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3C-SiC hetero-epitaxial growth on undulant Si(0 0 1) substrate

Hiroyuki Nagasawa*, Kuniaki Yagi, Takamitsu Kawahara

R&D Center, EO Company, Hoya Corporation, Akishima, 3-3-1 Musahino, Tokyo 196-8510, Japan

Abstract

A novel technique to eliminate planar defects in the 3C-SiC hetero-epitaxial layer on Si substrate was developed. Before growing 3C-SiC, countered slopes oriented in the [1 1 0] and [$\bar{1}$ $\bar{1}$ 0] directions were formed over the entire surface of Si(0 0 1) substrate (undulant-Si). In the initial stage of 3C-SiC growth, step flow epitaxy occurred on the surface slopes of the substrate, reducing the anti-phase boundaries. Continuous, twin boundaries (TBs) were arranged in parallel along the (1 1 1) or ($\bar{1}$ $\bar{1}$ 1) planes. The twin boundaries were eliminated through combination of the countered TBs with 3C-SiC growth. Finally, no planar defects were observed on the surface of 200-μm thick 3C-SiC grown on "Undulant-Si". © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Cubic silicon carbide (3C-SiC) is an attractive wide-band-gap semiconductor for high-frequency and high-efficiency electronic devices, due to its isotropic electron mobility and high-saturation velocity of electrons [1,2]. Moreover, among SiC polytypes, 3C-SiC is the only material that can be grown on a Si substrate, giving it a significant advantage in the low-cost fabrication of large-diameter wafers [3–5]. However, device applications using 3C-SiC grown on Si substrate have lagged significantly behind those using hexagonal-type SiC, owing to the difficulty in eliminating planar defects generated at the interface between 3C-SiC and the Si substrate, where a 19.8% mismatch in the lattice constant exists. Although numerous studies have investigated 3C-SiC hetero-epitaxy, little has been reported on drastically reducing the planar defects.

We developed an effective technique that eliminates planar defects in 3C-SiC hetero-epitaxial layers on Si(0 0 1) substrates. This paper describes the fundamental principle used to eliminate planar defects, and then describes a concrete means of realizing this principle. Finally, it discusses the efficacy of the method and its mechanism, referring to morphological studies of grown 3C-SiC surfaces.

2. Principle underlying the elimination of planar defects

Planar defects generated at the interface between 3C-SiC and Si substrate can be classified into two types: anti-phase boundaries (APBs) and twin boundaries (TBs). An APB in 3C-SiC is the

*Corresponding author. Tel.: +81-42-546-2756; fax: +81-42-546-2742.

E-mail address: nags@rdc.hoya.co.jp (H. Nagasawa).

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interface between two domains that correspond to each other through the exchange of Si and C atoms [6]. The crystal structure of each adjoining domain bounded by an APB is equivalent, except that it is rotated 90° around the [0 0 1] axis. TBs in 3C-SiC are a coherent interface between different stacking sequences of Si-C pairs that correspond to hexagonality [7].

Since APBs and TBs tend to propagate along four equivalent {1 1 1} planes, Si(0 0 1) is commonly used as a substrate for 3C-SiC growth, in order to decrease the density of planar defects with increasing thickness through mutual canceling [3,8]. However, elimination of planar defects in 3C-SiC using Si(0 0 1) has not been achieved. This occurs because when a certain domain expands in the [1 1 0] direction, the adjoining domain inevitably expands in the [$\bar{1}$ 1 0] direction. Thus, to eliminate planar defects, we must manipulate domain expansion so as to enhance it in a specific direction.

Step flow epitaxy of 3C-SiC on a slightly misoriented Si(0 0 1) substrate is generally recognized as one technique for enhancing domain expansion in a specific direction. In fact, step flow epitaxy of 3C-SiC on misoriented Si(0 0 1) substrate in the [1 1 0] direction has resulted in APB elimination, which is never achieved with a well-oriented Si(0 0 1) substrate [9]. Nevertheless, although 3C-SiC growth occurred on misoriented Si(0 0 1) substrate, TBs could not be eliminated, because the TBs parallel the (1 1 1) plane, and there is a reduced possibility of the TBs vanishing by combining TBs with increasing 3C-SiC thickness.

The first significant step in eliminating planar defects in 3C-SiC is to eliminate APB via step flow epitaxy using the misoriented slopes of Si(0 0 1) substrate. More importantly, TBs must not be arranged in only (1 1 1) plane. In other words, to effectively eliminate the TB at the intersection of TBs, it is necessary that TBs paralleling the (1 1 1) or ($\bar{1}$ $\bar{1}$ 1) planes must disperse in the 3C-SiC layer of equal density. To satisfy these conditions, Si(0 0 1) whose surface forms countered slopes oriented in the [1 1 0] and [$\bar{1}$ $\bar{1}$ 0] directions is thought to be an effective substrate for 3C-SiC growth. This paper refers to such Si(0 0 1) substrates as "Undulant-Si".

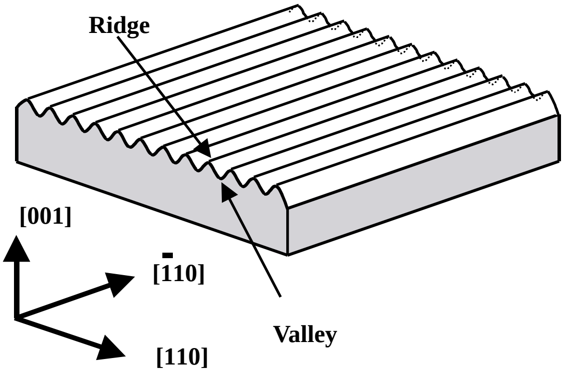

Fig. 1. Schematic structure of the surface of "Undulant-Si".

To ensure the effects of the "Undulant-Si" substrate, the entire surface of Si(0 0 1) must be covered with continuous undulations, in which the ridges are aligned in the [$\bar{1}$ 1 0] direction, as shown in Fig. 1. Although the ($\bar{1}$ 1 0) cross-section of each undulation is not necessarily symmetric, the areas of the slopes oriented in the [1 1 0] and [$\bar{1}$ $\bar{1}$ 0] directions must be equal to avoid TB collimation in a specific plane.

3. Experimental procedure

To confirm the effects of the "Undulant-Si" substrate on the elimination of planar defects in a 3C-SiC epitaxial layer, well-oriented Si(0 0 1)$\pm$0.3° (Just-Si) and Si(0 0 1) misoriented 4° towards the [1 1 0] direction (Off-Si) were used as references.

The "Undulant-Si" substrate was prepared in the following manner. The entire surface of "Just-Si" substrate was scraped with diamond slurry 15 μm in diameter in the [$\bar{1}$ 1 0] direction with a loading of 0.1 kg/cm^2 to form continuous undulations, with ridges aligned in the [$\bar{1}$ 1 0] direction. The scraped Si substrate was then oxidized at 1100°C for 5 h in a dry-oxygen stream at atmospheric pressure, to remove crystal defects introduced by the scraping process. Finally, the 200-nm thick oxidized layer was removed by exposure to 5% HF solution for 10 min. The "Undulant-Si" surface formed was inspected by atomic force microscope, and this confirmed that the ridge–ridge spaces ranged between 400 and 700 nm, and that the ridge–valley heights ranged between 7 and 26 nm.

A cold-wall-type, low-pressure CVD system was employed for 3C-SiC epitaxial growth on Si substrates. Before 3C-SiC growth, each substrate was carbonized in a flow of 10 sccm C_2H_2 and 100 sccm H_2 to convert the surface into a thin 3C-SiC layer. After 5 min of carbonization, a 3C-SiC layer was grown on the Si substrate using 50 sccm SiH_2Cl_2, 10 sccm C_2H_2, and 100 sccm H_2. The temperature and pressure during above processes were kept at 1350°C and 100 mTorr, respectively. An epitaxial layer about 200-μm thick was obtained on the Si substrate after continuing the 3C-SiC growth process for 5 h.

In order to observe the morphology of the 3C-SiC grown, using a transmission optical microscope, the Si substrate under the 3C-SiC layer was selectively removed in $HF+HNO_3$ solution.

4. Results and discussion

The surface of the 3C-SiC layer grown on "Just-Si" substrate exhibited a mosaic-like morphology, as shown in Fig. 2a. The adjoining domains had similar shapes, although they were rotated 90°, so that their long sides were oriented in the $\langle 1\,1\,0 \rangle$ directions. For the 3C-SiC layer on the "Off-Si" substrate, scale-like steps were seen, uniformly oriented at an obtuse angle in the [1 1 0] direction, as shown in Fig. 2b. Unlike the 3C-SiC epitaxial layers on "Just-Si" or "Off-Si" substrates, the 3C-SiC grown on "Undulant-Si" substrate had a mirror-like surface, through which the undulations on the reverse side were clearly observed, as shown in Fig. 2c.

To simplify the discussion of the morphological discrepancies among the three types of substrate, we first consider the transition in shape of a 3C-SiC nuclear generated on "Just-Si" substrate (Fig. 3). Since 3C-SiC grew epitaxially on the Si(0 0 1) face, the {1 1 1} facets of 3C-SiC nuclei were clearly aligned with the Si{1 1 1} planes. However, the {1 1 1} facets of 3C-SiC are polar faces, Si faces (blank portion in Fig. 3), or right-angled C faces (solid portion in Fig. 3). If the C

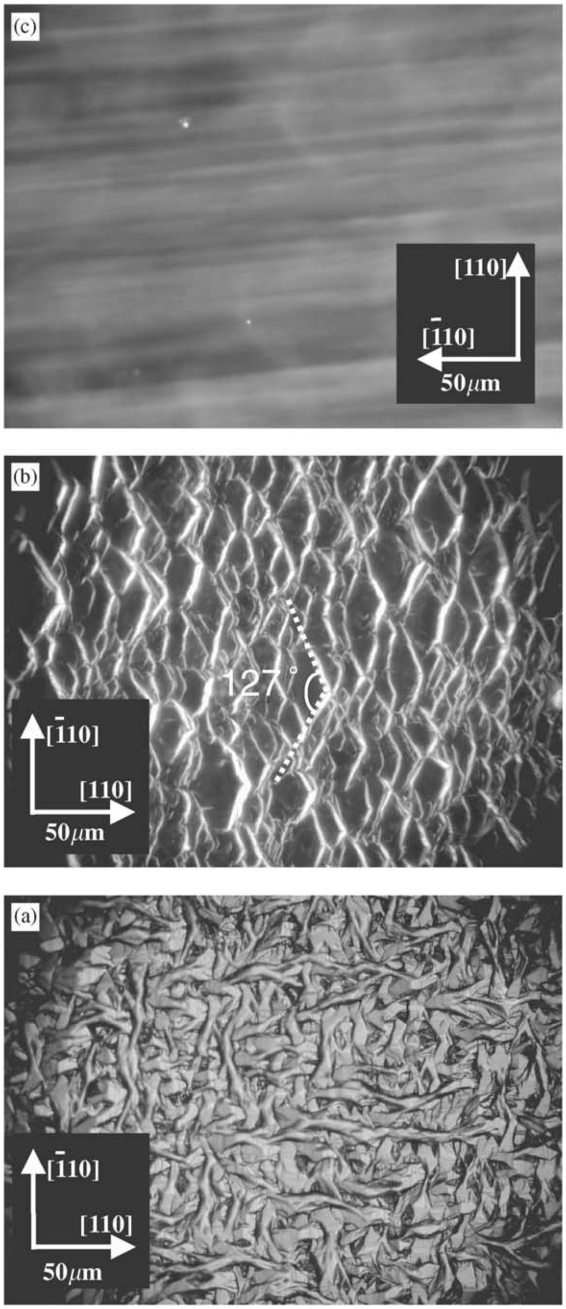

Fig. 2. Optical micrographs of the 3C-SiC surfaces on (a) "Just-Si", (b) "Off-Si", and (c) "Undulant-Si" substrates.

faces parallel the ($\bar{1}$ 1 1) and (1 $\bar{1}$ 1) planes, the Si faces must parallel the ($\bar{1}$ $\bar{1}$ 1) and (1 1 1) planes. Since the surface free energy of the C face

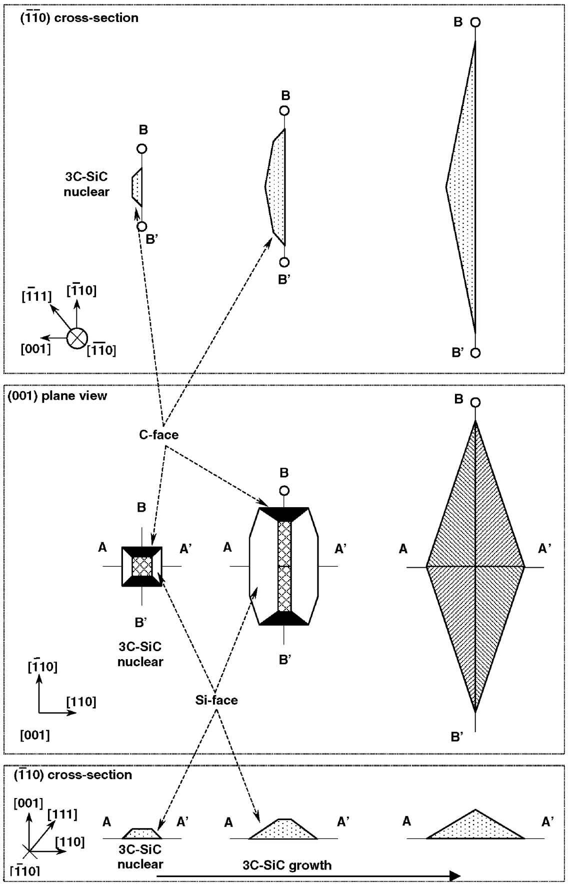

Fig. 3. Shape transition of a 3C-SiC nuclear on “Just-Si”. The 3C-SiC nuclear gradually expand into a pyramidal shape from left to right.

(300 erg/cm^2) is significantly lower than that of the Si face (2200 erg/cm^2), the C faces grow faster than the Si faces [10]. As a result, the 3C-SiC nuclear gradually expand into a pyramidal shape, transforming the Si face into an obtuse angle and the C face into an acute angle with 3C-SiC growth, as shown in the (0 0 1) plane view in Fig. 3. In actuality, however, the carbonization process employed in the initial stage of 3C-SiC growth involved multinucleation growth, not single nucleation growth. Moreover, the process was unable to orient the specific polar face in the desired direction. Thus, a mosaic-like surface formed on the surface of 3C-SiC grown on the “Just-Si” substrate, suggesting a high APB density.

On the other hand, scale-like steps of the 3C-SiC surface were seen on “Off-Si,” in which the obtuse angle was oriented in the [1 1 0] direction, demonstrating APB elimination. Since the observed obtuse angle of 127° is equivalent to the intersection angle of the (3 1 1) and (1 3 1) planes deformed from the (1 1 1) Si face, if APBs exist on the surface of the 3C-SiC, an acute angle of 53° corresponding to the intersection angle of the $(3\,\bar{1}\,1)$ and $(1\,\bar{3}\,1)$ planes deformed from C face must also be observed in the scale-like steps.

The reason that APBs are eliminated from 3C-SiC grown on “Off-Si” substrate is as follows: High-density APBs appear to be generated through multinucleation growth in the initial stage of 3C-SiC epitaxy, even using an “Off-Si” substrate. However, C face expansion upstream (i.e., in the $[\bar{1}\,\bar{1}\,0]$ direction) is blocked by the Si face of the adjoining domain already formed upstream. Therefore, only domains in which the C face orient toward the $[\bar{1}\,1\,0]$ and $[1\,\bar{1}\,0]$ directions are able to expand by merging with each other, eliminating APBs. Thus, we conclude that the (1 1 1) plane of 3C-SiC grown on “Off-Si” is a Si face.

However, the elimination of TBs on the surface of 3C-SiC grown on “Off-Si” has not been verified. To confirm this, the surface of 3C-SiC grown on “Off-Si” was inspected by optical microscopy after etching at 500°C with molten KOH for 5 min. This procedure is commonly used to make planar defects conspicuous. However, the scale-like steps of the 3C-SiC surface grown on the “Off-Si” substrate hinder observation of the etch-pits corresponding to planar defects. Thus, the surface of 3C-SiC grown on the “Off-Si” substrate was polished slightly to form a mirror-like surface before KOH etching. As shown in Fig. 4a, a high density of etch-pits, exceeding 2×10^5/cm^2, was observed on the etched surface of 3C-SiC grown on the “Off-Si” substrate. Since the shape and density of the etch-pits were similar to those of the scale-like steps before polishing, it was thought that the intersections of TBs on the surface corresponded to the scale-like steps. All the remaining TBs in 3C-SiC grown on “Off-Si”

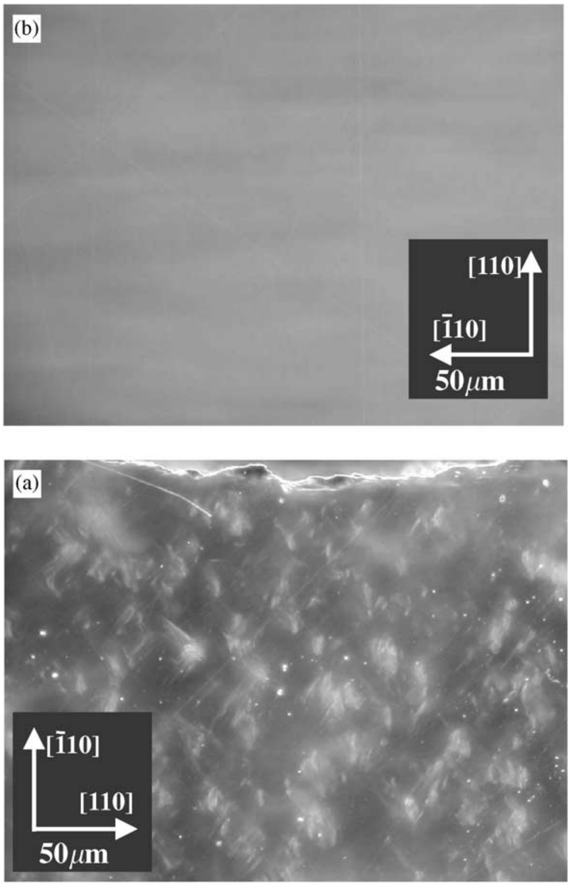

Fig. 4. Optical micrographs of the 3C-SiC surface after etching with molten KOH at 500°C for 5 min on (a) "Off-Si", and (b) "Undulant-Si".

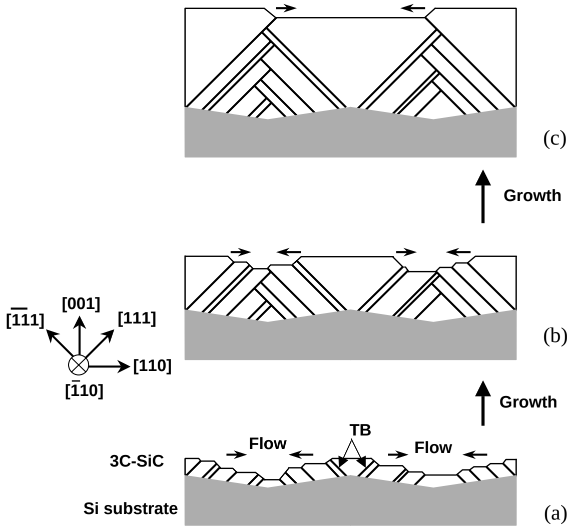

Fig. 5. Model of the elimination of TBs in the 3C-SiC layer on "Undulant-Si" with 3C-SiC growth. The ($\bar{1}$ 1 1) cross-sectional structure of 3C-SiC changes from (a) to (c) as growth progresses.

substrate were thought to parallel the (1 1 1) plane, because the steps prevent the propagation of TBs parallel to the ($\bar{1}$ $\bar{1}$ 1) plane, while no countered steps exist for TBs parallel to the (1 1 1) plane.

In contrast to 3C-SiC growth on "Off-Si" substrate, remarkable elimination of both APBs and TBs on "Undulant-Si" was confirmed. When molten KOH etching was performed on 3C-SiC grown on "Undulant-Si" substrate, virtually no etch-pits were observed, as shown in Fig. 4b. The mechanism for the elimination of planar defects is as follows. First, the APBs generated in the initial stage of 3C-SiC growth are eliminated on each slope on "Undulant-Si" by the same mechanism as described for the "Off-Si" substrate. Although TBs remain in the 3C-SiC layer after all APBs have been eliminated, these parallel the (1 1 1) or ($\bar{1}$ $\bar{1}$ 1) planes, forming countered steps on the surface, as shown in Fig. 5a. Thus, TB density, that is the density of steps, on the surface of 3C-SiC grown on "Undulant-Si" substrate decreases with increasing 3C-SiC thickness, through the combination of steps, as shown in Figs. 5b and c.

The most significant aspect of 3C-SiC growth on the "Undulant-Si" substrate is that the vanishing probability of TBs paralleling (1 1 1) is quite similar to that of TBs paralleling ($\bar{1}$ $\bar{1}$ 1), unlike the case of 3C-SiC growth on "Off-Si" substrate. Thus, the mirror-like surface of 3C-SiC itself indicates a low TB density.

Employing undulant substrates eliminates planar defects during the growth of not only 3C-SiC, but also that of other compound crystals. It is necessary to study further the dependence of planar defect density on epitaxial layer thickness with changes in the structure of the undulant substrate surface (i.e., varying ridge–ridge spacing or ridge–valley height), in order to discuss the mechanism for the elimination of planar defects more quantitatively.

5. Summary

We developed a novel technique that eliminates planar defects in 3C-SiC hetero-epitaxial layers on Si(0 0 1) substrates. To eliminate TBs as well as APBs, 3C-SiC was grown on an "Undulant-Si" substrate, whose surface formed countered slopes oriented in the [1 1 0] and $[\bar{1}\,\bar{1}\,0]$ directions. During the initial 3C-SiC growth, step flow epitaxy occurred on the surface slopes of the substrate, reducing the number of APBs. Moreover, TBs paralleled the (1 1 1) or $(\bar{1}\,\bar{1}\,1)$ planes, forming steps on the surface. Thus, the density of TBs could be decreased by combining TBs as 3C-SiC thickness increased. As a result, few planar defects were observed on 200-μm thick 3C-SiC grown on "Undulant-Si". The most significant aspect of 3C-SiC growth on an "Undulant-Si" substrate is that the probabilities of TBs paralleling (1 1 1) and $(\bar{1}\,\bar{1}\,1)$ vanishing were quite similar. Thus, the mirror-like surface of 3C-SiC itself indicates a low TB density.

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