, which contains...
mostly defect information from the substrate due to the limited x-ray penetration depth (~20 μm based on photoelectric absorption). The white lines distributed in Fig. 1(d) are due to residual polishing marks. All of the TSDs have one-to-one correspondence among Figs. 1(b), 1(c) and 1(d) (some of them are marked by hollow triangles for reference), except for the one marked by the solid triangle in Fig. 1(d). By comparing the two topographs in Fig. 1(b) and 1(d), one can notice that a TSD which is present in the substrate (marked by solid triangle) disappears after CVD growth and a linear defect is newly nucleated, lying roughly parallel to the step-flow direction. The approximate position of the TSD by looking from above the epilayer is marked by circles in Fig. 1(b) and 1(c). The distance from the disappeared TSD to the oval shaped etch pit associated with the linear defect intersecting the epilayer surface [see the inset in Fig. 1(c) for high-magnification micrograph] corresponds to the dimension of the basal plane along the off-cut direction. This provides direct evidence for the deflection of TSDs at the substrate/epilayer interface into closely spaced Frank partial dislocations separated by a Frank fault.

Figure 1. (a) Back-reflection x-ray topograph showing linear defects observed in the CVD grown epilayer parallel to the step-flow direction. (b) A magnified linear defect from the boxed region in (a). (c) The corresponding etch pattern of epilayer surface. (d) Back-reflection x-ray topograph from the substrate side.

3.2. Deflection of BPDs into TEDs

As we discussed above, TSDs can be converted into Frank partial dislocations (separated by Frank faults) on the basal plane. On the other hand, at the same substrate/epilayer interface a BPD on the basal plane can be converted into TED propagating roughly along c-axis. The sample studied for this experiment consisted of a 2 μm thick epilayer deposited using CVD. Monochromatic synchrotron x-ray topographs were recorded from the epilayer using

Figure 2. (11-28) grazing-incidence x-ray topograph showing a BPD, which is converted into TEDs at both ends.
the (11-28) reflection. X-ray topographs were recorded in grazing incidence such that the penetration depth allowed for imaging of the whole epilayer thickness down to beyond the interface.

**Fig. 2** shows an example where both ends of a half loop of BPD are converted into TEDs. The Burgers vectors of the two TEDs are the same since they belong to a half loop but their line senses are anti-parallel. Based on the line direction and Burgers vector, the configurations of the two TED segments have been simulated [10], as indicated in the insets. The simulations match very well with the topographic images. The extra atomic half planes associated with the TED segments are indicated in the figure. Many other similar examples have been examined as well and most of the BPDs are confirmed to convert into TEDs, which is consistent with previous studies indicating a 70%-90% conversion rate [11].

### 3.3. Nucleation of TEDs and BPDs at scratches

The influence of substrate surface scratches on the quality of CVD grown 4H-SiC homo-epitaxial layers has been studied using a combination of post-growth Monochromatic Synchrotron X-ray Topography (MSXT) and KOH etching. X-ray grazing topographs were recorded in order to image the whole epilayer as well as the interface. Fig. 3(a), 3(c) and 3(e) are (11-28) grazing-incidence MSXT images from the epilayer surface and Fig. 3(b), 3(d) and 3(f) are the corresponding etch pit patterns. The [11-20] off-cut direction is vertical in Fig. 3. Some examples of the nucleation of dislocations along scratches can be clearly seen in Fig. 3 and it is observed that the orientation of the scratch with respect to the off-cut direction exerts influence over the process. When scratches were parallel to the off-cut direction, they manifested themselves on the topographs as a single white band of contrast and on KOH etch patterns as a single, dense row of etch pits along the direction of the scratch. For scratches inclined to the off-cut direction, X-ray topography reveals a similar single white band but with additional linear features attached which project along the off-cut direction while KOH etching reveals a similar dense row of etch pits with a less dense row parallel to it at some distance away (see Fig. 3). Figs. 4(a) and 4(b) shows enlarged topographic and etch pit images from a similar region to Fig. 3. Fig. 4(b) reveals a distribution of six paired TED etch pits (marked with hollow arrows) and a single TED etch pit paired with a single BPD etch pit located at a distance along the off-cut direction (marked with solid arrows). These configurations are consistent with a row of TEDs propagating directly from the scratch to the epilayer surface (approximately along the epilayer surface normal) combined with occasional BPDs which propagate from the scratch to the epilayer surface on the basal plane. A model has been presented for a possible mechanism for this process and is to be published in a separate paper [12].

![Figure 3](image-url)

**Figure 3.** Synchrotron X-ray topographs ((a), (c) and (e)) and corresponding etch pit patterns ((b), (d) and (f)) recorded from epilayers grown on a scratched substrate surface. (a)-(b) show a scratch parallel to the off-cut direction while (c)-(f) show scratches inclined to the off-cut direction.
3.4. Nucleation of TSDs pairs and Carrot at scratches

MSXT and KOH etching pattern of some other samples reveal that TSDs can also be nucleated along substrate surface scratches. There are two scratches visible in Figs. 5(a) and 5(b). On the topographs both of them have linear features attached to them which project along the off-cut direction. X-ray topography reveals the lower one as a single white band which is similar to the cases we discussed above. Compared with the etch pit pattern, it is clear that only TEDs and BPDs nucleated along it. But the upper one manifested itself on the topographs as a single but wider white band of contrast. The corresponding etch pit pattern confirmed that some other dislocations whose pits are bigger and deeper than TED etch pits were also nucleated along the scratch. Fig. 5(c) shows an enlarged area and it is observed that these dislocations appear as large hexagonal pits which correspond to elementary TSDs [9].

A nucleation mechanism for screw dislocations at inclusions has been previously proposed by our group [13]. Here we extend this approach to explain the observed nucleation of TSDs along scratches. As shown in Fig. 6, this model assumes that the scratch groove is not uniform but has a graded bottom. Atomic steps which approach these local surface indentations can collapse, as shown in Fig. 6, creating two screw dislocations of opposite sign which have Burgers vector magnitude equal to the magnitude of the step disregistry.
Fig. 7 shows an example of nucleation of TSDs along the scratch where the density of the nucleated TSDs is relatively low. It reveals clearly a distribution of five TSD pairs (indicated by pairs of arrows) which confirms our proposed mechanism. It is interesting that carrot defects are found to be associated with the nucleated TSDs for the two pairs in the upper region of Fig. 7. For each pair, a carrot defect is connected with one of the TSDs which is shifted from the position of the scratch groove. This is consistent with our previously proposed mechanism for the formation of carrot defects [14]. The updated nucleation mechanism for carrot defects at scratches will be published in a separate paper [15].

Figure 7. Etch pit pattern showing five pairs of TSDs and two of them are attached with carrot defects.

4. Conclusions

The deflection of TSDs and BPDs from substrate into Frank partials and TEDs, respectively, in the epilayer, has been confirmed. The influence of surface damage associated with scratches on the substrate surface has been investigated. We have demonstrated that various kinds of dislocations can be nucleated along the scratches which can propagate into the epilayers. Nucleation mechanisms are proposed although further studies will be needed to fully understand the processes. This latter work underlines the importance of good surface preparation prior to CVD growth.

Acknowledgment

This work was supported in part by ONR Grant Nos. N000140010348, N000140110302, and N000140211014 and by subcontract to Dow Corning Corporation under ONR contract (Dr. P. Maki) Nos. N0001405C0324 and DAAD1701C0081. Topography experiments were carried out at the Stony Brook Synchrotron Topography Facility, Beamline X-19C, at the NSLS (Contract no. DE-AC02-76CH00016) and Beamline XOR-33BM, Advance Photon Source, Argonne National Laboratory, which is supported by U.S. Department of Energy, Office of Basic Energy Sciences under Contract No. W-31-109-ENG-38.

Reference