Investigation of dislocations in 8° off-axis 4H-SiC epilayer*

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This paper reports that the etching morphology of dislocations in 8° off-axis 4H-SiC epilayer is observed by using a scanning electronic microscope. It is found that different types of dislocations correspond with different densities and basal plane dislcation (BPD) array and threading edge dislocation (TED) pileup group lie along some certain crystal directions in the epilayer. It is concluded that the elastic energy of threading screw dislocations (TSDs) is highest and TEDs is lowest among these dislocations, so the density of TSDs is lower than TEDs. The BPDs can convert to TEDs but TSDs can only propagate into the epilyer in spite of the higher elastic energy than TEDs. The reason of the form of BPDs array in epilayer is that the big step along the basal plane caused by face defects blocked the upstream atoms, and TEDs pileup group is that the dislocations slide is blocked by dislocation groups in epilayer.

Keywords: elastic energy, basal plane dislcations, threding edge dislocations, threading screw dislocations

PACC: 6170G, 8160C

1. Introduction

Conventional 4H-SiC epilayer is produced on commercial substrates, which is 8° off-cut toward the [11$\bar{2}$0] direction, by chemical vapour deposition (CVD). It is widely recognised that there are high-density of defects in SiC epitaxial material. These defects include threading edge dislocations (TEDs), threading screw dislocations (TSDs) and basal plane dislocations (BPDs). The BPDs existed in SiC epilayers are primarily propagated from the substrates.[1] By x-ray topography using synchrotron radiation, Ohno *et al.*[2] observed that TEDs in the substrate propagated into the epitaxial layer, however BPDs in the substrate mostly converted to TEDs, and the rest are propagated as BPDs in the epitaxial layer. The relationship between dislocations and electrical properties of materials is very close.[3] It was reported that BPDs propagated from the substrate will cause nucleation of stacking faults in SiC bipolar diodes during forward operation, leading to the degradation of forward voltage drop of these devices,[4−6] while TEDs affect hardly to them. Ha *et al.*[7] observed the same phenomenon and suggested that the conversion was the image force in the epilayers between flowing growth steps and BPDs. Ohno *et al.*[8] also reported that low C/Si and high growth rate can enhance the propagation of BPDs. They thought that the step-flow growth was enhanced under such conditions, which will promote propagation of BPDs.[8] While, Tsutpmu *et al.*[9] reported that the BPDs density can be decreased by fast epitaxy. The reason for this contradiction is not clear at present. It does not have a consistent understanding of the reason why some dislocations converted in epilayers and the others propagated.

In this paper, based on the experimental results, in terms of Klapper's theorem and crystal structure of 4H-SiC, mechanism of conversion and propagation of dislocations in epilayers are discussed. The reason why BPD array and TED pileup produced in epilayer are studied.

2. Experiments

Homoepitaxial growth was carried out on commercially available 8° off-axis 4H-SiC (0001) Si-face substrate, which was supplied by SiCrystal.AG Co. in Germany, by using horizontal hot-wall chemical vapour deposition CVD reactor. Hydrogen was used

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as carrier gas. Silane (SiH_4) and propane (C_3H_8) were used as precursors. The flow rate of silane was 20 ml/min, and propane was 10 ml/min.[10] The chamber temperature and pressure were kept at 1550 ℃ and 9.6×10^3 Pa during growth, respectively. The epilayer was etched by molten KOH at 500 ℃ for 5 min. Four kinds of etch pits were observed by scanning electronic microscope (SEM), which are (a) large hexagonal pits corresponding TSDs, (b) small hexagonal pits corresponding TEDs, (c) shell-like etch pits corresponding $B_{\rm MD}$ with line vector along $[10\bar{1}0]$, and (d) shell-like etch pits corresponding $B_{\rm TSD}$ with line vector along $[11\bar{2}0]$. Good definition images of these dislocations are shown in Fig. 1(a), which are marked as a,b,c and d, respectively. There is BPDs array along the direction perpendicular to $[11\bar{2}0]$ in Figs. 1(a) and 1(b), respectively. In Fig. 1(b), some TEDs arrays lie along some certain crystal directions in the epilayer which is $< 1\bar{1}00 >$.

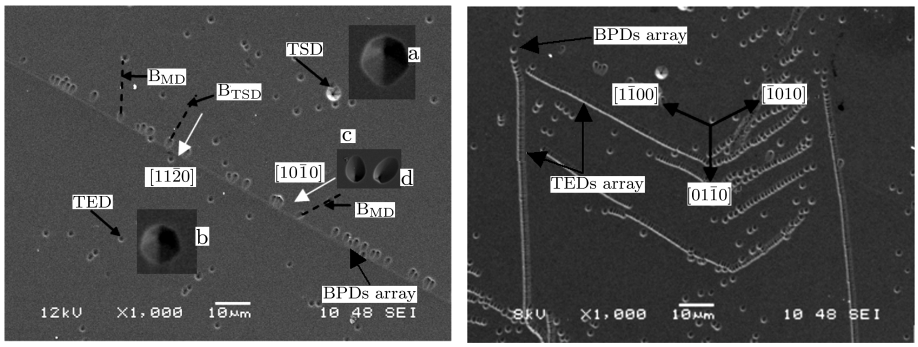


Fig. 1. Etch pits of 4H-SiC epilayer observed by SEM. White arrow is the direction of dislocation line and black dashed line is dislocation line.

3. Discussion

As shown in Fig. 1, the density of TEDs is the highest among these dislocations, whereas the density of BPDs is the second, and the density of TSDs is the third. As is well known, the dislocations in 4H-SiC epilayer by homoepitaxial growth method are primarily propagated or converted from the substrates. Which kinds of dislocations can propagate into epilayer? Which kinds of dislocations can convert to in epilayer? What is the connection between the dislocation density and the type? Why does BPD array and TED pileup group form in epilayer? These questions will be discussed in the following.

According to the Klapper's theorem,[11] the direction of dislocation extension in the epilayer must be according to the conservation of burgers vector and the principle of the lowest energy. For a straight dislocation propagating in the epilayer, its elastic energy per unit growth length W can be written as[12]

$$W = \frac{E}{\cos\alpha}, \tag{1}$$

here E is the elastic energy per unit length of dislocation line, and α is the angle between the dislocation line and the growth direction.

(1) For the TEDs and TSDs, their elastic energies per unit length of dislocation line $E_{\rm TED}$ and $E_{\rm TSD}$ can be written as[13]

$$E_{\rm TED} = \ln(r_0/r_1)(G\boldsymbol{b}_{\rm TED}^2)/4\pi(1-\nu), \tag{2}$$

$$E_{\rm TSD} = \ln(r_0/r_1)(G\boldsymbol{b}_{\rm TSD}^2)/4\pi, \tag{3}$$

here r_0 and r_1 are the radiuses of dislocation core and dislocation elastic force-field, respectively. For TED and TSD, the value of $\ln(r_0/r_1)$ is the same. The G is shear modulus, and ν is Poisson's ratio. For 4H-SiC, ν is 0.2. $\boldsymbol{b}_{\rm TED}$ and $\boldsymbol{b}_{\rm TSD}$ are the burgers vector of TED and TSD, respectively. The crystal structure of 4H-SiC is hexagonal, $\boldsymbol{b}_{\rm TED}$ is equal to a(a = 3.07 Å, 1 Å = 0.1 nm) and $\boldsymbol{b}_{\rm TSD}$ equal to $1c$ (c = 10 Å). Let A represent $\ln(r_0/r_1)G/4\pi$, then Eqs. (2) and (3) become

$$E_{\rm TED} = 11.75 \text{ A}, \tag{4}$$

$$E_{\rm TSD} = 100 \text{ A}. \tag{5}$$

Obviously, $E_{\rm TSD} >> E_{\rm TED}$. Due to the epilayer grown on an 8° off-axis substrate, for TED and TSD, both angles between the dislocation line and the growth direction are 8° (see Fig. 2).

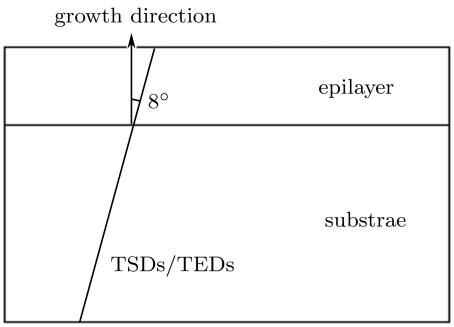


Fig. 2. The schematic diagram of TSDs/TEDs propagation.

According to Eq. (1), $W_{\rm TED}$ and $W_{\rm TSD}$ can be calculated and they are 11.87 A and 100.98 A respectively, i.e., $W_{\rm TSD} >> W_{\rm TED}$. It indicates that more TEDs must be existed in epilayer and substrate, and TEDs can not convert to TSDs due to the lower elastic energy. The former explains our observation that the density of TEDs is higher than TSDs, also the same phenomenon in substrate was observed by Daisuke *et al.*[14] The latter explains the reason why TEDs in the substrate propagate into the epitaxial layer, which was observed by Ohno *et al.*[8] Due to the differentia of the burgers vector (the direction of burgers vector of TED perpendicular to [0001], the burgers modulus is 3.07. The burgers vector of TSD is parallel to [0001], the burgers modulus is 10), TSDs can propagate into epilayer but can not convert to TEDs, in spite of the elastic energy of TSDs higher than TEDs. This inference will be verified in the following study.

(2) For BPDs, there are different dislocation types determined by the angle between the dislocation line and the burgers vector of the dislocation. If the angle is 0°, the dislocation is screw-type BPD (marked as $\rm B_{TSD}$), and if the angle is 90°, it is edge-type (marked as $\rm B_{TED}$). It is mixed-dislocation (marked as $\rm B_{MD}$) if the angle is neither 0° nor 90° (see Figs. 1 and 3).

The atoms glide easily along $< 11\bar{2}0 >$ because the direction of close-packed atoms in hexagonal structure is $< 11\bar{2}0 >$. It is implicated that the burgers vectors of the most BPDs are $< 11\bar{2}0 >$. Suppose the line vector of BPD is $[11\bar{2}0]$, and the burgers vector is $1/3\ [11\bar{2}0]$ (see Fig. 3), that is to say the angle between the dislocation line and burgers vector is 0°, then the BPD is $\rm B_{TSD}$. In this work, we have observed $\rm B_{TSD}$, as shown in Fig. 1. Daisuke *et al.*[14] confirmed that BPDs are mostly pure screw dislocations lying along $< 11\bar{2}0 >$ with the burgers vector of $1/3 < 11\bar{2}0 >$ in substrate, by x-ray topography. Jacobson *et al.*[15] observed that BPDs in the epitaxial layers lie parallel to the off-cut direction corresponding to screw dislocations. Ohno *et al.*[8] observed the same phenomenon and suggested that for a screw-type BPD.

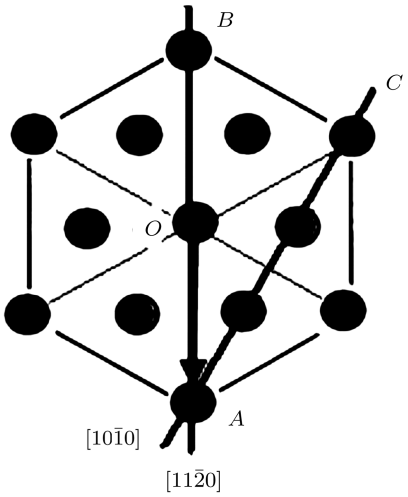


Fig. 3. The C–A is the dislocation along $[10\bar{1}0]$, B–A is along $[11\bar{2}0]$, O–A is the burgers vector with $[11\bar{2}0]$.

Suppose the line vector of BPD is $[10\bar{1}0]$, and the burgers vector is $1/3\ [11\bar{2}0]$ (see Fig. 3), that is to say the angle between the dislocation line and burgers vector is 30°, which is the $\rm B_{MD}$. As shown in Fig. 1. Daisuke *et al.*[14] reported that the BPDs along $< 1\bar{1}00 >$ are $\rm B_{MD}$s. The E and W of the two BPDs will be calculated respectively as follows.

For $\rm B_{TSD}$, the E of $\rm B_{TSD}$ is 9.42 A (according to Eq. (3)), α is 82°. Substituting these values into Eq. (1), we find that the $W_{\rm B(TSD)}$ is 67.69 A. For $\rm B_{MD}$, the dislocation line is neither perpendicular to the burgers vector nor parallel to, thus the burgers vector of $\rm B_{MD}$ can be dissociated to edge type and screw type dislocation, that is $\boldsymbol{b}_{\rm m} = \sin\theta \cdot \boldsymbol{b}_{\rm m} + \cos\theta \cdot \boldsymbol{b}_{\rm m}$[13] ($\theta$ is the angle between the $\rm B_{MD}$ line and burgers vector which is $[11\bar{2}0]$. $\boldsymbol{b}_{\rm m}$ is the burgers vector of mixed dislocation), as can be seen in Fig. 4.

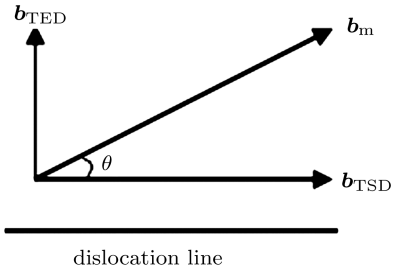


Fig. 4. The $\boldsymbol{b}_{\rm m}$ was dissociated to edge type and screw type dislocation.

Its elastic energy per unit length of dislocation

line $E_{\rm MD}$ can be written as

$$E_{\rm B(MD)} = (\ln r_0/r_1)(G(\sin\alpha' \cdot \boldsymbol{b}_{\rm m})^2)/4\pi(1-\nu) + (\ln r_0/r_1)(G(\cos\alpha' \cdot \boldsymbol{b}_{\rm m})^2)/4\pi. \quad (6)$$

Figure 5 showed the relationship between $B_{\rm MD}$ line and growth direction, where α' is the angle between the $B_{\rm MD}$ line and the growth direction, β is the angle between $B_{\rm MD}$ line and the $[11\bar{2}0]$ direction, γ is the angle between the $[11\bar{2}0]$ direction and the growth direction. By geometry, α' is found to be

$$\cos\alpha' = \cos\beta \cdot \cos\gamma. \quad (7)$$

The elastic energy per unit growth length $W_{\rm B(MD)} = E_{\rm B(MD)}/\cos\alpha'$, that is 97.9 A.

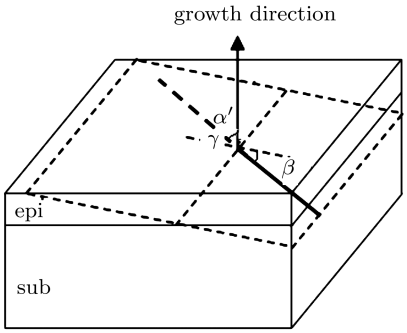


Fig. 5. The schematic diagram of $B_{\rm MD}$ in substrate and epilayer where α' is the angle between the $B_{\rm MD}$ line and the growth direction, β is the angle between $B_{\rm MD}$ line and the $[11\bar{2}0]$ direction, γ is the angle between the $[11\bar{2}0]$ direction and the growth direction.

From the results hereinbefore, we have found that $W_{\rm B(MD)} > W_{\rm B(TSD)} > W_{\rm TED}$. According to Klapper's theorem, it is necessary to analyse whether the convertible condition agrees with the conservation of burgers vector. For $B_{\rm MD}$s and $B_{\rm TSD}$s, the burgers vector are perpendicular to [0001], the value is 3.07 Å. For TEDs, its burgers vectors are perpendicular to [0001], and the value is 3.07 Å too. So this convertible condition agrees with the conservation of burgers vector. The two conditions indicate that both $B_{\rm MD}$s and $B_{\rm TSD}$s can convert to TEDs. Many researchers had reported this phenomenon. As can be seen from Figs. 1(a) and 1(b), there are some BPDs array. Why do BPDs array form in epilayer? A big step along basal plane caused by defects (may be stacking faults) will affect the deposition speed on both sides of it. In the condition of step-flow growth, this big step will block the upstream atoms. These atoms will pile up fast in front of this big step. In this case, stress is formed in this situation because that these atoms have no enough time to arrange according to the perfect crystal structure. In order to decrease stress, atoms arrange in the form of BPD array along basal plane. But the atoms deposit slowly at the place of downstream of the big step, thus no BPD array is formed at this place. As can be seen from Figs. 1(a) and 6.

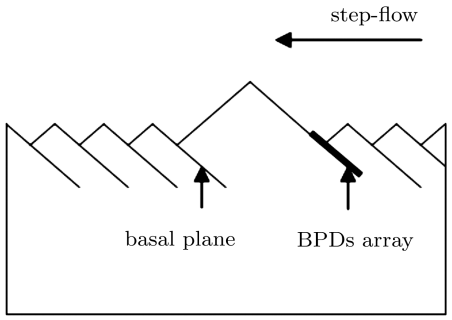


Fig. 6. The schematic diagram of the generation of BPDs array.

Due to the elastic force-field of dislocation groups, the slide of dislocations along $< 1\bar{1}00 >$ is blocked. Thus, dislocations plie up in the front of dislocation groups. The interval between the two TEDs among pileup group according to the relation of Eshelby–Frank–Nabarro, which is written as[16]

$$x_i = D\pi^2 i^2/8n\tau_0. \quad (8)$$

Here i is the ordinal of dislocation, x is the distance between the first dislocation and random one of pileup group, D and τ_0 are constants. It is concluded that the interval between the adjacent TEDs increases with the ordinal of dislocation. This is observed in Fig. 1(b).

4. Conclusion

In this paper, the reason why some dislocations converted in epilayers and others propagated is discussed. The elastic energies of these dislocations per unit growth length have been calculated. From the calculation in this paper, the elastic energy of TSDs is highest and that of TEDs is lowest among these dislocations, so the density of TSDs is lower than TEDs. The TSDs along $< 0001 >$ can propagate into epilayer but can not convert to TEDs, in spite of the elastic energy of TSDs higher than TEDs; basal plane mix dislocations ($B_{\rm MD}$s) and TSDs ($B_{\rm TSD}$s) can convert into TEDs because the convertible condition agrees with the conservation of burgers vector and the principle of the lowest energy. The reason why BPD array

existed in epilayer is also discussed. It is concluded that the big step along basal plane caused by defects (may be stacking faults) affects the deposition speed on both sides of it. Thus, BPD array formed. Because the dislocations slide is blocked by dislocation groups, the TEDs pileup group formed.

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