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Atomic Arrangement at 3C-SiC/Si (100) Interface Analyzed by Aberration-Corrected Transmission Electron Microscopy and *Ab Initio* Calculations

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Silicon carbide (SiC) is a promising material for future power devices due to its wide band gap, high electric breakdown field, and other outstanding semiconductor properties. 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 substrate [1]. A high density of defects are, however, induced in the crystal due to the large differences in thermal expansion coefficients and lattice mismatch between SiC and Si. To understand the formation mechanism of the defects, it is important to determine the atomic structure at the interface. In the present study, the 3C-SiC/Si (100) interface has been analyzed at an atomic level by aberration-corrected transmission electron microscopy (TEM) and *ab initio* calculations.

A SiC thin film is grown on a Si (100) substrate by chemical vapor deposition (CVD). For cross-sectional observations, the sample is thinned in [011] and [001] directions of the Si substrate by mechanical polishing followed by 3 kV Ar-ion milling. High-resolution TEM (HRTEM) observations are conducted in a thermal-field emission 200-kV TEM (JEM-2100F) equipped with an imaging aberration corrector (CEOS GmbH). *Ab initio* calculations are carried out by using a program package, STATE (Simulation Tool for Atom Technology) [2, 3].

Figure 1 shows a TEM image from a [011] direction of the Si substrate. The SiC layer about 150 nm in thickness is grown on the substrate. Figure 2 shows a diffraction pattern from an interfacial area 100 nm in diameter. This indicates that the SiC layer is hetero-epitaxially grown on the Si substrate and that the crystalline structure is cubic. In a HRTEM image shown in Fig. 3, it is successfully observed that a fourfold-periodic structure is formed at the interfacial area surrounded by white frames. However, the atomic structure cannot be analyzed directly from the image, since the image contains artificial contrasts. After removal of the artificial contrasts in the image by Image Subtraction & Deconvolution (ISD) method [4, 5], it is revealed that a fivefold-periodic structure is formed at the SiC side of the interface. These periodic structures are attributed to the ratio of the lattice parameters between Si and SiC (nearly 5 : 4). ISD method is also applied to a [001] HRTEM image. Based on these results, an atomic arrangement model at the interface is created. Structural optimizations are conducted for the model by the *ab initio* calculations.

In summary, the periodic structures formed at the 3C-SiC/Si (100) interface are observed by the aberration-corrected TEM. The structure model is achieved by using ISD method and the *ab initio* calculations. The result is an important finding for the growth control of 3C-SiC on Si substrates, and expected to provide valuable information for understanding of the formation mechanism of the interfacial defects.

References

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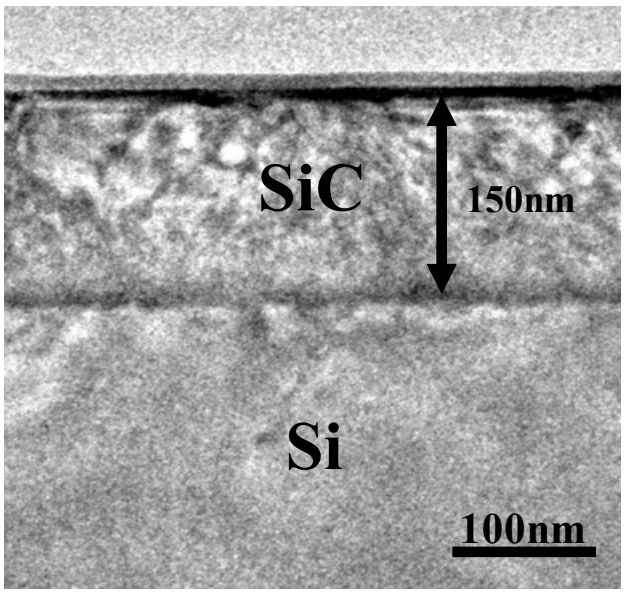

FIG. 1. TEM image observed along the [011] direction of the Si substrate.

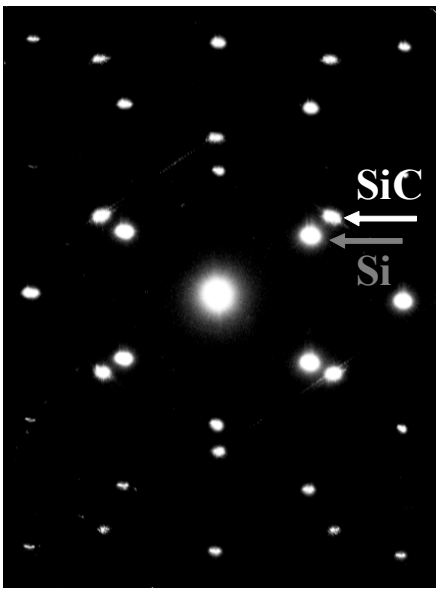

FIG. 2. Selected area diffraction pattern from an interfacial area 100 nm in diameter. Cubic SiC is hetero-epitaxially grown on Si substrate.

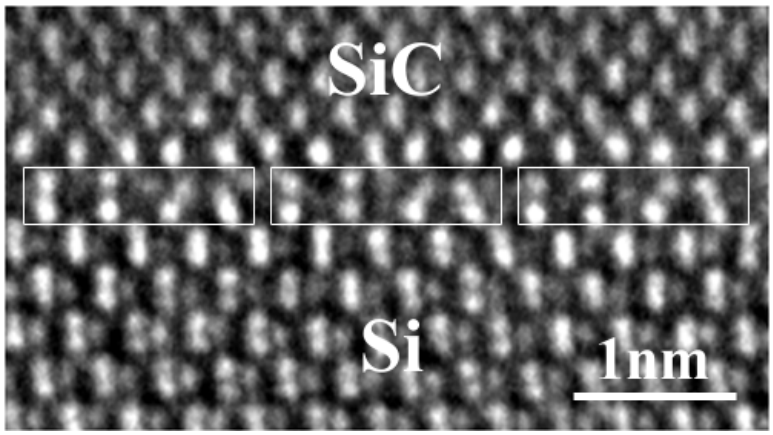

FIG. 3. Aberration-corrected HRTEM image along the [011] direction. Fourfold-periodic structure is formed at the interface.