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Analysis of Atomic Arrangement at 3C-SiC/Si(001) Interface by Aberration-Corrected Transmission Electron Microscopy

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1. Introduction

Silicon carbide (SiC) exhibits several outstanding properties such as wide band gap, high electron breakdown field and high electron saturated drift velocity. Among various polytypes of SiC, cubic SiC (3C-SiC) has an advantage that a large-area single crystal can be hetero-epitaxially grown on a Si [001] substrate [1]. A high density of stacking faults is, however, induced in the grown crystal due to the large difference in thermal expansion coefficients (8 %) and lattice mismatch between SiC and Si (a_{SiC} : a_{Si} = 0.436 nm : 0.543 nm ≒ 4 : 5). To reduce them, it should be important to understand the defect formation mechanism, therefore first of all, to know the atomic arrangement at the interface. In the present study, the 3C-SiC/Si(001) interface has been studied by utilizing aberration-corrected transmission electron microscopy (TEM).

2. Experimental

A SiC film about 150 nm in thickness was grown on a Si(001) wafer by chemical vapor deposition after carbonization of the silicon surface. For cross-sectional TEM observations, the sample was thinned in the [110] and [100] directions by mechanical polishing followed by 3 kV Ar-ion milling. High-resolution TEM (HRTEM) observations were conducted in a thermal-field emission 200-kV TEM (JEM-2100F) equipped with an imaging aberration corrector (CETCOR). After recording the images at defocus values of + and - 3nm, a newly developed image processing method called "image subtraction and improved deconvolution (ISD) method" [2,3] was applied to them for eliminating artificial image contrast and for direct imaging of the atomistic structures at the interface.

3. Results and Discussion

Figures 1 (a) and (b) show a cross-section TEM image and the corresponding diffraction pattern from the [110] direction, respectively. These indicate that the SiC layer is hetero-epitaxially grown on the Si substrate with the relationship of (001)[110]SiC//(001)[110]Si despite the 4:5 Si–to–SiC matching ratio. In the SiC film, many {111} stacking faults originating at the interface were observed.

Figures 2(a) and (b) show aberration-corrected HRTEM images from the [110] and [100] directions after the ISD processing, respectively. Atom positions constituting long-periodic structures are visible clearly as shown by arrows and deformed circles. As expected from the lattice mismatch and the diffraction pattern in Fig. 1(b), an ordered structure having periods four times longer than

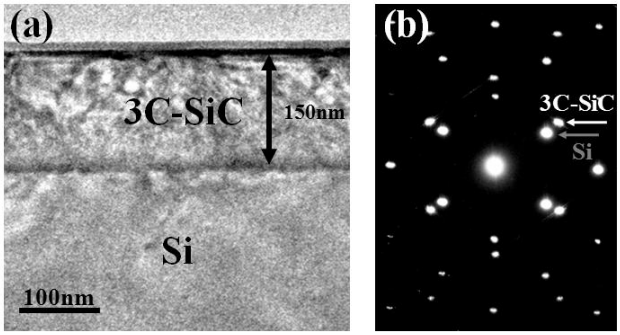

Fig. 1 (a) TEM image of the 3C-SiC film from the [110] direction of the Si substrate. (b) Selected area diffraction pattern from the interfacial area.

those of the silicon lattice, in other words, five times longer than those of the silicon carbide lattice has been formed at the interface.

Based on these results, three-dimensional (3D) atomistic positions at the interface have been reproduced as shown in Fig. 3 [4]. Atomic configurations significantly different from the Si and SiC bulk are formed within approximately three atomic layers, as indicated by black arrows in Fig. 3 All Si and C atoms involved in the model are fully coordinated with sp^3 bonds, which are distorted at the interface region. Based on the model, we have simulated images as shown in Figs. 2(c) and (d), which are in good agreement with the experimental images.

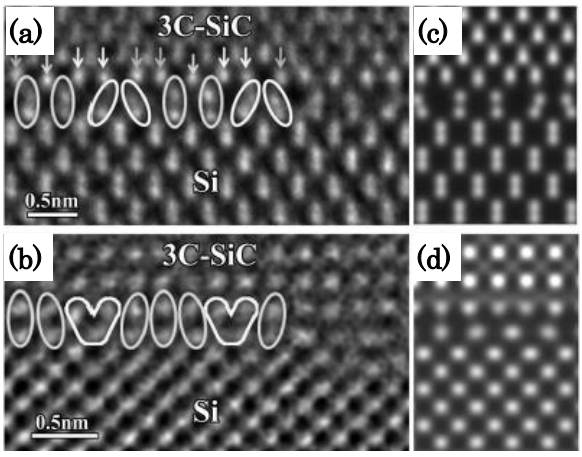

Fig. 2 Aberration-corrected HRTEM images after the ISD processing from [110] (a) and [100] directions (b). (c) and (d) are the corresponding image simulations based on the constructed 3D atomic configuration shown in Fig. 3.

The most important characteristic seen in the [110]- and [1-10]-projections is that a misfit dislocation is formed by the connection of two extra {111} half planes. This is generally referred to as a Lomer dislocation. At the Lomer dislocation core, Si–Si bonds and C-C bonds parallel to the interface are seen in the [110] and [1-10]-projections, respectively. From the viewpoint of formation energy, such irregular bonding to bulk structures is considered to be more appropriate than formation of dangling bonds. In addition to the Lomer dislocations, a different kind of simple misfit edge dislocations with the [100] and [010] directions are seen in the [100] and [010] projections. The strain field induced by the 2D misfit between Si(001)-(4×4) and SiC(001)-(5×5) is relaxed by the 2D network of the four kinds of dislocations parallel to the interface.

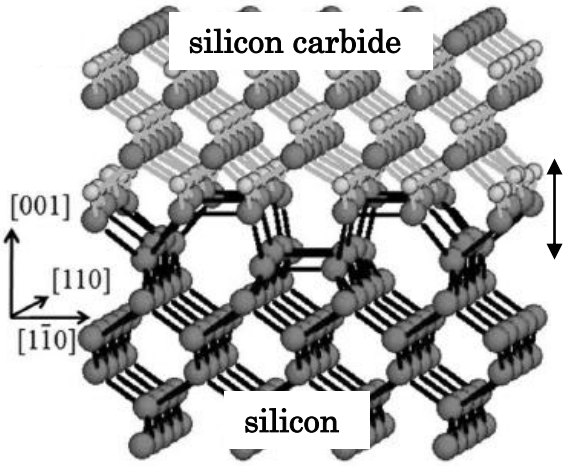

Fig. 3 Atomic configuration model of the 3C-SiC/Si(100) on the basis of Figs. 2(a) and (b).

In a previous research, two kinds of structure models have been proposed for the interface on the basis of calculations [5], in which only carbon-rich and neutral configurations at the interface have been taken into account. On the other hand, our interface model has a silicon-rich configuration. It should be also noted that the theoretical model was observed previously by HRTEM [6] but only in narrow areas less than 2nm wide, even if we ignore the uncertainty coming from artificial contrast in the images. On the other hand, in our experiments, the periodic structure has been observed in some areas extending for about 10 nm without stacking faults. The difference implys that the interface structure clarified in the present study is more stable than the theoretical models.

4. Conclusions

In the present study, the 3D atomic configuration of the long-period structures at the 3C-SiC/Si(001) interface has been clarified by aberration-corrected TEM images combined with the ISD method. The remarkable feature of the interface is that the 2D misfit between Si(001)-(4×4) and SiC(001)-(5×5) is relaxed by the 2D network of misfit dislocations; simple edge dislocations with the [100] and [010] directions and Lomer dislocations with the [110] and [1-10] directions. We hope that the results achieved here will serve as a foundation for future research to improve the quality of 3C-SiC thin films grown on Si(001) substrates.

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