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Realization of minimum number of rotational domains in heteroepitaxied Si(110) on 3C-SiC(001)

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Structural and morphological characterization of a Si(110) film heteroepitaxied on 3C-SiC(001)/Si(001) on-axis template by chemical vapor deposition has been performed. An antiphase domain (APD) free 3C-SiC layer was used showing a roughness limited to 1 nm. This leads to a smooth Si film with a roughness of only 3 nm for a film thickness of 400 nm. The number of rotation domains in the Si(110) epilayer was found to be two on this APD-free 3C-SiC surface. This is attributed to the in-plane azimuthal misalignment of the mirror planes between the two involved materials. We prove that fundamentally no further reduction of the number of domains can be expected for the given substrate. We suggest the necessity to use off-axis substrates to eventually favor a single domain growth. © 2016 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4939692>]

Silicon carbide (SiC) is an interesting wide band-gap material due to the outstanding mechanical and electrical properties that this material has to offer.^{1,2} Compared to other SiC polytypes, cubic SiC (3C-SiC) can be heteroepitaxially grown on low-cost silicon (Si) substrates.³ In the last decades, 3C-SiC has been drawing attention for micro-sensing applications for Micro-Electro-Mechanical-Systems (MEMS) and Nano-EMS (NEMS).^{4–7} Our group investigated the benefit of growing a Si epilayer on top of 3C-SiC/Si heterostructure to design MEMS devices benefiting from the properties of 3C-SiC.^{8–10} Indeed, the difference in reactivity between Si and 3C-SiC is advantageous for devices fabrication.¹¹ This offers a high chemical selectivity between the two layers, where the Si epilayer can be used as a sacrificial layer and the 3C-SiC layer can serve as an etch-stop layer. However, 3C-SiC and Si feature a large lattice mismatch (20%), a difference in thermal expansion coefficient (8%) as well as different crystallographic structures (zinc blende vs. diamond, respectively). We shall note here that the diamond Si belongs to the $Fd\bar{3}m$ space group and the cubic phase of SiC corresponds to the $T^2_d-F\bar{4}3m$ space group. These differences lead to a wide range of defects characterizing the 3C-SiC film (stacking faults, micro-twins, and antiphase domains). The formation of antiphase domains (APDs) is one of the most serious issues limiting the development of 3C-SiC/Si devices. It has been shown that the APDs tend to annihilate with increasing 3C-SiC film thickness.^{12–14} Generally, for MEMS/NEMS devices, the hetero-interface between the layers has to be smooth in order to avoid or limit the roughness transfer from one layer to the subsequent one, hence, avoid the process variability. Furthermore, the improvement of the material crystal quality

strengthen its mechanical properties. Therefore, the 3C-SiC and the Si layers have to show a smooth surface with a good crystalline quality. It is well-known that the APDs in the 3C-SiC layer drastically increase the roughness of the surface.¹⁵ Recently, we showed that the presence of APDs on the 3C-SiC surface leads to domain formation in the Si layer rotated by 90° around the growth direction.¹⁶ The presence of APDs on the 3C-SiC surface is then expected to increase the roughness of the subsequent Si layer due to irregular domain boundaries which are detrimental for MEMS/NEMS structures. In addition, the heteroepitaxy of Si on 3C-SiC is shown to occur in a columnar growth mode.^{16,17} This means that increasing the film thickness does not lead to any improvement of the crystal quality. The methods to improve the surface state and the final Si film quality are thus limited. Tuning the growth conditions can lead to an improvement of the crystalline quality and reduce the surface roughness to a certain extent.¹⁸ In fact, the best way to significantly ameliorate the final Si film quality and surface morphology at the same time is to completely eliminate the APDs on the 3C-SiC surface. However, the difference in symmetry between two materials (3C-SiC(001) and Si(110) in this case) leads to the formation of several domains in the grown layer.

The minimum number of domains that (must) form in the epilayer is fundamentally determined by the symmetry mismatch between the substrate and the epilayer.^{19,20} This minimum number falls from group theory and exists regardless of the kinetics, dynamics, and thermodynamics of the growth process. A large and representative number of reported epitaxial systems following group theory expectations has been corroborated in Ref. 19. Many substrate and epilayer combinations have a minimum number of domains larger than one. Various effects including approximately fulfilled symmetries can lead to additional domains.¹⁹ Such domains can also be generated in the layer depending on the

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growth conditions. It is fair to say, that any additional domain represents more grain types and increases disorder, typically leading to a degradation of the crystalline quality of the epilayer which is generally undesired. The attractive goal of decreasing the number of domains in the heteroepitaxial layer below the minimum limit for a given substrate orientation can only be achieved when the substrate symmetry is changed, typically reduced. For a desired substrate orientation, an off-cut of a few degrees can (i) provide the necessary break in symmetry, leading to a reduction of the number of domains,¹⁹ possibly down to one, and (ii) preserve the out-of-plane epitaxial relationship and desired epilayer growth direction.

In this letter, the morphological and structural features of the Si(110) epilayer grown on APD-free 3C-SiC(001) surface were investigated. Relying on group theory, and due to the in-plane azimuthal misalignment of the mirror planes between the 3C-SiC(001) film and the Si(110) epilayer, we will show that fundamentally the Si(110) layer must contain at least two domains.

The Si epilayer was heteroepitaxially grown on a 11 μm -thick 3C-SiC(001)/Si(001) template provided by NovaSiC.²¹ The 3C-SiC layer thickness was determined non-destructively by Fourier transform infrared spectroscopy (FTIR). The 3C-SiC layer is expected to exhibit a single domain. The growth of the Si layer was performed by chemical vapor deposition in a hot wall reactor by a mixture of SiH_4 (1 sccm) and H_2 (10 slm) at 900 °C. The pressure was kept constant at 900 mbars during the growth process. Detailed information of the Si growth conditions can be found elsewhere.¹⁸ The Si film thickness was 0.4 μm as measured by FTIR.

The surface morphology of both the 3C-SiC and Si layers was determined using tapping mode atomic force microscopy (AFM) (VEECO Dimension 3100). The crystal orientation determination of the Si film with respect to the 3C-SiC film was performed with a Panalytical X'Pert Pro diffractometer using Cu $K\alpha$ radiation (0.154 nm) and by rotating the sample around the Φ axis at fixed 2θ and χ values.

Figure 1 shows large scale optical microscopy images of different 3C-SiC thicknesses heteroepitaxially grown under the same conditions and their corresponding AFM images. It is widely admitted that, in addition to the worsening of the crystal quality, the presence of APD domains on the 3C-SiC surface increases its roughness due to the presence of irregular anti-phase boundaries (APBs) between the two domains.¹²⁻¹⁴ A reduction of the surface roughness with the increase of the film thickness is obvious from the AFM images in Figure 1.

Figure 2 shows the amplitude derivative AFM images of the 3C-SiC and the Si surfaces. It is well-known that the local 3C-SiC surface (i.e., APB-free) shows a smooth morphology characterized by atomic steps. In our case, the atomic steps can be observed on the single domain 3C-SiC surface (11- μm thick film), showing a rms roughness limited to 1 nm (Figure 2(a)). Since the domain formation in the Si epilayer is strictly linked to APDs on the 3C-SiC surface,¹⁶ reducing the APB-density on the 3C-SiC surface is expected to reduce the roughness of the top Si film. In Figure 2(b), the Si layer is shown to be smooth, the corresponding rms roughness of this surface is only 3 nm, compared to a faceted surface obtained in other work¹⁷ and a roughness of above

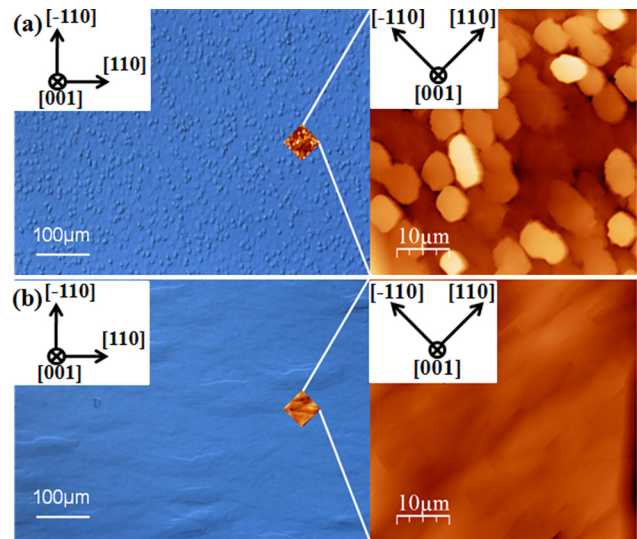


FIG. 1. Optical microscopy images (left) and atomic force microscopy images (right) ($50 \times 50 \mu\text{m}^2$) (a) of a 1.5 μm -thick 3C-SiC surface, (b) of a 11 μm -thick 3C-SiC surface. The insets depict the AFM images adapted to the optical images scale.

15 nm typically obtained using similar growth conditions on thin ($\sim 1 \mu\text{m}$) 3C-SiC films. This low roughness value is desired for subsequent devices fabrication.

Structural study using XRD was performed on this heterostructure in order to investigate the domains repartition in the Si film and their epitaxial relation with the 3C-SiC domain underneath it. The growth direction of the 3C-SiC film is along the [001] axis while the top Si layer is oriented along the [110] direction as already reported in literature.^{16,17} The azimuthal Φ -scan of the asymmetric (111) peaks (i.e., $2\theta = 35.69^\circ$, $\chi = 54.74^\circ$) of 3C-SiC(001) shows four peaks separated by 90° in Φ . These peaks are attributed to the diffraction of the {111} set of planes in 3C-SiC(001) (cf. Fig. 3(a)).

For a defect-free Si(110) crystal, two (111) peaks separated by 180° in Φ should appear at $\chi = 35.26^\circ$. However, for a Si epilayer grown on 3C-SiC(001) film, eight peaks are usually observed.¹⁶ The presence of these eight peaks is attributed to two reasons: (i) the presence of domains rotated by 90° around the growth direction which increases the number of peaks from two to four and (ii) each domain has a twinned counterpart rising the number of peaks to eight.^{16,17} In Figure 3(b), the azimuthal Φ -scan of the asymmetric (111) peaks of the Si(110) epilayer (i.e., $2\theta = 28.54^\circ$ and $\chi = 35.26^\circ$) shows only four peaks. These four peaks are attributed to the

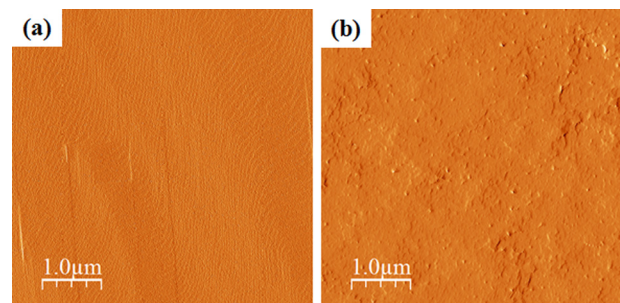


FIG. 2. Atomic force microscopy amplitude derivative images ($5 \times 5 \mu\text{m}^2$) (a) of an 11 μm -thick 3C-SiC surface (rms roughness limited to 1 nm), (b) of the Si epilayer surface (rms roughness 3 nm) grown on 3C-SiC.

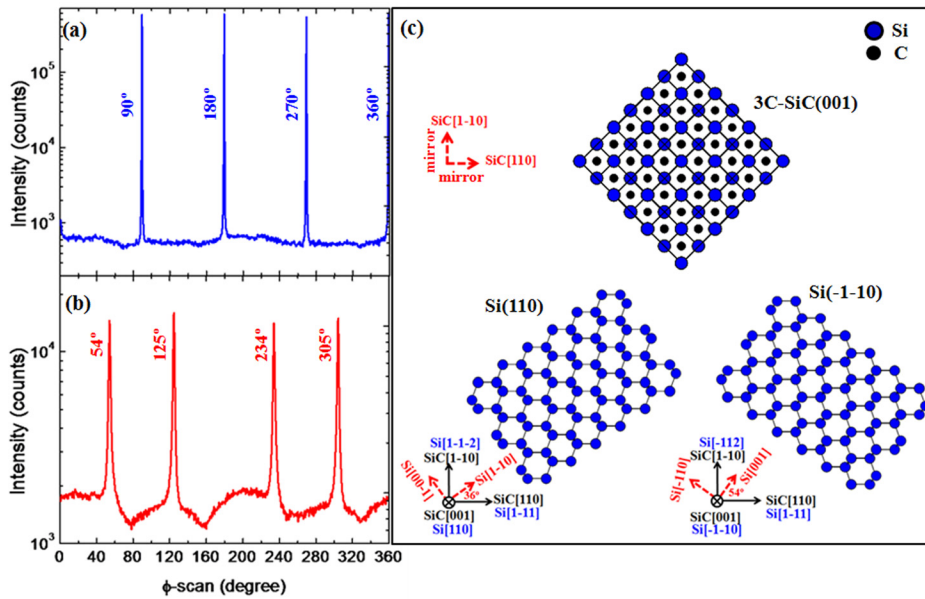


FIG. 3. Azimuthal XRD scans recorded along the asymmetric $\{111\}$ planes for (a) 3C-SiC(001) film (i.e., $2\theta = 35.69^\circ$ and $\chi = 54.74^\circ$) and (b) Si(110) film (i.e., $2\theta = 28.45^\circ$ and $\chi = 35.26^\circ$). The 3C-SiC surface exhibits a single domain. (c) Atomic representation of the 3C-SiC surface and the two Si domains. The epitaxial relation between the 3C-SiC film and the Si epilayer is indicated near the black arrows. The position of the mirror planes in each layer, respecting the given epitaxial relation, is indicated by dashed red arrows.

presence of two domains having a twin relation with respect to each other (domains are grown along the $[-1-10]$ direction instead of the $[110]$ direction). Based on the peak positions of the Si epilayer relatively to those of the 3C-SiC film, the epitaxial relationship between the 3C-SiC and the Si is thus: 3C-SiC[001] parallel to Si[110], 3C-SiC[110] parallel to Si[1-1-2], and 3C-SiC[1-10] parallel to Si[-11-1]. By defining surface lattice super cells, this orientation relationship shows a low lattice mismatch between the two materials.¹⁷ The difference in the lattice constant between $3 \times a_{\text{Si}[-112]}$ and $2 \times a_{\text{Si}[-1-10]}$ is 8%, while this difference drops to only 1.9% between $a_{\text{Si}[-11-1]}$ and $a_{\text{Si}[-110]}$. An atomic illustration of the two domains in the Si(110) epilayer and the 3C-SiC(001) film, taking into consideration the epitaxial relation between the two materials, is given in Fig. 3(c).

It has been shown that group theory can serve to predict the minimum number of rotational domains in heterostructures. A unified theory, based on the difference in symmetries between the two involved materials, has been developed by Grundmann *et al.* and it has been proved to be in agreement with many heterostructure systems.^{19,20} The formation of rotation domains in heterostructures strictly depends on the difference in symmetries between the film and the substrate.^{19,20} The minimum number of rotation domain in heteroepitaxy can be derived from the mismatch of the rotational symmetry between the substrate and the film. The substrate and the epilayer shall have a C_n , C_m symmetry, respectively, with regard to the surface normal, where n and m are integers with possible values $\{1,2,3,4,6\}$. The rotational domains result from the mismatch of the rotational symmetries across the interface of the involved materials. In our case, a 180° rotation around the Si[-11-1] axis was observed leading to the formation of two domains in the Si epilayer. This rotational domain was observed despite the same $2mm$ two-dimensional point group symmetry of 3C-SiC(001) and Si(110). We note that, for APD-free 3C-SiC(001) surface, the symmetry is $4mm$ for the first monoatomic layer only while this symmetry is reduced to $2mm$ for the infinite half space.^{19,22} At the early stage of Si nucleation, the Si adatoms interact with several monoatomic layers of the 3C-SiC surface

so that the $2mm$ symmetry has to be considered for the 3C-SiC(001). The Si(110) surface and half-space both show a $2mm$ symmetry. A simple formula can be used to calculate the minimum expected number of domains (N_{RD}) given in Ref. 20

$$N_{\text{RD}} = \text{lcm}(n, m)/m,$$

where lcm denotes the least common multiple, n denotes the C_n symmetry of the substrate, and m denotes the C_m symmetry of the epilayer.

Taking into consideration the mentioned formula and the symmetry of the 3C-SiC and the Si epilayer, the number of rotation domains in the Si epilayer must be equal to one. However, due to the aforementioned epitaxial relation between the Si epilayer and the 3C-SiC film, the mirror symmetry planes of the 3C-SiC(001) film (i.e., (110) and $(1-10)$ planes) and the Si(110) epilayer (i.e., (001) and $(1-10)$ planes) are misaligned. A rotation of 36° exists between the Si(1-10) plane and the 3C-SiC(110) plane (the 3C-SiC(110) plane coincide with the Si(1-11) plane) as depicted in Fig. 3(c). Doubling the number of domains in the epilayer is generally induced by the presence of the substrate mirror symmetry, except when the mirror plane of the substrate and that of the epilayer are aligned.¹⁹ In the case of misalignment, the mirror operation of the substrate is no longer mirror symmetry for the epilayer. Increasing the number of domains by a factor of two has been observed in the case of gallium nitride (GaN) on germanium (Ge), where the GaN lattice has been observed to be rotated by 4° compared to that of Ge.²³ The Ge mirror plane generated the presence of two GaN domains rotated by $\pm 4^\circ$ around the mirror plane (i.e., 8° compared to each other). In our case, an angle of 36° exists between the mirror symmetries of the 3C-SiC(001) and the Si(110). Thus, the mirror symmetry of the 3C-SiC surface allows the equivalent nucleation of Si domains rotated by $\pm 36^\circ$. These two domains have the same probability of presence and expansion. This is confirmed by the nearly identical intensities of the twinned domain compared to that of the main domain as

attested by the XRD azimuthal Φ -scan (Fig. 3(b)). This consideration highlights that, since the nucleation, the two domains have an equal probability of existence. Thus, the presence of the second domain in the Si layer is rather attributed to the angular misalignment of the mirror planes between the two materials than to the low formation energy of μ -twins in the Si layer.

The surface reconstruction has been shown to switch from $(n \times m)$ to $(m \times n)$, where $n, m = [1, 2, 3, \dots]$, between two antiphased domains on the 3C-SiC surface.²⁴ Thus, the surface can be treated as two local surfaces showing a 2 mm symmetry each, rotated by 90° around the growth direction. Therefore, the number of expected domains increases to four in the Si epilayer as previously reported for the Si layer heteroepitaxial on 3C-SiC.¹⁶

In the case of APD-free 3C-SiC(001) layer, the minimum number of domains that can be obtained in the Si epilayer is equal to two. This underlines that the growth was performed under the optimized conditions. Since these two Si domains are equally energetically/crystallographically favorable, further improvement seems to be impossible under our conditions. However, breaking the mirror symmetry of the 3C-SiC by using a specific off-cut is expected to favor eventually the growth of only one domain at the expenses of the second domain.

In summary, we reported the growth of a Si epilayer on an APD-free 3C-SiC(001) surface. The surface morphology of the Si film shows an rms roughness of only 3 nm. The APD-free 3C-SiC results in a reduction of the number of domains in the Si layer by a factor of two. The experimental results shown here are in complete agreement with group theory expectations. The minimum number of domains in the Si layer on 3C-SiC APD-free layer is expected to be two. This highlights that the Si layer grown under these conditions reveals the minimum number of domains that can be expected on on-axis 3C-SiC/Si(001). To proceed to further domain annihilation, off-axis substrates are suggested to favor the growth of one of the two domains.

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