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S. W. King, C. Ronning, R. F. Davis, et al.



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X-ray photoelectron diffraction from (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ (0001)_{Si} 6H–SiC surfaces

S. W. King, C. Ronning, and R. F. Davis^{a)} Department of Materials Science and Engineering, North Carolina State University,

Raleigh, North Carolina 27695-7919

R. S. Busby and R. J. Nemanich

Department of Physics, North Carolina State University, Raleigh, North Carolina 27695

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High-resolution $(\pm 1^{\circ})$ x-ray photoelectron diffraction (XPD) patterns were obtained along high symmetry azimuths of the (3×3) and $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ reconstructed $(0001)_{Si}$ 6H–SiC surfaces. The data were compared to XPD patterns obtained from (7×7) Si (111) as well as to models proposed for the (3×3) and $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ 6H–SiC reconstructions. Forward scattering features similar to those observed from the (7×7) Si (111) were also observed from the $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ 6H–SiC $(0001)_{Si}$ surface. Additional structures were found and attributed to the substitution of carbon atoms for silicon. Unlike (1×1) and (7×7) Si (111) surfaces, the XPD patterns of (3×3) and $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ SiC $(0001)_{Si}$ surfaces are different which is due to the presence of an incomplete bilayer of Si on the (3×3) surface. The most significant difference with the Si system is the equivalence of the $[10\overline{10}]$ and $[01\overline{10}]$ azimuths in the (3×3) structure. These results are consistent with a faulted Si bilayer stacking sequence which was proposed based on scanning tunneling microscopy observations. © 1998 American Institute of Physics. [S0021-8979(98)01423-6]

I. INTRODUCTION

X-ray photoelectron diffraction (XPD) is a new technique for probing the local atomic structure of metal and semiconductor surfaces with atomic specificity.¹⁻³ XPD experiments essentially consist of performing angle-dependent x-ray photoelectron spectroscopy (XPS) measurements. Anisotropies in the angular dependence of the intensity of emitted photoelectrons in single crystals are created by scattering on the potential of the nucleus of nearest-neighbor atoms. This effect creates intensity enhancements along crystallographic and surface-adsorbate bond directions. This technique has been successfully employed in the determination of surface adsorption sites for various atoms and molecules on metals and semiconductors as well as for studying a number of different epitaxial growth systems.¹⁻⁶ XPD has been applied in this research to study the atomic structure of (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ reconstructed $(0001)_{si}$ 6H–SiC surfaces.

Silicon carbide is a wide-band-gap compound semiconductor of considerable importance to the development of high-temperature, high-frequency, and high-power electronic devices.⁷ However, these applications are currently limited in part, by a variety of line, planar, and macroscopic defects in this material. By analogy with silicon, it is likely that many of these defects originate and/or nucleate on the SiC surface during growth. Therefore, a detailed understanding of the atomic structure of the SiC surface is desired. This has in part been provided for the (0001) surface of 6H–SiC by many recent scanning tunneling microscopy (STM) studies^{8–15} which have identified a variety of different surface reconstructions: (3×3) , $(\sqrt{3} \times \sqrt{3})R30^\circ$, (9×9) , (6 × 6), and $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$.

By analogy to the group III adatom $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ Si (111) reconstructed surfaces, 16-19 it has been proposed that the $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC (0001) surface reconstruction is due to a bulk terminated (0001) 6H-SiC surface with a 1/3 ML (monolayer) coverage of silicon or carbon adatoms in the T_4 position, as shown in Fig. 1.^{20,21} Recent STM investigations by Owman and Martensson¹⁰ and Li and Tsong¹² confirmed the threefold symmetric unit cell; however, they were unable to resolve the chemical identity of the adatom or determine the exact position of the adatom (i.e., T_4 or H_3). Owman and Martensson¹⁰ observed that the reconstruction was not composed of a mixture of Si and C adatoms or a mixture of T₄ and H₃ sites. These findings are complementary to the theoretical results of Northrup and Neugebauer.²² Their supercell calculations using the density functional method showed that for $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ (111) 3C-SiC surfaces, Si adatoms are preferred over C adatoms and that the T_4 site is favored over the H_3 site by both Si and C adatoms. In contrast, semiempirical, self-consistent quantum mechanical cluster calculations by Badziag^{23,24} showed that for the $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC (0001)_{Si} reconstructed surface a triangle of C atoms centered on the T₄ position is energetically more favorable than single C or Si adatoms.

Kaplan²⁰ originally proposed a model for the (3×3) 6H–SiC $(0001)_{Si}$ surface based on Auger electron spectroscopy (AES) data for a SiC surface terminated by a bilayer of silicon [Fig. 2(a)]. Based on analogy to the (7×7) Si (111) DAS model, Kaplan proposed a (3×3) unit cell which consists of two adatoms, six rest atoms (three dimers), and eight silicon atoms in the second layer positioned approximately

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FIG. 1. Top down view and schematic illustration of various adatom adsorption sites for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ reconstructed (0001)_{Si} 6H–SiC surface.

directly over the silicon atoms of the SiC substrate. However, the recent STM results of Kulakov *et al.*¹³ detected only one maxima (i.e., one adatom) in the (3×3) unit cell which is in contrast to the model proposed by Kaplan which



FIG. 2. Top down views of models proposed by (a) Kaplan (Ref. 20), (b) Kulakov *et al.* (Ref. 13), and (c) Li and Tsong (Ref. 12) for the (3×3) reconstructed $(0001)_{Si}$ 6H–SiC surface.

would predict two maxima. Based on this discrepancy, Kulakov et al.¹³ proposed a modified structure which was consistent with the AES results of Kaplan and their STM data. Their model for the (3×3) surface consists of a unit cell with 1 adatom, 3 rest atoms, and 7 silicon atoms located approximately on top of the silicon atoms of the SiC surface [see Fig. 2(b)]. This model includes three dimers and three dangling bonds (two unsatisfied Si bonds from the SiC substrate, and one dangling bond from the adatom) compared to the four dangling bonds in the model by Kaplan [Fig. 2(a)].²⁰ However, Kulakov et al.¹³ did observe stacking faults in their (3×3) reconstructed surface which had a structure essentially like that of the (3×3) model proposed by Kaplan.²⁰ Using STM, Li and Tsong¹² also confirmed the presence of one maxima in the (3×3) unit cell, but in contrast they concluded that the (3×3) reconstruction consisted of only 4/9 ML coverage of silicon for the (0001)_{Si} 6H–SiC surface. Accordingly, they attributed the (3×3) surface to extra Si-C tetrahedra on the surface distributed in a (3×3) pattern [see Fig. 2(c)] rather than a bilayer of silicon.

In this article, we report the first XPD patterns obtained from $(0001)_{Si}$ 6H–SiC surfaces. The XPD patterns obtained from the (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ $(0001)_{Si}$ 6H–SiC surfaces are compared with those obtained from (7×7) Si (111) surfaces and the above described models for these SiC reconstructions.

II. EXPERIMENT

The experiments described in this article were conducted in an integrated surface analysis and growth system which has been previously described.²⁵ The 6H-SiC wafers used in this study were *n*-type ($N_d = 10^{18}$ /cm³), cut-off axis (4° toward $\{11\overline{2}0\}$) and contained an $\approx 1 \ \mu m \ n$ -type 6H epilayer $(N_d = 10^{17}/\text{cm}^3)$ which had been thermally oxidized to a thickness of ≈ 1000 Å. The backside of the SiC wafer was sputter coated with tungsten after removal of the thermal oxide with a 10 min dip in 10:1 H₂O:HF solution. The tungsten coating was necessary to improve the heating efficiency of the SiC wafer by our tungsten filament heater as SiC is transparent in the infrared. The SiC wafers were subsequently given an ex situ clean consisting of ultrasonification in trichloroethylene, acetone, and methanol for 10 min each, followed by a 10 min 10:1 buffered HF vapor clean to remove any native oxides. Each SiC wafer was then loaded into the SiC atomic layer epitaxy (ALE) system and annealed in 10⁻⁶ Torr SiH₄ for 15 min at 1050 °C. This produced an oxygen free (3×3) reconstructed surface. The $(\sqrt{3})$ $\times \sqrt{3}R30^{\circ}$ reconstruction was generated by annealing the (3×3) surface in ultrahigh vacuum (UHV) in the ALE system at 1050 °C for about 10 min.

After either the (3×3) or the $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ surface had been prepared, the SiC wafer was transferred in situ to the XPS system. XPD patterns were acquired by rotating the SiC wafer about various polar and azimuthal angles using a computer-driven goniometer with five degrees of freedom (*x*, *y*, *z*, θ , and ϕ). The positions of the x-ray source and electron energy analyzer were fixed. Though the angular acceptance of the lens of the electron energy analyzer (VG CLAMII)



FIG. 3. XPS spectra of Si 2*p* and C 1*s* core levels from (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ (0001) 6H–SiC surfaces.

was $\pm 7^{\circ}$, an angular resolution of $\approx \pm 1^{\circ}$ was achieved by geometric constraints via grounding the lens and using smaller channeltron acceptance slits. The SiC XPD patterns were acquired by monitoring the Si 2*p* and C 1*s* core levels photoexcited by Al *K* α radiation ($h\nu = 1486.6 \text{ eV}$). Polar scans along high symmetry azimuths were acquired in increments of 0.9° from -35° to 70°. To ensure that the system was operating properly, XPD spectra were first acquired from Si (100) and Si (111) surfaces. Sharp features with full width at half maximum (FWHM) $\cong 3^{\circ}$ were easily resolved and were found to be in excellent agreement with Ref. 26.

III. RESULTS AND DISCUSSION

A. Chemical analysis of (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC $(0001)_{Si}$

Before photoelectron diffraction spectra were acquired from the (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ surfaces, a detailed chemical analysis of these two surfaces was performed using AES, XPS, ultraviolet photoelectron spectroscopy (UPS), low-energy electron diffraction (LEED), and electron energy loss spectroscopy (EELS). The details of the findings of this study are described in a separate paper.²⁷ For clarity, we provide a brief summary of the XPS results here. The XPS spectra obtained from the Si 2*p* and C 1*s* core levels from both the (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ surfaces are displayed in Fig. 3. One important feature to note in the Si 2*p* spectra is the presence of a small low binding energy peak at ≈ 99.5 eV for the (3×3) surfaces and the lack thereof for the $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ surface. The peak at 99.5 eV is indicative of some Si–Si bonding at the SiC surface. A detailed examination of the attenuation of the main Si–C Si 2*p* peak by the Si–Si peak, indicates the presence of $\approx 1.3-1.4$ ML of excess silicon on the SiC surface.²⁷ This is in excellent agreement with the AES results of Kaplan²⁰ which also indicated the presence of an almost complete bilayer of Si on top of SiC for the (3×3) reconstructed 6H–SiC surface.

Finally, it is also important to note that for the C 1s spectra in Fig. 3, no graphitic/non-Si–C bonded carbon was detected for either the (3×3) or $(\sqrt{3}\times\sqrt{3})R30^\circ$ surface. This is in contrast to the results of others^{28,29} which have observed the formation of some "graphitic" carbon for $(\sqrt{3}\times\sqrt{3})R30^\circ$ surfaces. In our study, we believe our lack of observation of graphitic carbon for the $(\sqrt{3}\times\sqrt{3})R30^\circ$ surface is related to the way in which we prepared the surface. In our case, the $(\sqrt{3}\times\sqrt{3})R30^\circ$ reconstruction was generated by annealing a "silicon-rich" (3×3) surface. In previous cases, ^{28,29} where graphitic carbon was observed for $(\sqrt{3}\times\sqrt{3})R30^\circ$ surfaces, the surface was prepared by annealing a "carbon-rich" (1×1) surface. We note that we have also observed graphitic carbon from $(\sqrt{3}\times\sqrt{3})R30^\circ$ surfaces generated by this method.²⁷

B. Forward scattering from bulk terminated (111)/(0001) 3C/6H–SiC

Silicon carbide exhibits several different polytypes which differ only in the stacking sequence along the c axis. 6H-SiC is 66.6% cubic and exhibits an ABCB'A'C' stacking sequence which is similar to that of 3C-SiC differing only in the periodic stacking fault in the 6H structure. Accordingly, in a surface sensitive technique such as XPD which effectively only samples the first 10-20 Å of the surface, (0001) 6H-SiC and (111) 3C-SiC should be essentially indistinguishable. Therefore for simplicity sake, we will treat the (0001) 6H-SiC XPD spectra as if it were from (111) 3C-SiC. This is fortuitous as 3C-SiC and Si have related crystal structures and therefore comparisons can be made between XPD spectra from (111) Si and (111)/(0001)3C/6H-SiC. Accordingly, the expected forward scattering peaks along certain high symmetry crystallographic directions for bulk terminated (111) 3C-SiC, and (0001)Si 6H-SiC surfaces were calculated from the crystal structure and lattice parameters and are listed in Table I for both C 1s and Si 2p photoelectrons.

Figure 4 illustrates both the crystal structure of 3C/6H– SiC and the expected forward scattering peaks along the [1010], [0110], and [1120] azimuths. As Fig. 4(a) illustrates, the [1010] and [0110] azimuths are inequivalent. In the [1010] azimuth, a forward scattering peak at 35.3° is expected for both the C 1s and Si 2p core levels due to forward scattering by both C and Si atoms along the Si–C "atomic row." An additional forward scattering peak at 70.5° is expected in the [1010] C 1s spectra due to scattering by surface Si atoms. For the [0110] azimuth, a forward scattering peak at 54.7° for both the Si 2p and C 1s photoelectrons is expected due to scattering by Si and C atoms, respectively. An additional forward scattering peak at 29.5° is expected in the [0110] C 1s spectra due to scattering by surface Si atoms. For the [1120] azimuth, the primary forward scattering peaks

TABLE I. Expected XPD peaks from bulk terminated (111) 3C–SiC and $(0001)_{Si}$ 6H–SiC surfaces along [1010], [1120], and [0110] azimuths calculated using the crystal structures and lattice parameters.

Si 2p				
Ŷ	[1010]	[1120]	[0110]	Scatterer
	0°	0°	0°	C and Si
	35.3°			Si
			54.7°	Si
		58.5°		С
	70.5°			C and Si
		72.9°		С
C 1 <i>s</i>	_	_	_	
	[1010]	[1120]	[0110]	Scatterer
	0°	0°	0°	C and Si
			29.5°	Si
		31.4°		Si
	35.3°			С
		44.4°		Si
			54.7%	С
	70.5°			C and Si

for the Si 2*p* photoelectron are at 58.5° and 72.9° and are both due to forward focussing by a carbon atom. For the C 1*s* photoelectron, there are no forward scattering features which lie exactly in the [1120] azimuth. However, slightly out of plane forward scattering peaks at 31.4° and 44.4° can be expected for the C 1*s* photoelectron.



FIG. 4. Side of views of 3C/6H–SiC atomic structure along the (a) $[11\overline{2}0]$ and (b) $[10\overline{1}0]$ azimuths. Expected forward scattering peaks are illustrated.



FIG. 5. Si 2*p* x-ray photoelectron diffraction spectra from (a) ($\sqrt{3} \times \sqrt{3}$)*R*30°, (b) (3×3) reconstructed (0001)_{Si} 6H–SiC surfaces and (c) (7×7) Si(111) along several azimuths.

C. $(\sqrt{3} \times \sqrt{3}) R30^{\circ} 6H-SiC (0001)_{Si}$

Most of the forward scattering peaks expected from bulk 3C/6H-SiC were identified in the Si 2p XPD patterns obtained from the $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC (0001)_{Si} surfaces. For the [1010] azimuth [see Fig. 5(a) (top)], a broad peak at $36\pm1^{\circ}$ was identified which was consistent with forward scattering along the [011]/[1011] crystallographic axis (i.e., the Si-C atomic row). This feature was similar in appearance to the Si-Si atomic row forward scattering peak observed at 35° from (7×7) Si (111) [see Fig. 5(c) (top)]. However, unlike the (7×7) Si (111) surface [see Fig. 5(c) (top)], additional peaks at 29° and 42° were symmetrically observed on both sides of the [011]/[1011] forward scattering peak for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ 6H–SiC $(0001)_{Si}$ surface. As mirror symmetry is expected about the [011] atomic row due to the (100) glide planes,²⁷ these additional peaks are probably due to forward scattering from larger emitter-scatterer distances (i.e., higher order effects). Peaks of this nature were also observed at 15° and 59° along the [1010] azimuth for both (7×7) Si (111) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC (0001)_{Si} surfaces.

As with Si (111),³⁰ asymmetries were observed between Si 2p XPD spectra acquired along the [1010] and [0110] azimuths of $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC (0001)_{Si} (i.e., [1010] \neq [0110]). In the [0110] azimuth, the expected peak for forward scattering in the [100] direction was observed at 55° [see Fig. 5(a) (middle)]. Similar to Si (111),³⁰ higher electron intensities due to higher order forward scattering from larger emitter-scatterer distances were also observed between 10° and 40°. However, symmetry was not observed about the forward scattering peak at 55°.

In the [1120] azimuth [see Fig. 5(a) (bottom)], a mosaic of broad diffraction peaks of equal intensity were observed in the Si 2p XPD spectra. Most of these peaks were also



FIG. 6. C 1s x-ray photoelectron diffraction spectra from (a) ($\sqrt{3} \times \sqrt{3}$)R30° and (b) (3×3) reconstructed (0001)_{Si} 6H–SiC surfaces along several azimuths.

present in the pattern of (7×7) Si (111) [see Fig. 5(c) (bottom)]. However, the expected peak at 58.5° (due to forward scattering along the [131] direction) has a "volcano" shape for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ 6H–SiC (0001)_{Si} surface and a rounded shape for the (7×7) Si (111) surface. As will be discussed later, this is related to the fact that for SiC, the scattering atom is carbon, whereas in Si the scatterer is a silicon atom.

C 1s XPD patterns obtained along the [1010] azimuth showed a single sharp peak at 35° which is in agreement with the expected value for forward scattering along the [011]/[1011] atomic row [see Fig. 6(a) (top)]. The sharpest and most intense peak in the C 1s XPD pattern along the [1120] azimuth at 30° is also in excellent agreement with the theoretical value.

The maximum anisotropy in intensity was observed in the $0^{\circ}/[0001]$ direction for both the Si 2p and the C 1s XPD patterns. For Si 2p and C 1s, the maximum anisotropy $(I_{\rm max} - I_{\rm min})/I_{\rm max}$ was $\approx 65\%$ and 40%, respectively. Higher order effects were also observed between 10° and 15° on both sides of the Si 2p and C 1s 0°/[0001] forward scattering peaks in a manner similar to (7×7) Si (111). The Si 2p $0^{\circ}/[0001]$ forward scattering peak from the $(0001)_{Si}$ 6H–SiC surfaces did not exhibit a volcano type shape but rather a flat sawtooth type shape [see Figs. 5(a) and 5(b)]. However, the C 1s 0°/[0001] forward scattering peak exhibited a volcano shape (see Fig. 6). A similar effect has been observed between Si 2p and C 1s spectra from (001) Si and 3C-SiC.^{26,31,32} The shape of this peak is strongly affected by the presence of scattering atoms surrounding the [111]/[0001] direction. As silicon is the nearest-neighbor atom to carbon along the [0001] direction, scattering by the former atoms probably induces the volcano shape observed in the C 1s XPD. For silicon atoms in SiC, carbon is the nearestneighbor atom, but the scattering factor of carbon is much weaker, hence the sawtooth structure. However, in pure silicon and diamond, all the atoms are either silicon or carbon and the volcano shape reappears.^{30,33,34} This also explains many of the differences between Si 2p XPD spectra from Si and SiC along the [1120] azimuth. Finally, it should be mentioned that the centroid of the Si 2p and C 1s 0°/[0001] forward scattering peaks were observed to vary by $\pm 2^{\circ}$. This is related to the fact that the SiC wafers were up to 4° off axis.

As previously mentioned, adatoms in T₄ or H₃ sites are commonly believed to be the origin of the $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ reconstruction. Unfortunately, we were not able to determine with any certainty whether any of the additional expected forward scattering peaks were due to Si or C adatoms proposed by the various models for the $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ reconstruction.^{22–24} Single scattering cluster simulations are necessary to determine the exact structure of the $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ reconstruction based on XPD data. The authors note that Pirri *et al.*³⁰ and Kuttel *et al.*³⁴ have experienced similar difficulties in distinguishing between XPD patterns from (7×7) and (1×1) Si (111) and (2×1) and (1×1) diamond (111), respectively.

D. (3×3) 6H-SiC (0001)_{Si}

In contrast to reconstructed and unreconstructed diamond and silicon surfaces,^{26,34} significant differences were observed between the Si 2*p* XPD patterns from (3×3) and ($\sqrt{3} \times \sqrt{3}$)*R*30° 6H–SiC (0001)_{Si} surfaces. In the [1010] azimuth, the Si 2*p* [001]/[1010] forward scattering peak at \approx 33° was observed from Si 2*p* XPD patterns from both (3 ×3) and ($\sqrt{3} \times \sqrt{3}$)*R*30° 6H–SiC surfaces [see Figs. 5(a) and 5(b) (top)]. However, peaks centered symmetrically at 29° and 42° were not observed from the (3×3) surface, which is more similar to the Si 2*p* XPD patterns obtained from (7×7) Si (111) [see Fig. 5(c) (top)]. Additionally, the sharp higher order diffraction peaks observed at 15° and 58° from the ($\sqrt{3} \times \sqrt{3}$)*R*30° surface were more broad and less intense for the (3×3) surface.

A volcano shaped peak centered at 35° was observed in the (3×3) C 1s XPD patterns in the [1010] azimuth instead of the one sharp peak centered at 35° as for the ($\sqrt{3}$ $\times \sqrt{3}R30^{\circ}$ 6H–SiC surface [see Figs. 6(a) and 6(b) (top)]. Sharper peaks centered symmetrically around the 35° volcano peak at ≈ 20 and 49° were also observed in the (3 $\times 3$ [1010] C 1s XPD pattern and are probably related to the higher order diffraction/forward scattering peaks observed about the 35° forward scattering peak in Si 2p XPD spectra for this azimuth. In the [1120] azimuth, a mosaic of sharp higher order features were found in the (3×3) C 1s XPD spectra instead of the single sharp peak centered at 30° observed in the $(\sqrt{3} \times \sqrt{3})R30^\circ$ reconstructed surface [see Figs. 6(a) and 6(b) (bottom)]. However, for [1120] Si 2p XPD patterns, there were no clearly identifiable differences between the (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC surfaces [see Figs. 3(a) and 3(b) (bottom)].

The largest differences between XPD of (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC surfaces were found in the [0110] azimuth. The Si 2*p* and C 1*s* XPD patterns from the (3 × 3) 6H–SiC surface along the [0110] and [1010] azimuths are identical, as can be seen in Figs. 5(b) and 6(b). This is in

TABLE II. Calculated forward scattering peaks for (3×3) reconstructed [111]/[0001] 3C 6H–SiC surfaces based on models proposed by Kulakov *et al.* (see Ref. 13) and Li and Tsong (see Ref. 12).

Si 2 <i>p</i> Kulakov [1120]	[1010]	[0110]	Li & Tsong [1120]	[1010]	[0110]
59.3° 51.5° 42.9° 38.2° 33.2°	66.2° 53.7° 29.5°	66.2° 53.7° 48.6°	59.3° 52.6° 42.9°	66.2° 29.5°	48.6°
C 1 <i>s</i> Kulakov [1120]	[1010]	[0110]	Li & Tsong [1120]	[1010]	[0110]
59.4° 39.3° 27.3° 25.3°	43.3° 30.8° 21.3°	38.0° 30.8° 25.3°	58.5° 39.3°	43.3° 30.8°	58.5°

contrast to the $(\sqrt{3} \times \sqrt{3})R30^\circ$ 6H–SiC surface in which the $[01\overline{10}]$ and $[10\overline{10}]$ azimuths were observed to be completely different [Fig. 5(a)].

To gain further insight into the nature of these differences, comparisons were made to previously proposed models for the (3×3) reconstruction based on recent STM images.^{12,13} Based on these models, a new set of forward scattering peaks were calculated for the (3×3) reconstruction. These are presented in Table II. As discussed in the introduction, Li and Tsong¹² have proposed that the (3×3) reconstruction is a result of 4/9 ML absorption of Si-C tetrahedra arranged in a (3×3) pattern [see Fig. 2(c)]. This model does not predict the observed equivalence of the $[01\overline{1}0]$ and $[10\overline{1}0]$ azimuths. Kulakov *et al.*¹³ proposed a different model for the (3×3) reconstruction which consisted of an incomplete bilayer of Si [see Fig. 2(b)]. We find the latter model for the (3×3) reconstruction to be in better agreement with our observed XPD patterns. This model specifically adds an additional Si–Si bilayer to the [011]/[1011] atomic row [see Fig. 7(a)]. As silicon has a larger nucleus it is a more effective scatterer than carbon. Therefore, an enhanced electron intensity along the [011]/[1011] chain should occur. This is exactly what we observed in both of our C 1s and Si 2p XPD patterns. The model proposed by Kulakov *et al.* also fails to explain the observed (3×3) equality of our [0110] and [1010] Si 2p and C 1s patterns. However, the model originally proposed by Kaplan²⁰ for the (3×3) reconstruction would explain the equivalence of the [0110] and [1010] XPD patterns [see Fig. 2(a)]. This is primarily a result of the stacking fault in this structure which produces Si-Si bilayers oriented in both directions [see Fig. 7(b)]. The presence of Si–Si bilayers oriented in both directions in turn can create forward scattering peaks at 35° in both the [0110] and [1010] azimuths as observed in our Si 2p and C 1s XPD spectra. The presence of this faulted silicon bilayer structure on SiC surfaces has actually been confirmed by Kulakov et al.¹³ They observed faults or domains of different orientation in their STM images of the (3×3) surface. The stacking structure in these domains is





FIG. 7. Side views along the $[11\overline{2}0]$ azimuths of the (3×3) reconstructions proposed by (a) Kulakov (Ref. 13) and (b) Kaplan (Ref. 20).

consistent with the model originally proposed by Kaplan²⁰ and is consistent with our observations of the equivalence of the $[01\overline{10}]$ and $[10\overline{10}]$ azimuths in our (3×3) XPD spectra.

As mentioned at the start of this section, the observation of clear differences between XPD patterns from (3×3) and $(\sqrt{3} \times \sqrt{3})R30^\circ$ reconstructed (0001)_{si} 6H–SiC surfaces is in contrast to reconstructed/unreconstructed Si and diamond surfaces for which no differences were observed.^{30,32-34} In the latter cases, the authors were trying to detect differences in surface reconstructions which are caused by a slight relaxation or repositioning of surface atoms. However, in our case, the differences we have observed between the (3×3) and $(\sqrt{3} \times \sqrt{3})R30^\circ$ are due to the presence of a partial bilayer/film of another material (i.e., silicon) lying over top of the SiC surface. This situation is perhaps more analogous to XPD studies of heteroepitaxial growth of different materials. Further, this technique may be extremely useful in further understanding the controlled growth of different SiC polytypes.

IV. CONCLUSIONS

High-resolution $(\pm 1^{\circ})$ XPD patterns were obtained along the high symmetry azimuths of (3×3) and $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ reconstructed $(0001)_{\text{Si}}$ 6H–SiC surfaces. The data obtained were compared to XPD patterns from (7×7) Si (111) as well as proposed models for the (3×3) and $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ 6H–SiC reconstructions. Forward scattering features similar to those observed from (7×7) Si (111) were observed from $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC $(0001)_{Si}$ surfaces. Additional features exist in the $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ 6H–SiC XPD patterns and were attributed to the substitution of carbon atoms for silicon atoms. Unlike (1×1) and (7×7) Si (111) surfaces, differences were observed between the XPD patterns of (3×3) and $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ SiC $(0001)_{Si}$ surfaces. The most significant difference was the equivalence of the [0110] and [1010] azimuths in the (3×3) structure. The faulted (3×3) structure proposed by Kulakov *et al.*¹³ is consistent with the measured (3×3) XPD patterns.

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