

# Study of Morphology Defects in 4H-SiC Thick Epitaxial Layers Grown on 4° off-Axis Si-face Substrates

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## Abstract

The crystallographic structure and origins of morphology defects observed in 4° off-axis Si-face thick 4H-SiC epitaxial layers were investigated by Nomarski microscope and Raman spectroscopy. The growth direction of these morphology defects is consistent with the step-flow direction, all of the defect include a certain core, which indicates that the defects were originated from certain cores. These cores of the morphology defects contain 3C poly-crystalline grains based on the Raman spectroscopy characterization. The head part of the defect formed during epitaxial layers growth and their formation is attributed to the foreign particles. The formation mechanisms of these obtuse morphology defects are discussed based on our model. It can be concluded that foreign particles fall down on the surface during the 4H-SiC epitaxy that disturb the normal step flow mode and lead to the 3C-SiC nucleation, which is the origination of the morphology defects.

## 1 Introduction

4H silicon carbide (4H-SiC) is a very promising candidate for application of high power, high frequency and high temperature electronic devices due to its superior physical properties[1-3]. The fabrication of high power SiC devices requires high-quality thick 4H-SiC epilayers[4]. In recent years, several groups have improved the epitaxy technology led to the smooth epitaxial surfaces on 4H-SiC substrates [5-7]. However, current SiC epitaxial wafers still contain morphology defects, which affect the overall quality of SiC devices including an increase of leakage current and a reduction breakdown voltage[8, 9]. The formation of the morphology defects is initiated by many factors such as the substrate defects, foreign particles and growth conditions and so on[10, 11]. Recently a kind of large morphology defects observed in 4° off-axis epilayers have been reported[12]. However, detailed structural analyses of the defects are not performed. The structures and origins of the large morphology defects need exhaustive investigation.

In this work, we present an intensive and thorough experimental study of the obtuse morphology defects in Si-face 4H-SiC epilayers by Nomarski microscope and Raman spectroscopy. The structures of these obtuse morphology defects are analyzed and their formation mechanisms are investigated based on our model.

## 2 Experiment

4H-SiC homoepitaxial layers were grown by a home-made vertical hot-wall CVD reactor[13]. Commercially available 10 mm×10 mm, n-type, Si-face 4H-SiC substrates oriented 4° off-axis toward [11-20] direction were used for

this work. The epitaxial growth was conducted by using a  $H_2 + SiH_4 + C_2H_4 + HCl$  gas system [14]. Homoepitaxial growth was maintained at 1550-1700°C with fluxes 30 slm, 80 sccm, 40 sccm for  $H_2$ ,  $SiH_4$  and  $C_2H_4$  respectively. The chlorine-additive was  $HCl$  and the  $Cl/Si$  ratio was fixed 1.0 for the crystal growth procedure. The  $C/Si$  ratio was also fixed 1.0 and the pressure was 80 Torr. After the growth stage, the samples were cooled down in an  $H_2$  ambient. The thickness of the epilayer was measured by cross-sectional Scanning electron microscope (SEM). The results indicate we obtained an epilayer with its thickness of 95.4  $\mu m$ . The morphological defects on these 4H-SiC epilayers were observed by Nomarski microscope and Raman spectroscopy.

## 3 Results and discussion

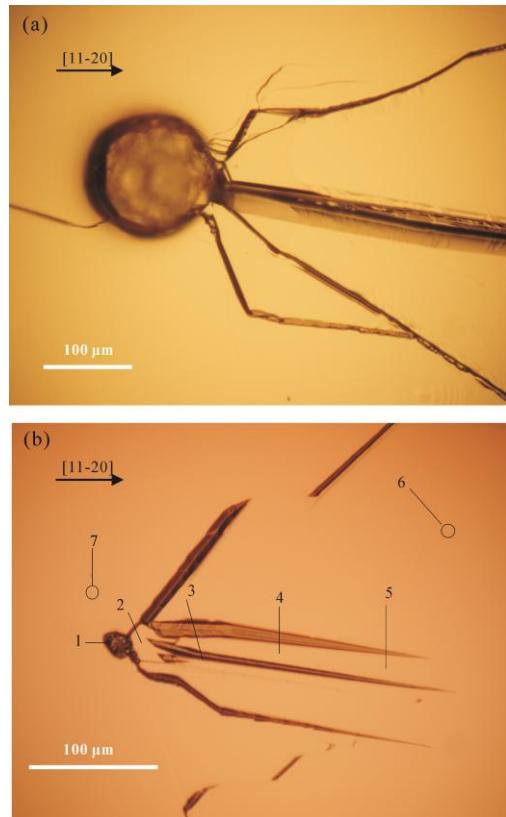


Fig.1 (a) Typical Nomarski microscope images of the morphology defect. (b) The measurement points of Raman spectroscopy.

Fig.1 shows the Nomarski micrographs of the morphology defect which is the typical surface morphological defects in the 95.4  $\mu m$  thick 4H-SiC homoepitaxial layers. As

seen in the figures, all the defects are arranged regularly along the step-flow direction. The defect shown in Fig.1 (a) was composed of a larger inclusive head and a morphology tail along the step-flow direction. The Fig.1 (b) shows the defect with a smaller inclusive head together with a morphology tail along the step flow direction as well as Fig.1 (a). The tail of the morphology defect consists of several prismatic structure as shown in Fig.1. The structures of the morphology defects are analyzed by Raman spectroscopy and the measurement points are shown in Fig.1 (b).

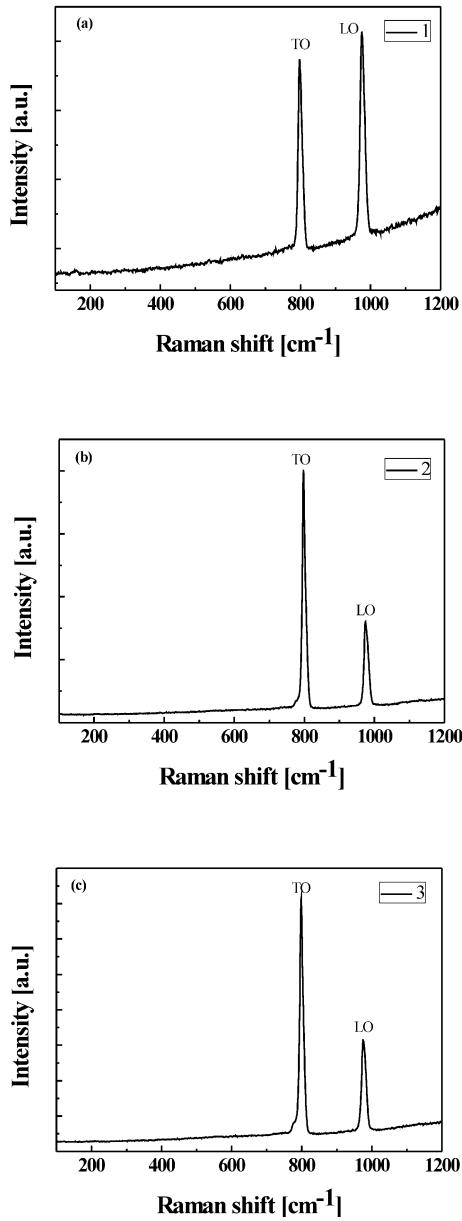


Fig.2 Raman spectra of different position of the morphology defect. The positions (labeled as 1~3) are seen in Fig.1(b).

The crystallographic structure of the defects is analyzed by Raman spectroscopy. The measurements of the defect are taken at six positions. Position 1 is located at the head of the defect. Four positions (labeled as 2~5) are evenly distributed

at the defect from head to the tail. Position 6 is located at the epilayer beside the defect but near to the head. Raman spectra of different positions of the morphology defect are shown in Fig.2 and Fig.3. It can be seen that the peaks of TO and LO modes for the spectrum at the defect from position 1 to 4 are similar and corresponding to the 3C-SiC, which indicates that these positions consist of 3C inclusion. However, the Raman peaks of the position 5 and 6 at 204 (TA), 610 (LA), 776 (TO), 796 (TO), and 964 (LO)  $\text{cm}^{-1}$  agree well with the 4H-SiC, which suggests the homoepitaxial growth of 4H-SiC at these positions.

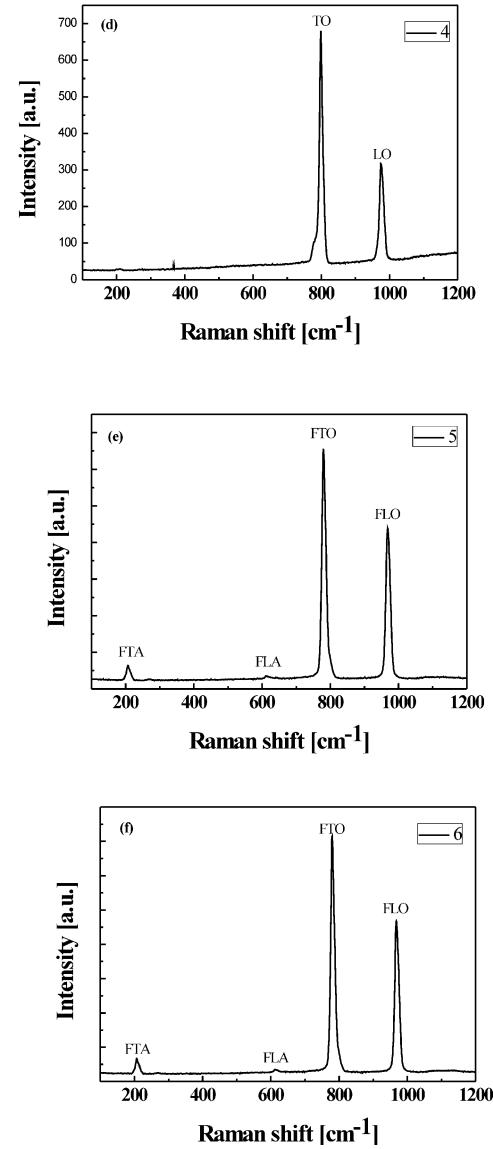


Fig.3 Raman spectra of different position of the morphology defect. Three positions (labeled as 4~6) are seen in Fig.1(b).

From the results of the Raman spectroscopy at different positions along the defect, it was found that the morphology defect was originated from 3C-inclusion[13]. The 3C-inclusion is big enough to disturb the step-flow epitaxial growth due to the high growth rate of two dimensional (2D)

nucleation[14, 15]. Then the epitaxial growth mode of the step-flow growth mode was interrupted in the region behind the head along the step flow direction on the basis of fluid dynamics[16]. These results are in agreement with a previous report by Takuro Tomita et al[17]. Furthermore, at position 6 beside the defect but near the head, the peaks observed are the typical peaks of 4H-SiC and no other peaks were detected. This indicates that in the region where the step-flow growth mode was not interrupted, it still shows the epitaxial nature with high crystal quality.

In order to find out the formation mechanism of the morphology defect, schematic diagrams describing the model are displayed in Fig. 4. In accordance with earlier papers reported [18, 19], morphology defects derive from the foreign particles are shown in the picture. When the foreign particle falls on the surface of the wafer, the steps are covered and the continuity of the steps is interrupted, as shown in Fig.4. With the growth mode of “Step-Controlled Epitaxy”, the Si and C atoms or molecules are first adsorbed to the terrace, then spread to the step and become nucleation in the corner of the step with lower level energy. Therefore, the nuclear structure will continue the crystal structure of the step, ensure that the crystal structure of the epitaxial layer in accordance with the substrate. However, when the foreign particle falls on the steps, the atoms or molecules adsorbed on the level cannot reach the steps, it is possible to have a two dimensional island formations in this area[20]. This should be attributed to the fact that the nucleation energy of 3C-SiC is lower than that of 4H-SiC. Therefore, two dimensional island nucleation are more likely to lead to the growth of 3C-SiC, eventually become the source of the morphology defects, as seen in Fig.4.

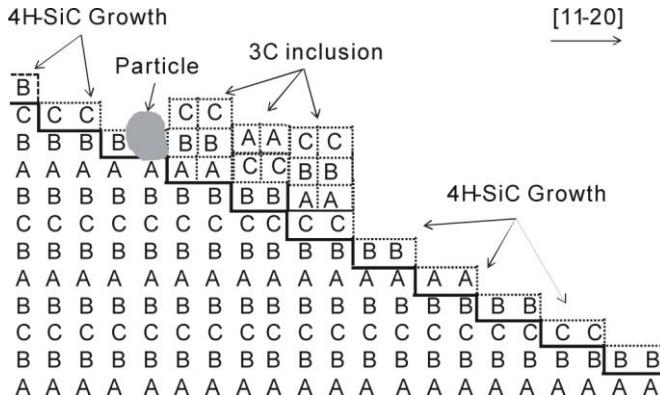


Fig.4 Illustration of the defect formation at the terraces with foreign particles during the 4H-SiC epitaxy.

From the above analysis of the morphology defects formation mechanism, it can be seen that the two dimensional island nucleation lead to the formation of 3C-SiC. However, two dimensional island nucleation is possible to cause the formation of 3C-SiC as well as 4H-SiC. The difference is the growth temperature. Therefore, increasing the growth temperature to reach or exceed the formation energy of 4H-SiC would reduce 3C-SiC nucleation. Meanwhile, another effect of the growth temperature is to increase the diffusivity of the adsorbed atoms to make it more active. Then the

adsorbed atoms can diffuse long enough to bypass the particles and become nucleation at the not covered steps near the particles, which prevents two dimensional island formation of the adsorption of atoms. It has been reported in the earlier literature to reduce the morphology defects by increasing the temperature[21]. Furthermore, increasing the flux of HCl gas can also decrease the formation of morphology defects[22, 23].

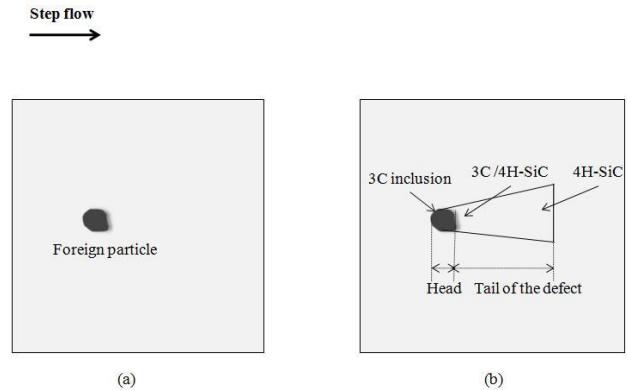


Fig.5 Plan view image of the formation mechanism of morphology defects introduced by foreign particles.

Fig.5 shows a typical plan view image of the defect formation process due to the foreign particles. At the first step, a particle of porous graphite foams which support the CVD deposition fall down on the surface of the wafer, this process can happen at any time in the epitaxy process, as seen in Fig.5(a). Then, with the increasing of the 4H-SiC epilayer, the foreign particle becomes a certain core which is the head of the defect. In the area where the step flow mode was disturbed, 3C-SiC nucleation happened, as shown in Fig.5(b). However, in the tail of the defect where the effect of the particle reduced and the normal step flow epitaxy carried out. In 2013, Chung et al. have reported that the origins of the morphology defects are the defect or the scratches in the 4H-SiC substrates [24]. However, we believe that the step mobility will be slower because of the foreign particles, meanwhile, the normal step flow mode will be disturbed during the 4H-SiC epitaxy. Then the atomic steps will bunch up. This is consistent with what our earlier paper reported[16]. As we can see from Fig.4, the formation of the 3C-inclusion area of the morphology defects is related to size and shape of the foreign particles. Also, when the particle fall down on the surface during the epitaxy is a critical factor to the length of the defects. Therefore, it can be concluded that foreign particles fall down on the surface during the epitaxy that disturb the step flow mode and lead to the 3C-SiC nucleation, which is the origination of the morphology defects.

#### 4 Conclusions

The morphology defects formed on Si-face 4° off-Axis thick 4H-SiC epitaxial wafers were characterized. Nomarski microscope and Raman spectroscopy were used to investigate the crystallographic structure and origins of morphology defects. All of these morphology defects were originated from certain cores. Moreover, the growth direction of the defects is

in accordance with the step-flow direction. The Raman spectroscopy results indicate that these cores of the morphology defects contain 3C poly-crystalline grains, which mean the head part of the defect formed during epitaxial layers growth and their formation is attributed to the foreign particles. The formation mechanisms of these obtuse morphology defects are discussed based on our model.

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