Characterization of a Basal-Plane Dislocation in 4H-SiC by X-Ray Three-Dimensional Topography and Transmission Electron Microscopy

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Abstract

The behavior of a basal-plane dislocation (BPD) in a thermally annealed 4H-SiC epilayer was investigated by X-ray three-dimensional topography and transmission electron microscopy. The two partials of a BPD changed their direction outward and formed a wider separation distance at the beginning of epitaxial growth. The partials maintained a virtually constant separation distance for most of the epilayer volume, but were constricted near the surface by high-temperature thermal annealing and then converted to a TED.

1. Introduction

In 4H silicon carbide (SiC) bipolar devices, basal plane dislocations (BPDs) in an epilayer trigger the expansion of Shockley-type stacking faults, causing forward voltage drop degradation of the devices [1]. A promising method to reduce BPD density in a 4H-SiC epilayer involves converting BPDs to threading edge dislocations (TEDs) [2]. X-ray three-dimensional (3D) topography has been applied to investigate the characteristic behaviors of BPDs and TEDs near epilayer/substrate (E/S) interfaces [3-7]. Using this method, we found that topography images of BPDs narrow just before the TED-TED conversion [3, 4, 6]. We also discovered that high-temperature annealing in Ar atmosphere drives the conversion of pre-existing BPDs to TEDs in 4H-SiC epilayers [8]. The question of how only a minority of BPDs in the substrate propagates into the epilayer and TED-TED conversion takes place by high-temperature annealing remains under discussion. This paper presents further analysis of BPD-TED conversion for a thermally annealed 4H-SiC epi-wafer, in which the detailed behaviors of a BPD near the E/S interface and in a volume of a thermally annealed 4H-SiC epilayer are examined by X-ray 3D topography and transmission electron microscopy (TEM).

2. Experimental

X-ray 3D topography measurements were conducted with \( \mathbf{g} = 1\ 1\ -2\ 12 \) on the synchrotron beam line BL24XU at SPring-8. This method uses an X-ray microbeam (\( E = 15 \) keV, diameter = 1-2 \( \mu \)m) and a special fine slit (V-slit) located near a sample [4]. Scanning the sample position under pinpoint X-ray diffraction measurement provides 3D topography, and varying the rocking angle gives the image of rocking-angle shifts (\( \Delta \omega \) map) [4]. The sample examined was an 8º off-cut (0001) Si-face 4H-SiC epi-wafer (10 \( \mu \)m-thick epilayer on a substrate). High-temperature annealing at 1800°C for 5 min was performed to convert the BPDs in the epilayer to TEDs after epilayer growth [8]. Prior to the 3D topography measurements, conventional synchrotron back-reflection X-ray topography was taken also with \( \mathbf{g} = 1\ 1\ -2\ 12 \) at \( E = 10.8 \) keV. Specimens for TEM observation were prepared using an FEI DB235 focused ion beam (FIB) system, while TEM analysis was conducted by the Hitachi H-9000UHR II with an acceleration voltage of 300 kV. Weak-beam dark-field images were obtained with \( \mathbf{g} = 1\ 1\ -2\ 12 \) at 0. The analysis of TED products was also conducted with \( \mathbf{g} = 2\ -1\ -1\ 0 \) and 1 -2 1 0.

3. Results and Discussion

The results of topography analysis are shown in Fig. 1 for a thermally annealed 4H-SiC epi-wafer. In conventional X-ray topography [Fig. 1(a)], BPDsub and BPDepi denote the parts of a BPD in the substrate and epilayer, respectively. A TED (TEDepi) to which the BPDepi converted near the downstream end is expected to be located in the dotted circle. The X-ray 3D topography image for the same position [Fig. 1(b)] confirms that the BPDsub and BPDepi propagate along the basal plane, and the BPDepi converts to TEDepi near the surface. Figure 1(c) provides the \( \Delta \omega \) maps for the vertical cross-sections at C1, C2, and C3. The \( \Delta \omega \) map for C1 exhibits a \( \Delta \omega \) pattern typical of a TED [3-7], while those at C2 and C3 correspond to TEDps [6, 7]. The \( \Delta \omega \) maps for C2 and C3 show that the strain field is more expanded in the epilayer than the substrate.

Figure 2 shows plan-view TEM images taken near the E/S interface and BPDepi-TEDepi junction. The two partials deviate from parallel changing in line directions outward at the E/S interface, and the separation distance widens when they enter the epilayer [Fig. 2(a)]. The separation distance peaks at \( \approx 100 \) nm, whereupon the right partial turns toward the left, forming a virtually constant separation distance of \( \approx 40 \) nm throughout most of the epilayer volume. This strongly suggests that some force arises to separate the partials at the beginning of epitaxial growth, which may hinder BPD-TED conversion at the E/S interface creating a wider stacking fault between the two partials [9] and
allowing BPD propagation into the epilayer.

In the gb product analysis under weak beam conditions, the Burgers vectors of the left and right partials are determined as \( b_1 = (a/3)[0 \ 1 \ -1 \ 0] \) and \( b_2 = (a/3)[1 \ 0 \ -1 \ 0] \), respectively. They point away from each other as indicated in Fig. 2(a). In this configuration, the separation of two partials is expected because the partials tend to be aligned with their Burgers vectors [10]. This coincides with observations showing that the line directions of the two partials change outward at the beginning of epitaxial growth. Although the separation width will be settled on a thermal equilibrium value in a volume of the epilayer, high-temperature heat treatment permits BPD_epi-TED_epi conversion in a near-surface region. The TEM image in Fig. 2(b) reveals that the separation distance of the two partials constricts; forming a pure screw-type BPD along the step-flow \([1 \ -2 \ 0]\) direction near the surface. Since the perfect BPD segment can easily make cross slip, promotion of BPD_epi-TED_epi conversion is expected near the surface by the cross slip of the segment toward the surface [8].

4. Conclusion

X-ray topography and TEM analyses were conducted for the propagation and conversion of a BPD during 4H-SiC epitaxial growth and high-temperature annealing. Topography analysis shows that the strain field around the BPD expands more in the epilayer than the substrate. TEM observation indicates that the two partials once separated near the E/S interface, whereupon one attracted the other. This strongly suggests that some force arises to separate the partials at the beginning of epitaxial growth. The separation distance of the partials was found to be constricted near the surface by high-temperature annealing, whereupon the BPD converted to a TED.

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