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Growth and characterization of SiC epitaxial layers on Si- and C-face 4H SiC substrates by chemical-vapor deposition

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High-quality Schottky junctions have been fabricated on n-type 4H SiC epitaxial layers grown by chemical-vapor deposition on C- and Si-face substrates in order to understand the effect of growth direction on the growth mechanism and formation of defects. Atomic force microscopy analysis showed dramatic differences between the surfaces of SiC epilayers grown on C and Si faces. There was a significant step bunching in the SiC grown on Si-face substrates. Current-voltage, capacitance-voltage, and deep-level transient spectroscopy (DLTS) measurements were carried out on the Schottky junctions to analyze the junction characteristics. The Schottky junctions on C-face SiC showed larger barrier heights than those on Si-face SiC, showing that each face has a different surface energy. The barrier heights of Ni Schottky junctions were found to be 1.97 and 1.54 eV for C-face and Si-face materials, respectively. However, the deep-level spectra obtained by DLTS were similar, regardless of the increased surface roughness of the Si-face 4H SiC. © 2005 American Institute of Physics. [DOI: 10.1063/1.2132520]

Recently, research has shifted to 4H SiC from 6H SiC due to its higher electron mobility with smaller anisotropy and relatively lower dopant ionization energies. 4H SiC also shows desirable features such as a wide band gap, high thermal conductivity, high breakdown field, and high-power device applications at high temperatures and high frequencies.1–4 Schottky diodes made on 4H SiC are highly useful in high-power rectifiers because of the high voltage (400–1100 V), low on-state voltage drop, low leakage current, and fast switching speed.5 Since there is a surface energy difference between (0001) C-face and (0001) Si-face substrates,6 there should be a difference in the electrical properties of devices made on these faces. Interface reaction is more active on the C face than on the Si face; therefore the interface state density is higher on C-face SiC. A similar kind of properties is also noticed on the Schottky junctions for N- and Ga-polarity GaN layers due to surface reconstruction.7

To prepare unintentionally doped SiC epitaxial layers, Si- and C-face 4H substrates (n~10¹⁸ cm⁻³) obtained from the Cree Research, Inc. were cleaned sequentially in acetone, xylene, and methanol using an ultrasonic bath, then cleaned with a Caro etch, rinsed in distilled water, and finally flushed with N₂. The SiC epitaxial layers were deposited on cleaned n-type off-axis 4H-SiC substrates, inclined 8° toward [11̅20] in order to avoid the formation of rough and mosaic patterns on the epilayer surfaces. The C- and Si-face substrates were etched under H₂ flow rates of 6 l/min at 1400 °C, not only to remove surface scratches incurred while polishing the substrates, but also to form a stepped pattern. 2% SiH₄ and 2% C₃H₆ in H₂ were used as source gases for Si and C, respectively. High-purity industrial-grade H₂ was used as a carrier gas and reductant for the growth of epitaxial layers. 2% N₂ in H₂ was used for nitrogen doping in the epilayers. To deposit epilayers, the substrate temperature and the reactor pressure were kept at 1550 °C and 80 Torr, respectively. A C/Si ratio of 1.0 was maintained in the gas phase. The nucleation growth rate is higher on C-face substrates than on Si-face substrates.

The Schottky junctions were fabricated on 5-μm-thick Si- and C-face SiC epitaxial layers employing a shadow

![AFM images of SiC epilayers grown with C/Si=1 on (a) C-face and (b) Si-face 4H SiC substrates by CVD.](image-url)
mask with diameters of 0.5, 1.0, and 1.5 mm. On the back sides of the SiC substrates, Ti (200 Å)/Ni(800 Å)/
Al (100 Å) metals were deposited by electron beam evaporation and then annealed at 1000 °C for 5 min in Ar to form
Ohmic contacts for current-voltage (I-V), capacitance-voltage (C-V), and deep-level transient spectroscopy (DLTS)
measurements. Ni (300 Å)/Au (500 Å) metals were deposited on the surfaces of Si- and C-face epitaxial layers as
Schottky junctions. The rectifying properties of the Schottky contacts were improved by annealing the samples at 500 °C
for 15–20 min in an Ar atmosphere. The surfaces of the grown layers were studied using an atomic force microscope
(AFM). The I-V measurements were done using an HP4145 parameter analyzer, and C-V measurements were carried out
using an HP4284A LCR meter in the 1 k–1 MHz frequency range. A DLTS system with a liquid nitrogen cryostat was used to characterize the defect levels in the temperature range from 70 to 700 K. For these experimental studies, 40
diodes with three different diameters of 0.5, 1.0, and 1.5 mm on each 1.1×1.1 cm² substrate were used, and 25–30 data
points were averaged. In order to obtain reproducibility, we have fabricated several samples and several runs using the
chemical-vapor deposition (CVD) system. The mapping studies on each 1.1 cm² substrate were used, and 25–30 data
measurements were done using an HP4145

The AFM analysis revealed that the SiC epilayer grown on a C face contained small and large nano-tube like struc-
tures, as shown in Fig. 1(a). The epilayers on Si faces showed large step heights, from step bunching, which are
20–30 times the unit-cell height (10.08 Å) of 4H SiC [Fig. 1(b)]. In general it has been reported in literature that the
heights are one or two times the bilayer of 4H SiC. In the present case the larger heights could be due to the combina-
tion of multiple step heights. It is evident from the AFM analysis that the Si-face epilayer showed greater surface
roughness than the C-face epilayer.

The diode current-voltage relationship governed by the thermionic emission theory is expressed as

\[ I = I_0 e^{\frac{q(V - I R_s) V}{kT}} \left[ 1 - e^{-q(V - I R_s) V/kT} \right], \]

where \( V \) is the applied bias, \( I \) is the measured current, \( I_0 \) is the saturation current, \( R_s \) is the specific on-resistance, \( \eta \) is the ideality factor, \( k \) is the Boltzmann constant, \( T \) is the temperature, and \( \phi_b \) is the barrier height. The leakage currents of C- and Si-face Schottky junctions were found to be \( 10^{-3} \) and
\( 10^{-2} \) A/cm² at −20 V, respectively, as shown in Fig. 2. By simulating experimental results, the specific on-resistance
was found to be 0.12 Ω cm² for the Si face and 0.3 Ω cm² for the C face. From the I-V data, there is a little difference in current transport properties between SiC grown on the C or Si face.

The barrier height was calculated from the C-V measure-
ments using the conventional plot of \( I/C^2 \) vs \( V \), as shown in Fig. 3, using the relations

\[ \phi_b = V_{bi} + \frac{kT}{q} \ln \left( \frac{N_C}{N_D} \right) + \frac{kT}{q} - \Delta \phi, \quad \Delta \phi = \sqrt{qE_m/4\pi\varepsilon_s}, \]

\[ E_m = qN_C\alpha\varepsilon_s + qN_D(\alpha - w)\varepsilon_s, \quad w = \sqrt{2\varepsilon_s V_{bi}/qN_D}, \]

\[ N_D = \frac{2}{q\varepsilon_s \left[ -(dI/C^2)/dV) \right] A^2}. \]

where \( V_{bi} \) is the built-in potential, \( N_D \) is the donor concentra-
tion, \( N_C \) is the effective density of states in the conduction band, \( \Delta \phi \) is the image force lowering of the barrier, \( E_m \) is the maximum electric field, \( \varepsilon_s \) is the dielectric constant of the semiconductor, \( \alpha \) is the distance of heavily doped region extension, \( w \) is the depletion width, and \( A \) is the area of the diode. The physical parameters of the C- and Si-face Schottky junctions obtained from the C-V measurements are shown in Table I. The carrier concentration was found to be \( 3.3 \times 10^{19} / \text{cm}^3 \) for the Si face and \( 6.6 \times 10^{15} / \text{cm}^3 \) for the C face.

### Table I. Physical parameters of C- and Si-face Schottky junctions.

<table>
<thead>
<tr>
<th>Face</th>
<th>( \phi_b ) (V)</th>
<th>( V_{bi} ) (V)</th>
<th>( E_m ) (10⁵ V/cm)</th>
<th>( W ) (μm)</th>
<th>( \Delta \phi ) (V)</th>
<th>( N_D ) (cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1.97</td>
<td>1.86</td>
<td>8.5</td>
<td>0.555</td>
<td>0.107</td>
<td>6.6×10¹⁵</td>
</tr>
<tr>
<td>Si</td>
<td>1.54</td>
<td>1.47</td>
<td>7.8</td>
<td>0.221</td>
<td>0.106</td>
<td>3.3×10¹⁶</td>
</tr>
</tbody>
</table>

FIG. 2. (Color online) I-V curves of Schottky junctions with 1 mm diameter fabricated on C-face and Si-face 4H SiC epilayers.

FIG. 3. (Color online) A plot of \( 1/C^2 \) vs \( V \) for Schottky junctions with 1 mm diameter fabricated on C-face and Si-face 4H SiC epilayers.
The DLTS spectrum shown in Fig. 4 is dominated by traps at <100 K due to Ti, and the $Z_1/Z_2$ trap at 330 K, which has been proposed to be related to the silicon antisite ($\text{Si}_C$) or carbon vacancy ($V_C$).\cite{11,12} Experimental work (Ref. 12) shows that increasing the carbon decreases the height of this peak, suggesting that the defect may be due to $\text{Si}_C$ or $V_C$. However, theoretical estimates for the formation energy, negative-$U$ nature, and acceptor nature may conflict with this assignment.\cite{13} Overall, there is a negligible difference between the deep-level spectrum in 4H SiC grown on the carbon or the silicon face.

The Arrhenius plot is shown in Fig. 5. The activation energy levels and capture cross sections were found to be $E_c = -0.14$ and $E_c = -0.63$ eV, and $7 \times 10^{-15}$ and $9 \times 10^{-15}$ cm$^2$ for Ti and $Z_1/Z_2$, respectively. There was also a trap at 0.64 eV, with a larger capture cross section of $4 \times 10^{-14}$ cm$^2$ superimposed on the peak at 330 K. This second trap at 330 K appeared in higher concentration in the SiC grown on the C face, with a 0.63/0.64 eV trap ratio between 2.5:1 and 2.7:1, and was barely detectable in the 4H SiC grown on the Si face. If both traps (0.63 and 0.64 eV) were due to the $Z_1$ and $Z_2$ levels, respectively, their concentrations would be expected to be the same, assuming identical formation energies on hexagonal and cubic lattice sites and identical densities of possible sites. The observation that they are not always present in a one-to-one ratio suggests that the traps comprising this peak are the $Z_1/Z_2$ trap at 0.63 eV and some other trap at 0.64 eV. There have been other reports of overlapping peaks in this region, with differing annealing temperatures of 600, 1200, 1400, and over 1700 °C.\cite{13,14,15} The different annealing temperatures indicate a variety of compositions. The trap at 0.3 eV was present in both samples. It is similar in character to the $P_3$ trap described in Ref. 14, although the concentration we measured is three orders of magnitude lower.

C/Si ratios outside of the windows of 2–6 for growth on the Si face and 2–3 for growth on the C face reportedly result in nonspecular growth.\cite{16} From the AFM images of the growth with C/Si ratio of 1, the surface with greater roughness was that of the Si face. Aside from the whiskers, growth on the C face is specular. From the difference in surface morphologies, one would expect that the defect structure might be different for the C- and Si-face SiC. However, the fact that the DLTS spectra were nearly identical indicates that formation of the macrosteps during growth on the Si face does not result in additional electrically active defects. 4H SiC has also been characterized for C/Si ratio of 2 on both C and Si faces, with no differences seen in either photoluminescence or DLTS in literature.\cite{17}

In summary, the AFM analysis distinguished a difference between the surface roughness of SiC epitaxial growth on C-face and Si-face 4H substrates. The Schottky junctions fabricated on C-face SiC epilayers showed a lower leakage current, as compared with that of Si-face epilayers. The traps Ti and $Z_1/Z_2$ with more or less the same concentrations were observed in C-face and Si-face Schottky junctions.

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