Characterization of V Shaped Defects in 4H-SiC Homoepitaxial Layers

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Abstract

Synchrotron white beam x-ray topography images show that faint needle-like surface morphological features observed on the Si-face of 4H-SiC homoepitaxial layers using Nomarski optical microscopy are associated with V shaped stacking faults in the epilayer. KOH etching of the V shaped defect reveals small oval pits connected by a shallow line which corresponding to the surface intersections of two partial dislocations and the stacking fault connecting them. Transmission electron microscopy (TEM) specimens from regions containing the V shaped defects were prepared using focused ion beam milling, and stacking sequences of (85), (50) and (63) are observed at the faulted region with high resolution TEM. In order to study the formation mechanism of V shaped defect, low dislocation density 4H-SiC substrates were chosen for epitaxial growth, and the corresponding regions before and after epitaxy growth are compared in SWBXT images. It is found that no defects in the substrate are directly associated with the formation of the V shaped defect. Simulation results of the contrast from the two partial dislocations associated with V shaped defect in synchrotron monochromatic beam x-ray topography reveals the opposite sign nature of their Burgers vectors. Therefore, a mechanism of 2D nucleation during epitaxy growth is postulated for the formation of the V shaped defect, which requires elimination of non-sequential $1/4[0001]$ bilayers from the original structure to create the observed faulted stacking sequence.

Keywords: CVD; epitaxial growth; stacking fault; defects; x-ray topography; HRTEM

Introduction

It is generally accepted that 4H-SiC will eventually replace silicon for the fabrication of next generation high power devices, with many 4H-SiC based devices already being designed and demonstrated to have enormous potential [1]. This relies on the delivery of high quality 4H-SiC epitaxial wafers, which are usually grown on the vicinal 0001 Si-face plane using chemical vapor deposition (CVD) homoepitaxy [2]. The quality of the epitaxial layers has improved due to several factors. First, for those defects inherited from the substrate, such as threading screw dislocations (TSDs) and micropipes (MPs), production of low defect density substrate wafers [3]

results in consequently low defect densities in the epitaxial layers. Second, ingenious engineering of the epitaxial growth process enables the conversion of defects from a harmful category to a less harmful one. For example, basal plane dislocations (BPDs) can cause the degradation of device performance by generating Shockley stacking faults [4]. BPDs are thereupon engineered to convert to threading edge dislocations (TEDs), which are electrically benign, by pre-growth etching [5] and interrupted growth [6]. Third, optimized growth conditions eliminate those defects generated in the epilayer or at the substrate/epilayer interface, such as triangular defects [7-10] and carrot defects [11-13]. Such progress in achieving better quality epilayers relies on a complete understanding of different kinds of defects, which involves locating the defects, characterization of their nature, and determining their origins. In this paper, we present the characterization of V shaped defects, which are occasionally observed in our studies of 4H-SiC epilayers, and their possible formation mechanism via 2D nucleation.

Experiment

Defects in four inch PVT-grown 4H-SiC substrate wafers are mapped and studied before epitaxial growth using synchrotron white beam x-ray topography (SWBXT), with both transmission geometry and grazing geometry. Then, 4H-SiC homoepitaxial layers with an n-buffer plus n-type drift structure are grown on the Si-Face of the substrate by CVD. The epilayer surface is first examined with Nomarski optical microscopy to check the existence of V shaped defects. Then, defects are imaged and studied using SWBXT, using the same imaging geometries as used for the substrate. Finally, the epitaxial wafers are etched using molten KOH to decorate the V defects. 11-20 cross-sectional TEM samples are made on the V shaped defects using the focused ion beam (FIB) technique and studied with high resolution TEM (HRTEM).

Results and Discussion

V shaped defects can be recognized using Nomarski optical microscope as faint needle-like surface morphological features, as shown in Fig. 1 (a). These are different from triangular defects which show area contrast [8-10]. After KOH etching, an etch pattern consisting of two oval pits connected by a shallow line is observed to be associated with the V shaped defect, as shown in Fig. 1(b). SWBXT studies reveal that these V shaped defects are actually stacking faults in the epilayer. In Fig. 1(c) of -1011 transmission image, dark contrast of triangular shape is associated with the V shaped defects. All such defects open towards the downstep direction and the height of the triangles corresponds to their projected length in the epilayer thickness, indicating that they are completely embodied in the epilayer. For comparison, there are two much larger stacking faults with dark contrast in the image and they are contained in the substrate [14-16]. The V shaped defects are out of contrast in Fig. 1(d) and are determined to be Frank faults with a fault vector of $n \times c/4[0001]$ ($n=1, 2, \text{ or } 3$), which satisfies contrast extinction criteria when $g \cdot R = \text{integer}$, where g corresponds to the reflection vector and R corresponds to the fault vector. Therefore, two oval pits in Fig. 1(b) correspond to the partial dislocations and the shallow line corresponds to the intersection of stacking faults with the sample surface.

Figure 1. (a) Optical micrograph shows the faint needle-like surface morphological features associated with the V shaped defect.; (b) Etch pit pattern of V shaped defect is composed of two small oval pits connected by a shallow line; (c) SWBXT images of $-101-1$ reflection recorded from a region containing V shaped defects; (d) SWBXT images of $10-10$ reflection recorded from the same region as Fig. 1 (c)

In order to study the origin of V shaped defect, 4H-SiC wafers before and after epitaxy growth were examined using SWBXT and images recorded from regions where V shaped defects form are carefully compared. Fig. 2(a) is a SWBXT grazing image of $11-28$ reflection recorded from a region on the silicon face of the epitaxial wafer containing several V shaped defects. The stacking fault is out of contrast and the partial dislocations associated the stacking fault show linear contrast. Fig. 2(b) shows a $11-28$ grazing image recorded from the same region before epitaxial growth. Several TSDs are marked with black circles and they are observed to appear at about the same locations before and after epitaxial growth, which suggests TSDs propagate along the threading direction from the substrate into the epilayer. By comparison, four V shaped defects are marked with white boxes and no defects are observed at the locations corresponding to the apexes of the V shaped defects which are expected to be their nucleation sites.

Figure 2. (a) SWBXT image recorded in grazing incidence ($g=11-28$) on the epilayer surface (Si-face) containing many V shaped defects. White boxes highlight four V shaped defects and black circles mark several TSDs; (b) same reflection recorded from the corresponding region on Si face of the substrate before epitaxial growth

Therefore, it is reasonable to consider that these V defects are newly generated in the epilayer instead of directly being inherited from defects in the substrate. If so, according to the law of Burgers vector conservation, the partial dislocations associated with the V defects should have opposite signs of Burgers vectors, and their net Burgers vector should be equal to zero. This has been verified through comparison in the contrast from the partial dislocations on synchrotron monochromatic beam x-ray topography images (SMBXT). Our simulation results of the contrast from dislocations with c-component of Burgers vector on basal plane indicate that dislocations with c-component of Burgers vector show black & white line contrast [17] and when the sign of the c-component changes the black and white contrast switches positions. It can be observed in Fig .3 that the partial dislocation on the left (L) side shows black-white contrast and the other one on the right (R) side shows white-black contrast, which suggests they have opposite sign c-component of Burgers vector.

Figure 3. SMBXT image of 11-28 reflection showing contrast from two V shaped defects. Reverse in back/white contrast from the two partial dislocaitons associated with V shaped defects reveals the opposite sign nature of their Burgers vectors

HRTEM studies have been carried out on V shaped defects and 11-20 cross-sectional TEM samples were made using the FIB technique. According to the Zhadnov notation [18], the lattice of perfect 4H-SiC should have a (22) stacking sequence. One sample made from a V shaped defect shows a (85) stacking sequence at the faulted region, as shown in Fig. 4(a). Another sample made from a different V shaped defect shows two faulted stacking sequences, (50) and (63), separated by 4 bilayers of perfect 4H-SiC (22) stacking sequence.

Figure 4. HRTEM images of V shaped defects showing: (a) (85) stacking sequence; (b) (50) and (63) stacking sequences

Fig. 5 shows how to transform the perfect (22) stacking sequence to an (85) faulted stacking sequence. Column I is the perfect (22) stacking sequence. Layer 7 is eliminated from column II and the new stacking sequence forms in column III; as a result, a (50) faulted stacking sequence is generated. Next, eliminate layer 11 and an (80) faulted stacking sequence can be generated, as shown in column IV and V. Finally, eliminate layer 17 and an (85) stacking sequence can be generated, as shown in column VI and VII. Each time a bilayer is eliminated, a distortion of $\frac{1}{4}c(0001)$ is induced to the lattice, so the total distortion is $\frac{3}{4}c(0001)$ in this case. During the transformation process no shift of the lattice on the 0001 plane is induced, which means no Shockley fault is generated. In a similar way, faulted stacking sequences observed in Fig. 4(b) can be artificially generated by eliminating layer 7 to form a (50) stacking sequence and eliminating layers 17, 21 and 23 to form a (63) stacking sequence, as shown in Fig. 6. Therefore, a distortion of $\frac{1}{4}c(0001)$ is associated with a (50) stacking sequence and a distortion of $\frac{3}{4}c(0001)$ is associated with a (63) stacking sequence. These results are consistent with the fault vectors determined by x-ray topography study.

Figure 6. Transformation from perfect (22) stacking sequence to (50) and (63) faulted stacking sequences

The artificial transformation from the perfect stacking sequence to the faulted one can be achieved during the actual crystal growth through 2D nucleation. Fig. 7 schematically shows the formation mechanism of a (50) stacking fault through 2D nucleation. 4H-SiC epitaxial growth is conducted on the vicinal (0001) plane and the step flow on the growth surface is sketched in Fig. 7(a). In Fig. 7(b), one SiC bilayer of wrong stacking sequence is nucleated on the growth surface (at layer 7) before the step flow arrives. As step flow continues, layer 8 at stacking position C merges into the 2D crystal on layer 7 which is also at stacking position C, because the same stacking sequences on each other is not allowed. Overall, it looks like that the original A step at layer 7 is overgrown by C step at layer 8, as shown in Fig. 7(c). Subsequently, the coming steps pile up on this distorted layer 8 and a (50) stacking fault forms as the one shown in Fig 7(d). Therefore, elimination of layer 7 can be realized through 2D nucleation of a single SiC bilayer on the growth surface and (50) can be generated as a result. The same processes of 2D nucleation can happen on layers 11 and 17 and thus an (85) stacking sequence will be generated. Similarly,

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