Misorientation dependent epilayer tilting and stress distribution in heteroepitaxially grown silicon carbide on silicon (111) substrate

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Abstract

The advantages and disadvantages of using off-axis substrates for heteroepitaxial growth of 3C-SiC on Si(111) substrates are investigated in this paper. 3C-SiC is deposited on on-axis and 4° off-axis 150 mm Si(111) substrates using low pressure chemical vapour deposition. The dependence of surface morphology, roughness, crystallinity, alignment between the epilayer and the substrate, and film stress are evaluated using atomic force microscopy, x-ray diffraction, and wafer curvature measurement. Highly parallel steps are observed on both on-axis and off-axis Si substrates after surface preparation, yet step density is doubled and step height is much larger (> 21 times of single step height) for 4° off-cut Si compared to on-axis Si. X-ray diffraction results indicate that SiC grown on on-axis Si substrates are well-aligned with the Si substrates, while the SiC grown on off-axis substrates are tilted positively by as large angle as 1.66°. The well-aligned SiC grown on on-axis Si substrate exhibits lower and uniform residual stress compared to the film grown on off-axis Si substrates, which exhibits a nonuniform distribution of higher stress. The stress distribution is found to be dependent on Si surface step direction and height. These misorientation dependent tilting and stress distribution mechanisms are expected to be applicable to other hetero-epitaxial growth systems with similar mismatch magnitude.

1. Introduction

SiC has wide energy gap and excellent physical, electrical, and chemical properties. SiC has more than 200 different polytypes, among them, 3C-SiC is the only SiC polytype that can be grown on large-diameter, low cost Si substrates. It offers the potential of integrating SiC-based electronics with mature Si technology and the 3C-SiC/Si structure can act as an excellent cost-effective template for graphene preparation [1,2]. In addition, as the research interest for fabrication of GaN-based blue light-emitting diodes is soaring up, the use of 3C-SiC/Si(111)

template for GaN growth shows great potential for reducing the intrinsic strain, improving crystal quality and obtaining large-area crack-free GaN films [3-6]. Consequently, there is a great need for an in-depth investigation of parameters that exert influences on the properties of the grown 3C-SiC. Relatively extensive investigations had been performed for the growth of 3C-SiC on on-axis Si(111) substrates, yet very limited knowledge and information are available in the open literature for the growth of 3C-SiC on off-oriented Si(111) substrates. It was shown that the surface roughness, stacking fault density, and stress magnitude were heavily dependent on the off-cut direction, where smoother SiC film with lower stress magnitude and less stacking fault density was achieved on off-axis Si substrate tilted towards [110] direction as compared with [112] direction [7,8]. Therefore, the merit of using either on-axis or off-axis substrates must be evaluated on a case-by-case basis. Although the differences in surface morphology, roughness, stress, crystalline quality had been reported for the growth of 3C-SiC on off-oriented Si, the root cause of them has not been investigated. In addition to that, tilting/inclination of the grown epitaxial layer relative to the substrate has been widely reported for hetero-epitaxial growth of other different materials [9-12], however, there is no investigation had been performed to evaluate the tilting degree of the hetero-epitaxially grown 3C-SiC film. Therefore, in this paper, we present a comprehensive study of the impact of the Si substrate misorientation on the surface morphology, crystal quality and orientation, and stress of deposited 3C-SiC using atomic force microscopy (AFM), x-ray diffractometry (XRD), and wafer curvature and stress measurements. Also, a mechanism for the observed misorientation-dependent properties of the grown SiC is proposed.

2. Experimental Details

The growth of 3C-SiC was performed on both on-axis (off-cut angle $< 0.5^\circ$) and off-axis (off-cut angle of $3.5 \pm 0.5^\circ$ towards $[110]$) 150-mm Si(111) substrates (both are p-type doped with resistivity in the range of $1\sim 10 \Omega \cdot \text{cm}$) using a custom-made low-pressure chemical vapour deposition reactor at a temperature of 1000°C . Si wafers were loaded into the reactor at 600°C as received (without pre-treatment). The temperature was ramped up at a rate of $5^\circ\text{C}/\text{min}$ under oxygen (100 sccm (standard cubic centimetre per minute)) in a pressure of 95 Pa to maintain the native oxide on the Si surface, which minimises the risk of carbon contamination of the silicon surface prior to a SiH_4 oxide removal process. The native oxide formed on the Si substrate surface was removed using low pressure SiH_4 at 1000°C to ensure a sharp 3C-SiC/Si interface. Following the removal of oxide, continued SiH_4 flow grows a fresh layer of Si on the activated Si substrate. This is then followed by a carbonisation step performed at 750°C to convert the clean Si surface into SiC layers. Epitaxial growth was then subsequently initiated at 1000°C using alternating supply epitaxy with SiH_4 and C_3H_6 as precursors. The details of this growth procedure are reported in Ref. 13 and 14.

XRD measurements were performed with a Panalytical Empyrean x-ray diffractometer, with a high resolution four-crystal Ge (220) asymmetrical incident beam monochromator, using Cu $K\alpha$ radiation ($\lambda = 1.5405980 \text{ \AA}$), and a PIXcel-3D detector with a fixed anti-scatter slit. The PIXcel detector is used in the Open Detector (OD) mode for the rocking curve and phi scan measurements. AFM measurements were performed using Park NX20 under non-contact mode. Cross-section transmission electron microscopy (TEM) characterisation was performed using FEI Tecnai F20 TEM (operating at an accelerating voltage of 200 keV). SiC cross-sectional slices were diced using diamond saw along the $[\overline{112}]$ direction, they were thinned down using sandpaper and finally by precision ion polishing system. The incident beam during TEM

observation was injected along $[\bar{1}10]$ direction. Due to excellent wafer thickness uniformity achievable with our optimised process (better than 99 % uniformity across 150-mm wafer), a Tencor Flexus 2320 system was used for monitoring wafer curvature prior to and after epitaxial growth. The scans were done along the diameter of 150 mm wafers with 10 mm edge exclusion. The biaxial stress for SiC films was calculated on the basis of the modified Stoney's equation [15-17], using the appropriate elastic moduli (E) and Poisson's ratios values: 170 GPa and 0.26 for Si(111).

3. Results and discussion

3.1 The morphology and roughness

Substrate surface morphology plays a very important role in the kinetics of epitaxy process and significantly impacts the crystalline quality of the grown film. The surface morphology and root-mean-square (RMS) roughness of Si substrates after in-situ surface preparation and grown SiC films at different process stages were characterised using AFM and are shown in Fig. 1 to Fig. 3.

Fig. 1 (a) shows the presence of step-like features on the on-axis Si surface after the in-situ Si surface cleaning using SiH_4 , with root mean square RMS roughness of ~ 0.17 nm over $1\ \mu\text{m} \times 1\ \mu\text{m}$ scan area. The origin of the small particulates that are evenly populating the surface is unclear and under current investigation. The terrace width ranges from ~ 155 to ~ 322 nm with an average step height of 0.31 nm, shown in Fig. 1 (b), indicating that a single step on Si(111) corresponds to double layers of Si atoms [18]. The calculated off-cut angle is therefore less than 0.1° , and no obvious step-bunching phenomenon was observed. The off-cut angle of the on-axis Si wafer was measured by XRD to be 0.06° , in a good agreement with AFM results and supplier specification. In contrast, Fig. 1 (c) shows that the in-situ cleaned off-axis Si wafer had a much larger RMS roughness of 1.55 nm. Highly parallel steps along $[\bar{1}10]/[1\bar{1}0]$ direction have been

observed on off-oriented Si substrates, the steps are normal to the wafer primary flat. From Fig. 1(d), it is clearly shown that the step density is twice as high as the step density on the on-axis wafer, with step spacing ranged from ~ 82 nm to ~ 117 nm and step height varied from 6.67 nm to 8.33 nm, which is more than 21 times higher than the step formed on on-axis Si. Its terrace width and step height are very similar to what reported for 4° off-cut Si(111) towards [110] [19], whose component vector in the (111) plane is $[11\bar{2}]$ direction. XRD measurement also confirmed that the off-cut angle of the off-axis Si wafer is $\sim 4.0^\circ$. Fig. 1 (c) and (d) clearly demonstrates that step bunching has occurred during the surface preparation step, most likely due to the larger off-cut angle and high temperature processing. Vicinal planes are clearly seen after removing the surface oxide from the 4.0° off-cut Si substrate. The initial surface roughness is therefore much higher for the off-axis Si substrate due to the denser and higher steps.

Fig. 1. Top-view AFM images and surface line profile of Si surface after in-situ cleaning: (a) top-view morphology of on-axis Si, (b) surface line profile of on-axis Si, (c) top-view morphology of $\sim 4.0^\circ$ off-axis Si, and (d) surface line profile of $\sim 4.0^\circ$ off-axis Si. The scan area is $1\ \mu\text{m} \times 1\ \mu\text{m}$.

Fig. 2. Top-view surface morphology of SiC films grown on on-axis Si substrate at various process stages: (a) after carbonisation (~ 3 nm), (b) after 8 ± 2 nm SiC growth, and (c) after 240 ± 5 nm SiC deposition. The scan area is $5\ \mu\text{m} \times 5\ \mu\text{m}$.

Fig. 3. Top-view surface morphology of SiC films grown on $\sim 4.0^\circ$ off-axis Si substrate at various process stages: (a) after carbonisation (~ 3 nm), (b) after 8 ± 2 nm SiC growth, and (c) after 240 ± 5 nm SiC deposition. The scan area is $5\ \mu\text{m} \times 5\ \mu\text{m}$.

After converting the Si surface into SiC by carbonisation (Fig. 2 (a)), the surface of the on-axis wafer surface is quite smooth with a RMS roughness around 0.11 nm (similar to in-situ cleaned Si surface) and the step-like features are still visible. The presence of steps after carbonisation indicates that the chemical reaction that forms SiC during the carbonisation does not significantly change the initial surface morphology. This SiC layer thickness was measured to be around 3 nm using ellipsometry. A key point in our carbonisation process is that the formed carbonisation layer is very thin due to optimized carbonisation conditions and relatively low carbonisation temperature.

Fig. 3 (a) shows that the step-like feature is also visible for SiC deposited on off-axis Si substrates. However, unlike the on-axis case where the RMS roughness was similar before and after carbonisation, the RMS roughness after carbonisation on off-axis Si substrate is increased to 3.08 nm, which is a significant change from the RMS roughness of 1.55 nm of the cleaned Si surface. This indicates that the Si surface and thin carbonised film (~ 3 nm) may not be stable during the cool down process—Si atoms might easily diffuse through the thin SiC layer and cause the formation of Si voids: the higher stress of the SiC grown on off-axis substrate may contribute to the formation of Si voids, which are absent in the SiC grown on on-axis substrate with similar thickness; the mismatch in thermal expansion coefficients between Si and SiC also introduces stress during the cool down process, which can also contribute to the formation of Si voids. This gives rise to an increase in roughness that is not seen with the thicker SiC films, which could be due to formation of Si voids in the case of the carbonised film (due to the much larger step height, the carbonisation conditions may need to be specifically optimized for off-axis wafers). With growth of thicker SiC films, the film become more robust and stable during the cool down process, so they retains their roughness characteristics. From TEM evaluation of

thicker SiC film grown on off-axis Si substrate, there are no Si voids having been observed at the SiC/Si interface, which supports the assumption that Si voids only occurred in thin carbonised film ($\sim 3\text{nm}$) if it is cooled down to room temperature.

Due to the island growth mode of SiC at the subsequent film growth stage, the step-like features of the carbonised layer disappeared and the surface became rougher with increasing film thickness. After $8 \pm 2\text{ nm}$ SiC deposition, the SiC surface is composed of fine grains and no clear pattern can be recognized in the AFM image in Fig. 2 (b) and Fig. 3 (b). No obvious difference can be observed in surface morphology for SiC film grown on on-axis and off-axis substrates. This indicates that the previously observed Si voids in the case of off-oriented substrates are either not formed or covered up by thin SiC growth. The trend of RMS roughness of Si substrates and deposited SiC film at different stages is shown in Fig. 4. The RMS roughness for the $8 \pm 2\text{ nm}$ SiC layer is around 0.98 nm , for SiC films deposited on both on- and off-axis substrates. For 70 nm SiC film, the RMS roughness data are also comparable at a value of $\sim 1.16\text{ nm}$. With the further increase in thickness, triangular features were observed on SiC with a thickness of $240 \pm 5\text{ nm}$ when using on-axis Si substrate (Fig. 2 (c)). In contrast, the SiC grown on off-axis substrate (shown in Fig. 3 (c)) had a vastly different morphology; it is anisotropic, with lines predominantly developed in the directions parallel to the initial Si surface steps. The RMS roughness is slightly smaller for $240 \pm 5\text{ nm}$ SiC grown on off-axis substrate (2.57 nm) than that on on-axis substrate (3.22 nm), even though both had comparable roughness values after 9 nm SiC deposition. The impact of substrate orientation on RMS roughness was further exemplified by increasing the deposited SiC film thickness, for a $\sim 625\text{ nm}$ SiC film, the RMS roughness reached a value of 6.06 nm for SiC grown on off-axis Si, compared with a value of 9.05 nm for SiC grown on on-axis Si. It seems to indicate that our growth conditions may be

better suited for SiC growth on off-axis Si substrates, where the denser steps on off-axis substrate enhanced step-flow growth mode rather than island growth. Despite the vastly different growth conditions, this observation is in agreement with what reported by Severino et al. [7] that a smoother film was deposited on off-axis Si than on-axis Si, where the root cause was attributed to enhanced lateral growth. Although the roughness is smaller when using off-axis substrate, the XRD evaluation (discussed in detail in Section 3.2) shows a significant tilting of the grown SiC layer relative to the substrate. The tilting of the grown layer might also contribute to the smaller roughness.

Fig. 4. RMS roughness of Si substrates and SiC films at various thicknesses. The inserted section is an enlargement of RMS roughness for thin SiC films (< 10 nm).

3.2 Crystallinity and alignment analysis

The orientation and crystalline quality of the SiC films were evaluated using high resolution XRD. From the 2θ - ω scan, it is confirmed that the SiC films are epitaxially grown on all Si(111) substrates, following the orientation of the Si substrate, no SiC(200) or SiC(110) peaks were found. However, this is only a rough characterisation. In order to accurately evaluate the degree of tilt between the grown epitaxial layer and the substrate, rocking curve (RC) scans at azimuthal angles ranging from 0° to 360° (relative to the wafer primary flat) with an increment of 30° were performed. The difference in omega position between Si(111) and SiC(111) peak was used to tell the tilting degree of the SiC epilayer using the the following Equation [10]:

$$(\omega_{SiC} - \omega_{Si})_{maximum} - (\omega_{SiC} - \omega_{Si})_{minimum} = 2\Delta\alpha_0, \quad \text{Equation (1)}$$

where ω_{SiC} is the omega angle of SiC(111) peak at a certain azimuthal angle, ω_{Si} is the omega angle of Si(111) peak at the same azimuthal angle, and $\Delta\alpha_0$ is the relative tilting angle of the

epilayer to the substrate, it is calculated from half the difference in the optimized ω angles at the Bragg condition, $(\omega_{SiC} - \omega_{Si})_{maximum}$ means the maximum difference between $\omega_{SiC(111)}$ and $\omega_{Si(111)}$, $(\omega_{SiC} - \omega_{Si})_{minimum}$ means the minimum difference between $\omega_{SiC(111)}$ and $\omega_{Si(111)}$, and the maximum and minimum value was achieved at an azimuthal angle of ϕ and $(\phi + 180)^\circ$ by rotating the sample to do a 360° ϕ scan. For 240 ± 5 nm SiC grown on on-axis wafer, the relative tilting angle is as small as 0.05° . In contrast, SiC grown on off-axis substrate, was positively tilted/inclined by 1.66° from the Si substrate [shown in Fig. 5, where $\Delta\omega$ is equal to $(\omega_{SiC} - \omega_{Si})$], which means that the grown SiC is $\sim 5.60^\circ$ tilted from the expected [111] direction. This type of tilting is usually named as Nagai tilt and has been widely observed in the heteroepitaxial growth of different materials on off-axis substrates, including GaN, AlGaAs, GaInAs, and GaAs [9-12]. For homoepitaxy on off-cut substrates, there is no misfit between the substrate and the epilayer, thus tilting does not occur. However, for hetero-epitaxial growth on off-oriented substrates, due to the presence of misfit, there may be a deviation of the growth direction of the epilayer relative to the substrate surface. For a step-controlled growth, it has been reported that the growth front is not normal to the substrate, but instead flows across the surface at an enhanced rate towards the tilt direction [20,21]. Growth of 3C-SiC on off-oriented Si(111) substrates has been reported, but the relative tilting has not been evaluated. These are the first results on the tilting of 3C-SiC grown on off-oriented Si(111) substrates. Therefore, this result demonstrated that the on-axis substrate is preferred over off-axis substrate for a better alignment between the epilayer and substrate.

Fig. 5. The difference in omega position between SiC(111) and Si(111) peaks at different azimuthal angles . Delta omega is equal to $(\omega_{SiC} - \omega_{Si})$ at a certain azimuthal angle. $\Delta\alpha_0$ is the

relative tilting angle of the epilayer to the substrate. For the SiC film grown on $\sim 4.0^\circ$ off-cut Si(111) substrate, the tilting angle is around 1.66° .

The full-width at half maximum (FWHM) of XRD rocking curve (RC) scans of the SiC (111) peak are shown in Fig. 6, a scattering distribution in the FWHM data versus different azimuthal angle was seen for 240 ± 5 nm SiC grown on on-axis and off-axis Si substrates, they have a similar average FWHM at $1.28^\circ \pm 0.08^\circ$, no obvious difference can be observed. Based on these data, it is difficult to deduce whether the SiC quality is worse or better in the directions parallel to the steps of Si substrate, compared to the directions normal to the steps; although the dependence on the step directions has been previously reported for GaN deposition [22].

Fig. 6 FWHM of RC scans of the SiC(111) peak for SiC films (240 ± 5 nm) grown on on-axis and off-axis Si substrates at different azimuthal angles.

3.3 Stress evaluation

It has been reported that stress magnitude in grown 3C-SiC is both orientation and off-cut direction dependent [7,8,17]. Stress measurements were performed at different azimuthal angles from 0° to 180° and the results are shown in Fig. 7. It is found that the stress distribution is quite uniform for SiC grown on on-axis Si with an average tensile stress of 676 MPa (242 nm thick SiC), yet non-uniform tensile stress distribution was observed for SiC grown on off-axis substrate, which ranged from 737 to 970 MPa (238 nm thick SiC). From the AFM image shown in Fig. 1(c), it can be seen that the steps on the off-axis Si surface are parallel to $[\bar{1}10]/[1\bar{1}0]$ direction. At zero degree of azimuthal angle, the curvature scan direction is normal to the steps (crossing the steps), while at 90° , the curvature scan direction is parallel to the steps. The crystalline quality evaluated by FWHM of RC using XRD measurements indicated that the film

quality is comparable at directions normal and parallel to the surface steps. Hence the impact of quality on stress distribution can be excluded. Therefore, the higher stress observed at 0° indicates that the surface step direction and height determine the magnitude of stress. Nonuniform distribution of stress has been previously observed for SiC films grown on off-axis substrates [7], but no clear explanation has been given, and the correlation with surface steps has not been previously investigated.

Fig. 7. The distribution of residual stress in SiC films (240 ± 5 nm) grown on on-axis and off-axis Si substrates.

3.4 Mechanism that determines epilayer tilting and stress distribution

For SiC on Si, the lattice mismatch is as high as $\sim 20\%$. The cross-section TEM image in Fig. 8 illustrates the formation of misfit dislocations at SiC/Si interface. These misfit dislocations help to relieve the in-plane stress caused by lateral lattice mismatch between the epilayer and the substrate. The stress caused by the mismatch in the normal direction (perpendicular to the interface) has to be accommodated by the deformation of the epilayer. For on-axis Si, the surface steps are of single monolayer high, whereas for off-axis Si, the step height is much larger ranged from 6.67 nm to 8.33 nm, which is more than 21 times higher than the step formed on on-axis Si. Also, the step density is nearly doubled in comparison to the on-axis Si. In addition, vicinal planes occur on off-axis Si, which introduces nonuniformity, and film growth can occur on both the (111) planes and the vicinal planes. As a result, a larger density of higher steps existing on the off-axis Si surfaces not only lead to a significant tilting of the grown layer, as shown by XRD measurements in section 3.2, but also cause a higher level and non-uniform distribution of residual stress in the grown film. Therefore, these results indicate that the surface step direction and height determine the magnitude and nonuniform distribution behaviour of stress.

Fig. 8. High resolution cross-section TEM image of the 3C-SiC/Si structure, injection beam is along $[\bar{1}10]$ direction . The line indicates the 3C-SiC/Si interface.

4. Conclusions

In summary, both positive and negative effects were observed for SiC grown on off-axis Si substrates. Highly parallel steps have been observed on well-oriented and off-oriented Si substrates after thermal oxide removal and Si deposition. The SiC films (~240 nm) deposited on an off-axis Si substrate has vastly different morphology in comparison with that deposited on an on-axis Si substrate. XRD measurements indicate that SiC films grown on-axis Si substrate is well-aligned with the Si substrate, while the SiC grown on $\sim 4^\circ$ off-axis substrate is tilted positively by 1.66° . The well-aligned SiC grown on on-axis substrate exhibited much lower and uniform residual stress compared to the SiC grown on off-axis Si. The nonuniform distribution of higher stress, present in films grown on off-axis wafers, is related to the presence of denser and higher steps in the Si substrate. These misorientation-dependent tilting and stress distribution mechanisms are expected to be applicable to other hetero-epitaxial growth systems with similar mismatch magnitude.

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Figure captions

Fig. 1. Top-view AFM images and surface line profile of Si surface after in-situ cleaning: (a) top-view morphology of on-axis Si, (b) surface line profile of on-axis Si, (c) top-view morphology of $\sim 4.0^\circ$ off-axis Si, and (d) surface line profile of $\sim 4.0^\circ$ off-axis Si. The scan area is $1\ \mu\text{m} \times 1\ \mu\text{m}$.

Fig. 2. Top-view surface morphology of SiC films grown on on-axis Si substrate at various process stages: (a) after carbonisation ($\sim 3\ \text{nm}$), (b) after $8 \pm 2\ \text{nm}$ SiC growth, and (c) after $240 \pm 5\ \text{nm}$ SiC deposition. The scan area is $5\ \mu\text{m} \times 5\ \mu\text{m}$.

Fig. 3. Top-view surface morphology of SiC films grown on $\sim 4.0^\circ$ off-axis Si substrate at various process stages: (a) after carbonisation ($\sim 3\ \text{nm}$), (b) after $8 \pm 2\ \text{nm}$ SiC growth, and (c) after $240 \pm 5\ \text{nm}$ SiC deposition. The scan area is $5\ \mu\text{m} \times 5\ \mu\text{m}$.

Fig. 4. RMS roughness of Si substrates and SiC films at various thicknesses. The inserted section is an enlargement of RMS roughness for thin SiC films ($< 10\ \text{nm}$).

Fig. 5. The difference in omega position between SiC(111) and Si(111) peaks at different azimuthal angles. Delta omega is equal to $(\omega_{\text{SiC}} - \omega_{\text{Si}})$ at a certain azimuthal angle. $\Delta\alpha_\theta$ is the relative tilting angle of the epilayer to the substrate. For the SiC film grown on $\sim 4.0^\circ$ off-cut Si(111) substrate, the tilting angle is around 1.66° .

Fig. 6 FWHM of RC scans of the SiC(111) peak for SiC films ($240 \pm 5\ \text{nm}$) grown on on-axis and off-axis Si substrates at different azimuthal angles.

Fig. 7. The distribution of residual stress in SiC films (240 ± 5 nm) grown on on-axis and off-axis Si substrates.

Fig. 8. High resolution cross-section TEM image of the 3C-SiC/Si structure, injection beam is along $[\bar{1}10]$ direction . The line indicates the 3C-SiC/Si interface.

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