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# Selective Growth and Schottky Diode Characteristics of β-SiC Single Crystal Films on Si (111) Substrates by Chemical Vapor Deposition

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Crack-free single-crystal epitaxial films of  $\beta$ -SiC(111) are selectively grown up to 5 µm thick on selectively-etched Si(111) substrates for the first time. Schottky barrier diodes are fabricated using Au as a Schottky metal (the diameter: 0.75 mm). The diodes show excellent rectification characteristics with reverse leakage\_currents of about 5 µA (1.1 x 10<sup>-3</sup> A.cm<sup>-2</sup>) at -5 V and 250 µA (5.5 x 10<sup>-2</sup> A.cm<sup>-2</sup>) at -10 V, which are one to two orders smaller than those of conventional  $\beta$ -SiC(100) Schottky barrier diodes. The ideality factor (n) is 1.4 - 1.6 and the Schottky barrier height 0.9 - 1.1 eV.

### 1. Introduction

Silicon carbide (SiC) is a wide-bandgap semiconductor with excellent thermal and chemical stabilities as well as high thermalconductivity. So, it has long been a prime candidate material for electronic devices operative at high temperatures where silicon devices cannot be used. 1) Recent success in large-area single crystal growth of  $\beta$ -SiC on Si substrates by CVD has led to a growing interest in device fabrications using B-SiC on Si.<sup>2,3)</sup> Various diodes and FETs have been vigorously fabricated and evaluated using  $\beta$ -SiC(100) films on Si(100) substrates. 4-10) But significant reverse leakage currents observed for p-n junction and Schottky barrier diodes made the device characteristics poor, especially at high temperatures.9) The improvement in crystal quality and surface morphology is greatly required.

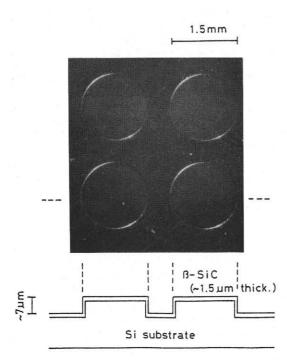
The authors consider that the (111) face of  $\beta$ -SiC is superior to the (100) face for layer-by-layer growth with smooth surface morphology because bulk crystals of  $\beta$ -SiC usually show a platelet shape with welldeveloped (111) faces. The CVD growth of  $\beta$ - SiC(111) on Si(111) substrates has been tried by a few researchers.<sup>2,3)</sup> Usually, the wafer shows severe warpage, and cracks appear in the film. Very few works have been reported on the device fabrication.

In the present paper, in order to reduce the internal stress in the film, selectivelyetched Si(111) substrates are used for the epitaxial growth of  $\beta$ -SiC(111). The warpage is reduced, and crack-free single crystal films up to 5 µm thick are selectively obtained for the first time. Schottky barrier diodes are fabricated and superior diode characteristics to conventional  $\beta$ -SiC(100) diodes are presented.

# 2. CVD Growth

Si(111) substrates with a selectivelyetched surface are used as shown in Fig. 1. The etching is carried out by reactive ion etching using  $CF_4$  and  $O_2$  gases with aluminum metal mask. The region outside the circles in Fig. 1 is etched off to a depth of about 7  $\mu$ m. The substrate size is 15 mm x 15 mm x 0.35 mm. The typical diameter of each circle is 1.5 mm.

The CVD growth is carried out using SiH,



(Cross-sectional view)

Fig. 1. Top view of  $\beta$ -SiC(111) single crystal film on selectivelyetched Si(111) substrate. The circle regions are non-etched.

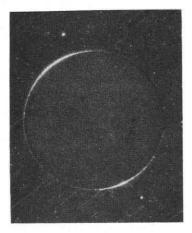


Fig. 2. Enlarged view of Fig. 1.

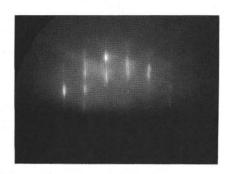


Fig. 3. RHEED pattern of β-SiC(111).

and  $C_{3}H_{8}$  source gases and a H<sub>2</sub> carrier gas. The substrate is placed on a SiC-coated graphite susceptor, which is heated by rf induction. Prior to CVD growth, the substrate surface is etched with a HCl gas at about 1100 °C and a thin carbonized "buffer layer" is formed on the surface at about 1350 °C in a flow of  $C_{3}H_{8}$ . Subsequently, the CVD growth is done at about 1350 °C. The flow rates of SiH<sub>4</sub>,  $C_{3}H_{8}$ , and H<sub>2</sub> are 1 SCCM, 1 SCCM, and 10 SLM, respectively. The growth rate is 1.5 µm/h.

Figures 1 and 2 show a typical result of CVD growth on selectively-etched Si(111) substrates. The film thickness is about 1.5  $\mu$ m. The grown film in each circle region shows a very smooth surface free from cracks. On the other hand, the film outside the circles has cracks as shown in Fig. 2. Thick films up to 5  $\mu$ m were grown without cracks in circle regions. Figure 3 is a typical RHEED pattern of the grown film in the circle, which shows epitaxially-grown  $\beta$ -SiC(111) single crystal with excellent crystal quality and surface flatness.

The wafer warpage is reduced as shown in Fig. 4. The wafer warps as a concave surface. The warpage is measured by Talysurf as a height from the center of the wafer. Two wafers with the circle diameters of 0.75 mm and 1.5 mm selectively-etched are compared with a non-etched wafer.

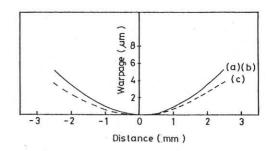


Fig. 4. Reduction of wafer warpage of β-SiC(111) on Si(111) using selectively-etched substrate. (a)Wafer using non-etched substrate. (b)(c)Wafer using selectively-etched substrate.(The circle diameters are (b)0.75 mm, (c)1.5 mm.)

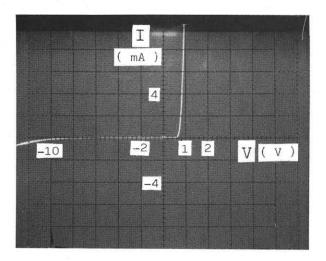


Fig. 5. Typical I-V curve of  $\beta$ -SiC (111) Schottky barrier diodes.

## 3. Schottky Barrier Diodes

Schottky barrier diodes are fabricated by evaporation of Au metal on the films in the circle regions. The film thickness is about 5  $\mu\text{m}$ . The diameter of Au metal is 0.75 mm. The backside ohmic contact for Si (n-type,  $\rho$ = 0.015  $\Omega$ .cm) is nickel metal. A typical I-V curve of the diodes is shown in Fig. 5. For comparison, a typical I-V curve of Schottky barrier diodes of  $\beta$ -SiC(100) on Si(100) by the same fabrication procedure is shown in Fig. 6. The  $\beta$ -SiC(111) diode has excellent rectification as compared with the  $\beta$ -SiC(100) diode. The reverse leakage currents are about 5  $\mu$ A (1.1 x 10<sup>-3</sup> A.cm<sup>-2</sup>) at -5 V and 250  $\mu$ A  $(5.5 \times 10^{-2} \text{ A.cm}^{-2})$  at -10 V, which are one to two orders smaller than those of  $\beta$ -SiC(100) diodes in Fig. 6 and reported by other researchers. 4,10) Values of the ideality factor (n) and the saturation current density obtained from the I-V characteristics are 1.4 - 1.6 and  $4 \times 10^{-8} - 2 \times 10^{-7}$  A.cm<sup>-2</sup>.

Typical C-V characteristics plotted as  $1/C^2$  - V are shown in Fig. 7. The Schottky barrier height is 0.9 - 1.1 eV. Ionized impurity concentration is 9 x  $10^{15}$  - 3 x  $10^{16}$  cm<sup>-3</sup> and increases from the surface of  $\beta$ -SiC towards the substrate as in Fig. 8, which is

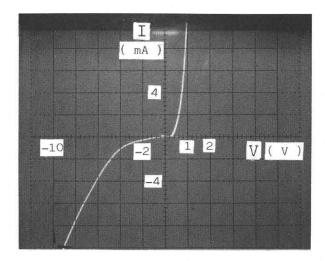


Fig. 6. Typical I-V curve of conventional  $\beta$ -SiC(100) Schottky barrier diodes.

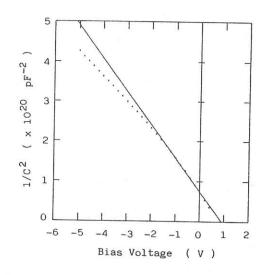
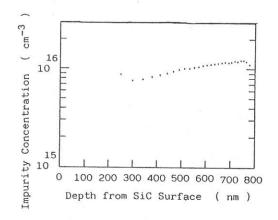
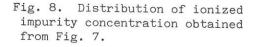


Fig. 7. C-V characteristics of  $\beta$ -SiC (111) Schottky barrier diodes.





#### calculated from Fig. 7.

#### 4. Discussion

Reported values of thermal expansion coefficient of β-SiC at 25 - 1500 °C are about 10 % larger than those of Si. But the wafer warpage of  $\beta$ -SiC(111) on Si(111) is observed during the CVD growth So, the warpage is not caused by the difference in thermal expansion coefficient but mainly by the tensile stress in the film due to the difference in lattice constant (20 %) between B-SiC and Si. On the other hand, the wafer of  $\beta$ -SiC(100) on Si(100) does not show warpage during the growth nor after cooling down to room temperature. Transmission electron microscope observation shows similar kinds of defects, mainly the {111} face stacking faults, in both  $\beta$ -SiC(111) on Si(111) and B-SiC(100) on Si(100). <sup>11,12)</sup> Therefore, in the case of  $\beta$ -SiC(100) on Si(100), internal stress is not stored in the film, or is relaxed in the interface between SiC and Si. A detailed mechanism is unknown at the present stage.

In the present study of  $\beta$ -SiC(111) on Si(111), cracks generate only in the region outside the circles as in Fig. 2, and release the internal stress of the wafer. Much smaller reverse leakage currents and smaller values of the n factor of the fabricated Schottky barrier diodes compared with conventional  $\beta$ -SiC(100) diodes<sup>4,10)</sup> show the superiority of  $\beta$ -SiC(111) on Si(111) in crystal quality and surface flatness.

Similar tendency of the distribution in impurity concentration in Fig. 8 is observed for the distribution in carrier concentration of  $\beta$ -SiC(100) on Si(100) by Hall measurements. Reverse leakage currents of  $\beta$ -SiC(111) Schottky barrier diodes decrease with increasing film thickness. So,  $\beta$ -SiC near the Si substrate contains a lot of defects and probably incorporates a lot of impurities, which affects the diode characteristics.

### 5. Conclusions

Crack-free  $\beta$ -SiC(111) single crystal films up to 5  $\mu$ m thick are selectively grown on selectively-etched Si(111) substrates. Schottky barrier diodes fabricated on the crack-free  $\beta$ -SiC(111) films show much more excellent rectification characteristics compared with conventional  $\beta$ -SiC(100) Schottky barrier diodes.

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