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Growth of single orientation 3C-SiC applying anisotropic step etching on a 4H-SiC substrate

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Abstract

The growth of a single-orientation 3C-SiC layer is demonstrated in anisotropic step etching of a 4H-SiC substrate with hydrogen. During etching, steps of one unit-cell height were formed on the substrate with a miscut toward the $[\bar{1}100]$ direction and an overgrown 3C-SiC layer exhibiting a single orientation. A possible mechanism for determining the orientation is proposed following a comparison of results from a substrate with a miscut toward the $[\bar{2}110]$ direction.

1. Introduction

The growth of high quality 3C-SiC on hexagonal SiC substrates is a lingering problem needing resolution in realizing various promising devices. One of the main difficulties has been the growth of 3C-SiC with a single in-plane orientation across all the wafer. With its double orientation, 3C-SiC is known to have a killer defect [1] at the boundary of the oriented crystals, often referred to as a double position boundary [2]. Neudeck and colleagues [3] have documented the theoretical expectation that a single-orientation 3C-SiC layer can be grown across terraces connected by a step of one unit-cell height. They argue that the orientations of the terminating layer of a substrate align along the same direction result in a single orientation for the overgrown 3C-SiC. Nakajima and colleagues [4] reported anisotropic step etching using H_2 to form bunched steps of one unit-cell height on a 6H-SiC substrate with a miscut to the $\langle 1\bar{1}00 \rangle$ direction (half unit-cell height in the $\langle 11\bar{2}0 \rangle$ direction). They attributed this anisotropic step-height formation to differences in desorption energy and dangling bond number on each step. To date, a few reports have discussed controlling the orientation of 3C-SiC layer using bunched step formation across a hexagonal substrate. In this presentation, we report the growth of a single-orientation 3C-SiC on a hexagonal substrate with steps of one unit-cell height. From an industry point of view regarding practical applications, and without any preparatory three-dimensional processing of the substrate surface, we applied a simple H_2 etching to a 4H-SiC substrate, which is the most commercially available polytype.

2. Experimental

The vender's specification of the wafer used was a 4-inch on-axis Si-face SI-type 4H-SiC (0001). Portions of size 3.3mm × 3.3 mm with miscuts to the $[\bar{1}100]$ and $[\bar{2}110]$ directions were selectively cut out and used for growth. The growth of 3C-SiC was performed using a hot-wall CVD reactor with a substrate temperature of 1370°C just after 30 minutes of H_2-etching. The C/Si ratio was maintained at 1 by regulating the precursors silane and propane. The growth thickness was controlled to 1 μm at a growth rate of 4 μm/h. Using an X-ray diffractometer, φ scans were performed on the 3C-SiC{113} covering an area of size 5 mm × 5 mm (the total growth area). The angle ψ was varied from 28.22° to 32.22° in 1° increments. In the following, the substrates on which the 3C-SiC layers are grown and have a miscut toward the $[\bar{1}100]$ or $[\bar{2}110]$ direction are designated correspondingly as g1 or g2. Separately prepared H_2-etched substrates with the same step orientation as the g1 and g2 substrates are referred to as e1 and e2, respectively.

3. Results and discussion

From the XRD φ scans taken of the g1 and g2 layers of 3C-SiC{113} [Fig. 1(a)], the former features three peaks having an angular interval of 120°, whereas the latter has six peaks with intervals of 60°. Thus, 3C-SiC in the g1 layer has three-fold rotational symmetry and a single orientation, whereas 3C-SiC in the g2 layer has two orientations with a tilt of 60° to each other.

From AFM images and cross-sectional profiles of the surfaces of the e1 and e2 [Fig. 1(b) and (c), respectively], the former exhibits a 1.0-nm-high step (one unit-cell height), whereas the latter exhibits a 0.5-nm-high step (half unit-cell height). Therefore, anisotropic step etching of the 4H-SiC substrate to form a bunched step of one unit-cell height along the $[\bar{1}100]$ direction was confirmed. We attribute the observed variation in crystal orientation [Fig. 1(a)] to differences in the bunched step height.

A mechanism by which the 3C-SiC orientation can be determined is possible (Fig. 2). We believe our experimental results [Fig. 1(a)] can be explained following similar views presented in Refs. [3] and [4]. The variation in energy during layer desorption is considered to be twice that in 4H-SiC because the stacking sequence is a simple repetition of k and h. The dangling bond number at the step edge differs between the $[\bar{1}100]$ and $[\bar{2}110]$ directions being two for the former and one for the latter. The variation in steps, as characterized by the combination of desorption energy and dangling bond number, is four along the $[\bar{1}100]$ direction and two along the $[\bar{2}110]$ direction, and appears repeatedly along each direction. The variation in steps therefore produces one slow-etching

layer and subsequently fast-etching layer(s). If fast-etching layers bunch beneath the slow-etching layer, the height of the bunched step is then equivalent to four layers (one unit-cell height) in the former and two in the latter, as observed in Fig. 1(b) and (c). On the 4H-SiC surface with half unit-cell-high steps, the orientation of the terminating layer differs by 60° in all neighboring terraces [Fig. 2(b); lower drawing]. In contrast, on surfaces with one unit-cell-high steps [Fig. 2(b); upper drawing], the same orientation is seen across the terraces as insisted by Neudeck and colleagues [3]. Assuming an overgrown SiC crystal inherits its orientation from the terminating layer of the substrate, which is expected from calculations [5], a 3C-SiC layer with a single orientation is established in the g1 layer, whereas two orientations develop in the g2 layer [Fig. 2(c)].

To the best of our knowledge, this is the first empirical demonstration using anisotropic step etching of single-orientation growth of 3C-SiC on a hexagonal substrate.

4. Conclusions

Growth of a single-orientation 3C-SiC on 4H-SiC sub-strate has been empirically demonstrated. Anisotropic step etching was used to form bunched steps of one unit-cell height. A mechanism was also presented for this growth based on the orientational relationship between the terminating layer on the bunched step and the grown 3C-SiC crystal.

References

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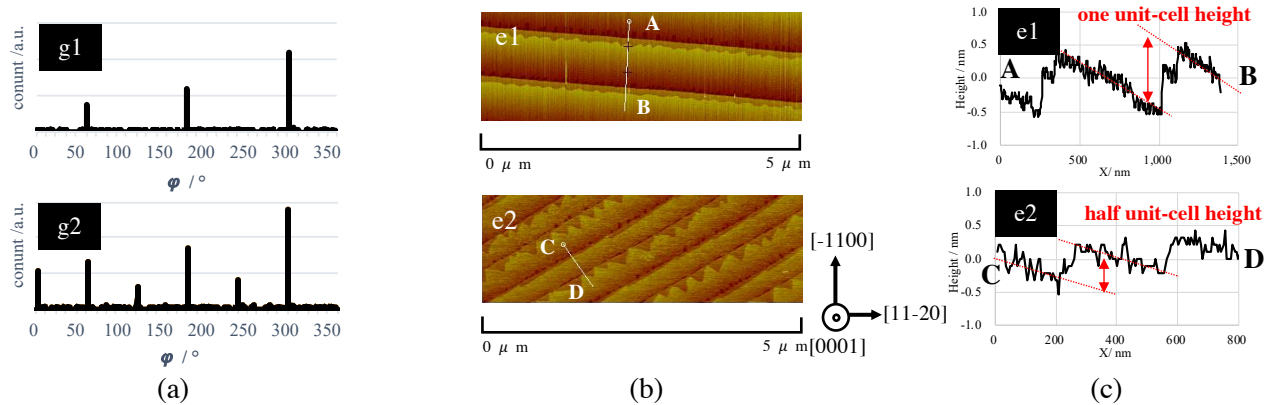[5] V. Heine, J. Am. Ceram. Soc., **74**(10) (1991) 2630.

Fig. 1. (a) XRD φ scans taken of the g1 and g2 layers of 3C-SiC{113}. (b) AFM images of the e1 and e2 surface layers after H$_2$ etching. (c) Cross-sectional profiles along the white lines in (b).
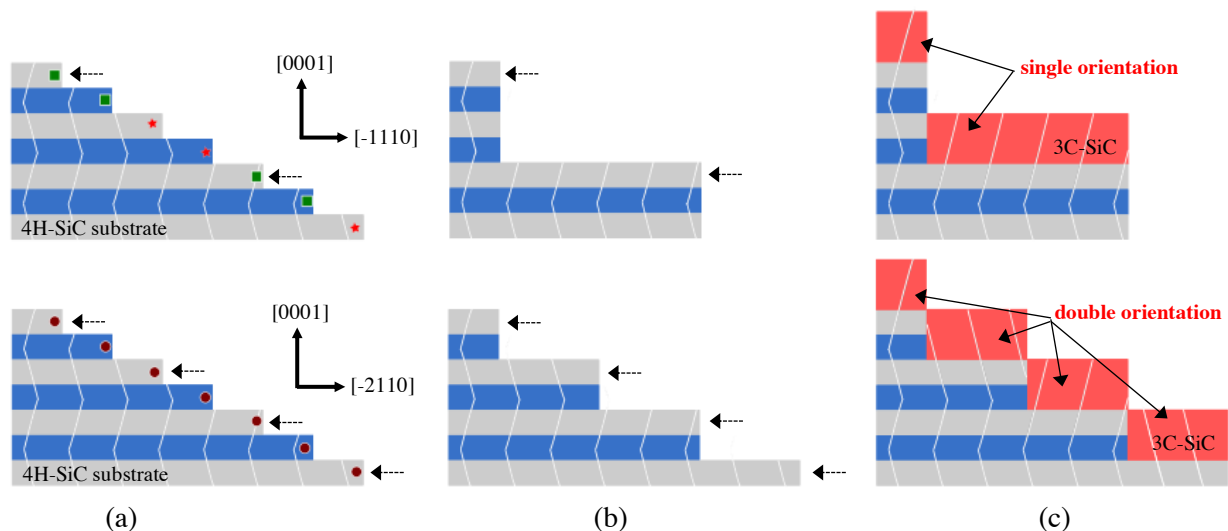

Fig. 2. Schematic of the mechanism for the determining the orientation of the grown 3C-SiC layer. Cross-sections (a) before H$_2$ etching, (b) after H$_2$ etching, and (c) after starting 3C-SiC growth. The upper and lower drawings correspond to the g1 and g2 layers, respectively. Symbols at step rises indicate the difference in dangling bond number. The dashed arrows mark the layer with slowest etching rate for each substrate, which has been chosen arbitrarily for illustration purposes.