



# Atomic-scale characterization of Si(110)/6H-SiC(0001) heterostructure by HRTEM



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## ABSTRACT

The atomic structure of Si(110)/SiC(0001) heterojunctions prepared on 6H-SiC(0001) was characterized by transmission electron microscopy and X-ray diffraction. An FCC-on-HCP parallel epitaxy is achieved for the Si(110)/SiC(0001) heterostructure with a growth temperature of 1050 °C and the in-plane orientation relationship is Si[1-10]//6H-SiC[11-20]. The pure edge misfit dislocations with a Burgers vector of  $\frac{1}{3} \langle 11-20 \rangle_{\text{SiC}}$  parallel to the interface are observed to accommodate the extreme lattice mismatch. Along the in-plane orientation Si[1-10]SiC[11-20], the Si/6H-SiC interface has a 4:5 Si-to-SiC matching mode with a residual lattice-mismatch of 0.26%. The misfit dislocation density at the Si/SiC interface is calculated as  $1.217 \times 10^{14} \text{ cm}^{-2}$ .

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## 1. Introduction

SiC semiconductor has attracted considerable attention because of its wide applications for various optoelectronic and electronic devices [1–4]. However, due to its wide bandgap, SiC is not sensitive to long-wavelength light ranging from most of the visible to the infrared region of the optical spectrum. This essentially limits its application for detection of visible and infrared light. A promising way to solve this problem is to adopt a Si/SiC heterostructure, in which Si is used as a non-UV light absorption layer [5,6]. At present, the SiC-based Si/SiC heterostructure is comparatively less studied [7–10], and the studies just focused on using Si/SiC heterostructure to improve the performance of the SiC SBD [8], or using Si/SiC heterostructure to solve the problem of SiC/SiO<sub>2</sub> interface defect states in SiC MOSFET [9,10], the non-UV photoelectric applications of the Si/SiC heterostructure are rarely reported.

In our previous work, it was found that the Si films on SiC substrates always have a polycrystalline structure with multiple preferential orientations at different growth temperatures [11,12]. Preferential growth orientation of  $\langle 110 \rangle$  can be achieved when the growth temperature increases to 1050 °C [11]. However, the atomic structure of the Si(110)/6H-SiC(0001) heterojunction along the in-plane orientation Si[1-10]SiC[11-20] has not been observed, which determines some important parameters such as the lattice

mismatch and the interface state density of the heterostructure. In this paper, the Si(110)/6H-SiC(0001) heterojunctions were prepared by low-pressure chemical vapor deposition (LPCVD). Transmission electron microscopy (TEM), X-ray diffraction (XRD) were employed to investigate the atomic structure of Si/SiC heterojunction.

## 2. Experimental

The Si/SiC heterojunctions were prepared on 6H-SiC(0001) substrates by LPCVD. An n-type doped (doping concentration of  $\sim 10^{17} \text{ cm}^{-3}$ ) 6H-SiC wafer with a thickness of 300 nm was purchased from II-VI Inc. The Si films were grown on 6H-SiC substrates at 1050 °C. Silane (SiH<sub>4</sub>) and hydrogen (H<sub>2</sub>) are used as a silicon source and a carrier, respectively. Prior to deposition, the 6H-SiC substrates were cleaned using the standard RCA method, and then treated in H<sub>2</sub> atmosphere at 1050 °C for 10 min. The growth pressure is maintained at 300 Pa during the Si/SiC heterostructure growth. The crystal orientation of the Si film was characterized by XRD (SHIMADZU XRD-7000). The atomic structure of the Si/SiC heterostructure interface was determined by high-resolution TEM (JEOL JEM-3010).

## 3. Results and discussion

Fig. 1 shows the XRD data of the Si film on the 6H-SiC substrate. There are four diffracted peaks at 28.45°, 35.5°, 47.5° and 75.5°.

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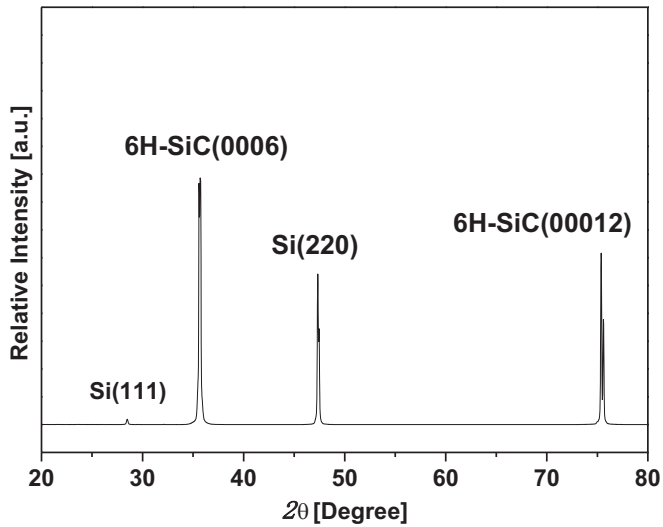


Fig. 1. X-ray specular  $\theta$ - $2\theta$  scans for Si/SiC(0001) heterostructures with the Si layer grown at 1050 °C.

According to the database of joint committee on powder diffraction standards, these peaks are from Si(111), 6H-SiC(0006), Si(220) and 6H-SiC(00012) respectively. The prominent presence of the Si(220) reflection is observed, and the intensity of the Si(111) reflection is relatively low. It is shown that when the Si layer was grown at 1050 °C, it is mainly  $\langle 220 \rangle$  oriented and the parallel-plane relationship is Si(110)//6H-SiC(0001).

The low magnification cross-sectional TEM bright-field image of the Si/6H-SiC heterostructure is shown in Fig. 2(a). In this image, the lower part belongs to the 6H-SiC substrate, while the upper part represents the Si thin film. The Si film has a rough surface with a thickness of 0.28–0.35  $\mu\text{m}$ . The Si/SiC heterostructure has a sharp interface and consist of columnar grains. The SAED patterns at the Si/6H-SiC interface corresponding to Si[001] SiC[1-100] zone axes are shown in Fig. 2(b). The diffraction spots can be categorized into two sets. One has a hexagonal close-packed (HCP) structure with a lattice constant of 3.08 Å, which is identical with the corresponding lattice constant of the 6H-SiC. The other belongs to the Si film with a face-centered cubic (FCC) structure. SAED patterns at the Si/6H-SiC interface clearly show the FCC-on-HCP orientation relationship of (110)[1-10]Si//{(0001)

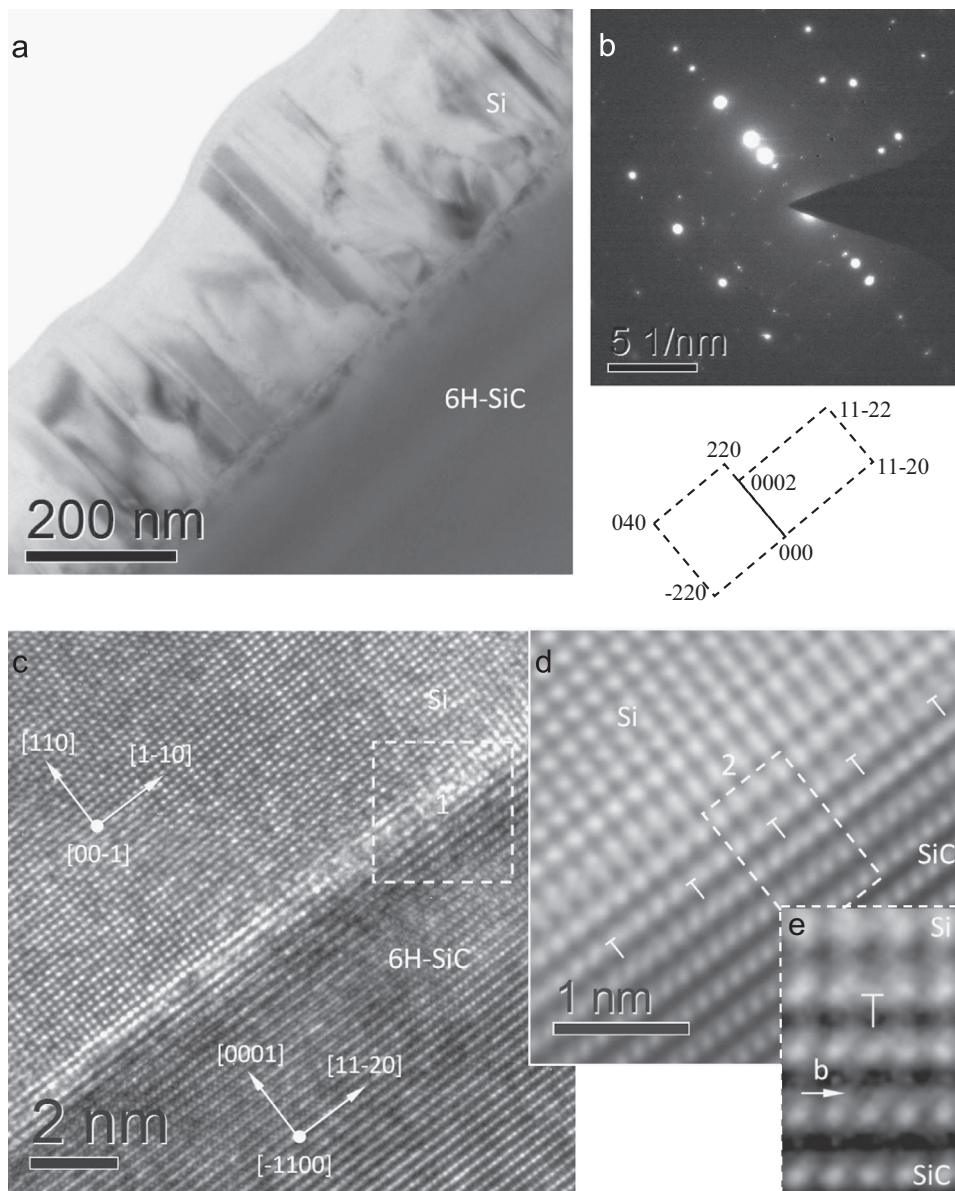


Fig. 2. TEM images and the SAED patterns of Si(110)/6H-SiC(0001) interface. Low magnification cross-sectional TEM image (a), SAED patterns (b), HRTEM image of the Si(110)/6H-SiC(0001) interface (c), the processed HRTEM images of region 1 (d) and region 2 (e) by using FFT and Fourier mask filtering technique. The SAED patterns at the Si/6H-SiC interface corresponding to Si[001] SiC[1-100] zone axes. The corresponding SAED pattern shows (220)[1-10]Si//{(0001)[11-20]SiC epitaxial relation.

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