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3C-SiC Island Growth on 4H-SiC Terraces: Statistical Evidence for the Orientation Selection Rule

B.J. Van Zeghbroeck[1,a*] and D.C. Bobela[2,b]

[1]University of Colorado, CB 425, Boulder, CO 80309, USA

[2]TrueNano Inc, 10850 Dover St, Ste 500, Westminster, CO 80021, USA

[a]bart@colorado.edu, [b]davidb@truenano.com

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Abstract. 3C-SiC islands were grown on atomically flat (111) 4H-SiC terraces and characterized by micro-Raman and FTIR. The islands initially have a triangular shape as defined by three {100} planes and over time evolve into hexagonal shaped islands. The triangular shape reveals the domain orientation of the island and is easily observed with an optical microscope. Examining 347 3C-SiC islands on 17 4H-SiC terraces we found that islands grown on the same terrace have the same domain orientation with 99.6% probability. The orientation of 3C-SiC islands grown on adjacent terraces was found to be close to random. This work confirms an orientation selection rule with high probability, suggesting that 3C-SiC can be grown without anti-phase domains or DPBs when grown on a single atomically flat 4H-SiC terrace, even when there are multiple nucleation sites.

Introduction

Cubic silicon carbide (3C-SiC) has been proposed as a promising material for high power MOSFETs due to its wide bandgap and high mobility. Compared to 4H-SiC MOSFETs, 3C-SiC MOSFETs have been shown to have a comparable bulk mobility, a modestly lower breakdown field and, more importantly, an up to five times higher channel mobility [1], resulting in a lower specific on-resistance and lower capacitance for devices with a breakdown voltage ranging from 600 V to 1,200 V [2].

Unfortunately, there are no commercially available 3C-SiC substrates. Instead, 3C-SiC is obtained by hetero-epitaxy on either silicon, on-axis 4H-SiC or on-axis 6H-SiC. Such heteroepitaxy of 3C-SiC typically results in the formation of anti-phase domains separated by domain boundaries (DPBs) and/or stacking faults, as the stacking sequence can either be ABCABC or ACBACB. Despite these defects, MOSFETs with a high channel mobility have been demonstrated, but such defects have been shown to be detrimental when fabricating large-area high-voltage devices with high yield [3,4].

A variety of approaches have been pursued to create large domains and reduce the number of stacking faults. Notable efforts that demonstrated high-quality 3C-SiC growth include the growth on atomically flat 4H-SiC or 6H-SiC terraces [5,6,7]. Ferro et al. argued that there is an "orientation selection rule" that states that the 3C-SiC stacking order simply continues the order of the underlaying 4H-SiC half-cell [6], be it that it randomly varies across a 4H-SiC substrate. Ideally, one could envision creating a single atomically-flat terrace, resulting in a single 3C-SiC domain across the terrace provided that the selection rule rigorously applies.

In this paper, we present experimental evidence supporting this selection rule, based on the observation of the domain orientation of small 3C-SiC islands grown on 4H-SiC terraces and finding that there is a very high probability of those islands having the same domain orientation, when grown on the same 4H-SiC terrace.

Experimental Procedure

Growth was performed by hot-filament CVD on 4H-SiC terraces that naturally form on a 4° off-axis 4H-SiC substrate under certain growth conditions as listed below.

Hot-filament CVD has been shown to result in 3C-SiC material quality that equals that of standard CVD as based on HR-XRD and Raman measurements [8,9,10], but distinguishes itself from CVD in that precursors (silane and propane) and the carrier gas (hydrogen) are cracked by the filaments at temperatures at or above 1800ºC. The presence of the resulting atomic hydrogen causes etching during growth [11], decorating defects, while the cracking of propane occurs independent of the substrate temperature. In experiments with a single filament, we also observe a lateral variation of the carbon-to-silicon ratio and the effect it has on the surface morphology and formation - or lack thereof - of triangular defects. Typical growth time is 30 min resulting in 10 µm thick epi layers.

The 4H-SiC terraces were obtained either by masking the substrate with a small 1 mm x 2 mm piece of 4H-SiC or at high carbon-to-silicon ratios which favor the formation of large (~100 µm) triangular defects. In either case, we observed nucleation of triangular 3C-SiC islands on these terraces which, depending on growth time and carbon-to-silicon ratio, evolve into hexagonal structures. These islands were imaged by optical and SEM microscopy as shown in Fig. 1 and data was collected regarding the orientation of the islands on each atomically-flat 4H-SiC terrace. The polytype was verified with micro-Raman and the 4H-SiC epi-layer thickness was confirmed to be 10 µm with FTIR as shown in Fig. 2.

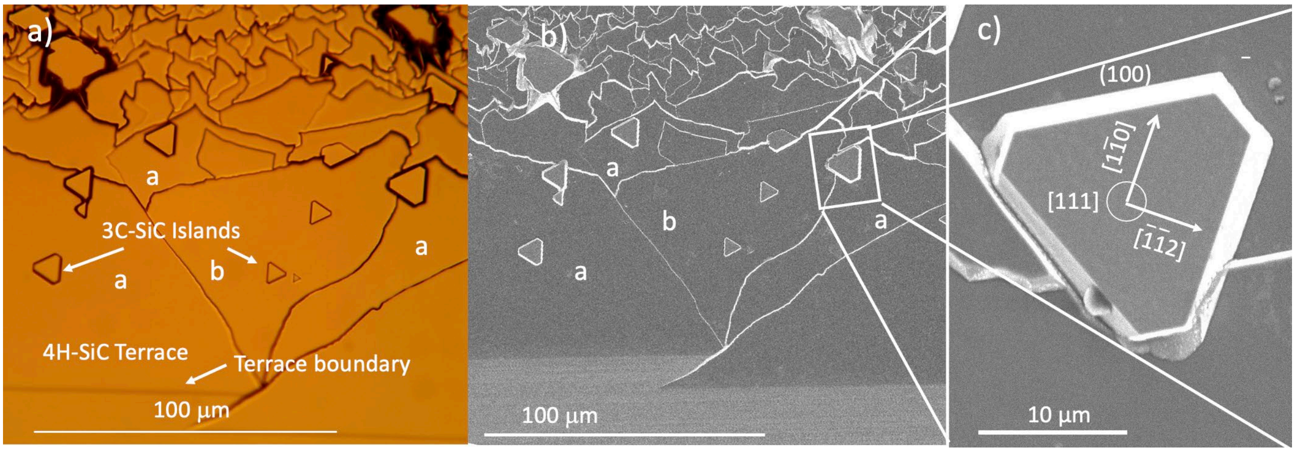

Fig 1: a) Top-down optical image showing 3C-SiC island growth on 4H-SiC, b) SEM of the same region, and c) Close-up of a single 3C-SiC island identifying the crystallographic planes and directions

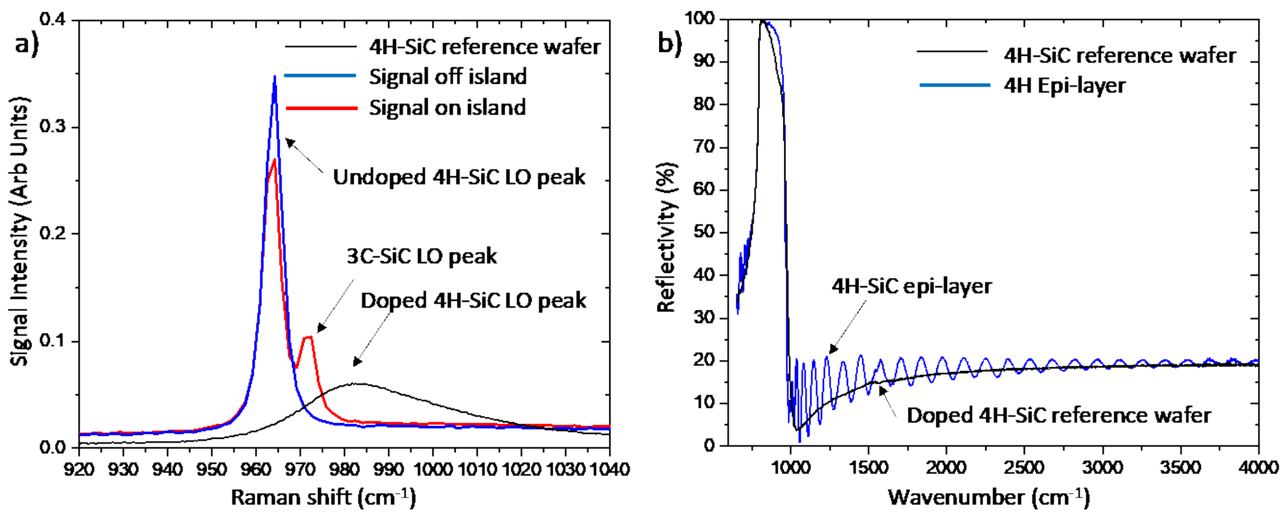

Fig 2: a) Micro-Raman spectra on and off a 3C-SiC island compared with an *n*-type doped 4H-SiC reference wafer, and b) Fourier transform infrared reflection (FTIR) measurement of the undoped 4H-SiC epi-layer on a doped 4H-SiC substrate, compared with a *n*-type doped 4H-SiC reference wafer.

Experimental Results

A first observation, as can be taken from Fig. 1b and Fig. 1c is that the atomically flat terraces can easily be identified by optical and SEM microscopy. The 4° angle of the terraces, relative to the substrate was also verified with a profilometer. Optical images show a different shade between the atomically flat terrace, which appears darker due to the 4° angle relative to the substrate and the 4H-SiC substrate region and revealing a clear line separating the two. SEM imaging shows a difference in structure between the flat terrace and the rougher surface of the 4H-SiC growth region.

A second observation is the clear triangular shape of the 3C-SiC islands, exhibiting a flat (111) top flanked by (100), (010) and (001) facets. These triangles vary in size depending on when nucleation took place and the larger ones evolve into hexagons like those observed when growing 3C-SiC on 3C-SiC mesas [8]. More relevant to our study, the triangles on the same 4H-SiC terrace align, pointing in the same direction, left or right i.e. forming small domains with opposite orientation. The difference here is that the domains have not grown together, making it easy to identify their orientation with an optical microscope, rather than using SEM contrast due to ion or electron channeling [12].

Next, we collected statistical data from two different samples: First using a sample that contains several triangular defects with each having three or less 3C-SiC islands as shown in Fig. 3a. What stands out compared to trangular defects reported in the litterature is the smooth 4H-SiC terrace within the triangle and a few well-defined 3C-SiC islands as confirmed by micro-Raman, instead of a rough mixed polytype region [13]. The angle of the triangle is typically close to 120°C, but can be quite different as shown in Fig. 3a and 4a, and also reported previously [13].

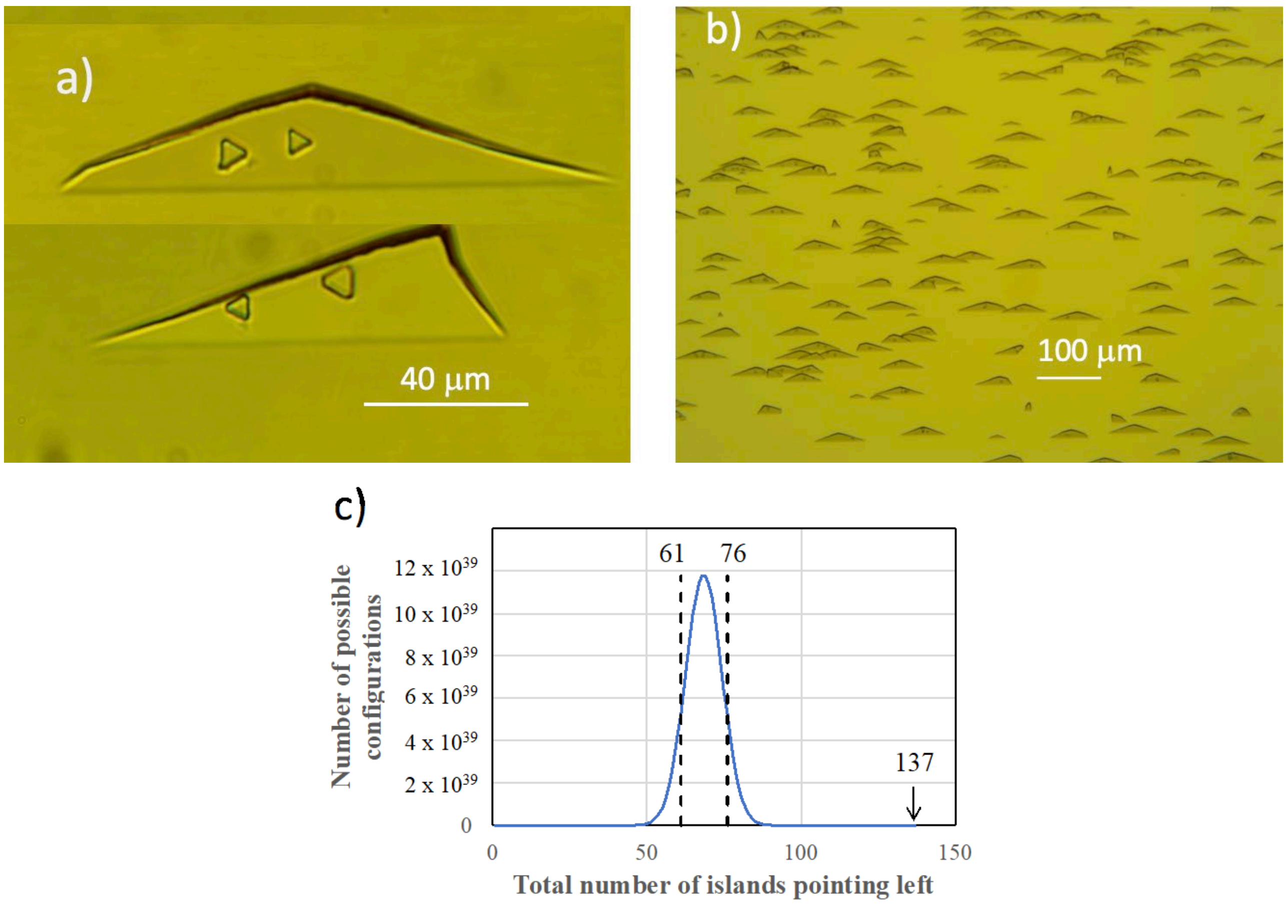

Fig 3: a) Typical triangular defects used to identify 4H-SiC terrace type based on the orientation of the triangular 3C-SiC islands, b) Image of a single image frame containing all 137 triangular defect terraces used to identify the domain orientation, and c) binomial distribution of configurations corresponding to the total number of islands pointing the same way.

We examined a total of 137 terraces in a single image frame as presented in Fig. 3b and counted 61/76 islands pointing to the left/right. Assuming an equal probability of islands pointing either way, the number of possible configuations as shown in Fig. 3c is given by:

$$\binom{n}{s} = \frac{n!}{(n-s)!\,s!}$$

Where n is the total number of terraces and s is the number of terraces where the islands point to the left. The probability of having the number of islands pointing to the left or right between 61 and 76 including both boundaries is then 82.86%. The 61/76 split is therefore consistent with an equal probability of islands pointing one way or the other.

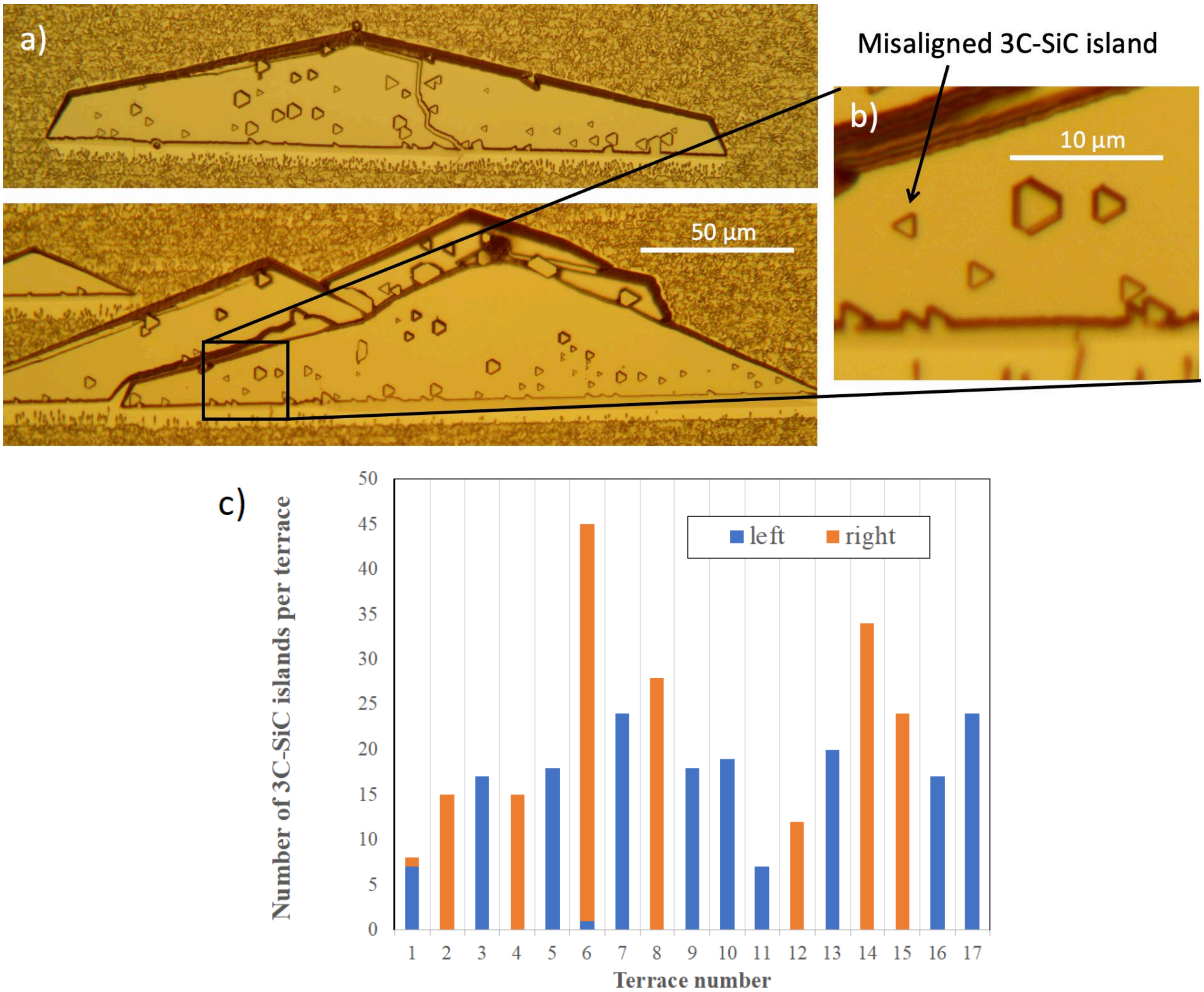

Fig 4: a) Example triangular defects with a large number of 3C-SiC islands including the upper one that contains two different 4H-SiC terraces, b) close-up revealing one of the few misaligned islands and c) number of islands and their orientation as observed on 17 terraces.

Second, using a sample grown with higher C:Si ratio that resulted in a larger number of triangular defects with more nucleation sites, we identifier the nucleation sites that did not align with all others on the same terrace. Examples of this type of triangular defects are shown in Fig. 4a. Noticeable is the very rough 4H-SiC growth around the triangular defect region, caused by the high and no-optimal C:Si ratio. The observed number of islands and their orientation on 17 terraces is shown in Fig. 4c. We only found 2 out of 347 nucleation sites to have the opposite orientation compared to all other nucleation sites on the same terrace, or less than 0.6%. A closer inspection of the two misaligned islands, like the one shown in Fig. 4b did not reveal an obvious reason for its orientation

Conclusion

Hot-filament CVD growth on 4°-off SiC was used to form atomically flat terraces due to step flow growth either by partially masking the substrate or by growing under carbon-rich conditions. We observed nucleation of 3C-SiC islands on these terraces, which are initially shaped as triangles, whose orientation reveals the domain orientation. A detailed count revealed a 61 versus 76 orientation split. In contrast, almost all islands on a shared terrace point the same way, indicating aligned domains. Quantitatively, we found that 99.6% of all 3C-SiC nucleation sites on a shared terrace had the same orientation. We therefore conclude that the domain orientation of the 3C-SiC nucleation sites follows the stacking sequence of the underlaying 4H-SiC half-cell with very high probability, while the orientation of 3C-SiC islands grown on adjacent terraces was found to be close to random.

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Disclosure

The authors disclose having a financial interest in TrueNano, Inc.

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