

Polarity Dependent Step Bunching and Structure of Hexagonal SiC Surfaces

J. Schardt, J. Bernhardt, M. Franke, U. Starke and K. Heinz

Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg,
Staudtstraße 7, D-91058 Erlangen, Germany

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Abstract. An overview of the atomic structure found on the hexagonal surfaces of 3C-, 4H- and 6H-SiC polytypes including polarity dependent step bunching and dangling bond saturation is presented. Bulk grown samples as well as CVD grown epilayers were investigated by quantitative low-energy electron diffraction (LEED) and Auger electron spectroscopy (AES). *Ex situ* chemical preparation methods generate bulk truncated surfaces with dangling bonds saturated by adsorbates. The surface layer arrangement and thus the surface morphology seems to depend only on the polarity of the sample but not on the polytype. The same behaviour is found for the dangling bond saturation. On the nominally Si-terminated (0001) surface of most of the 4H- and 6H-SiC samples, LEED structure analyses reveal that a linear layer stacking sequence is preferred (*step bunching*). Oxygen covers the topmost substrate atoms in most cases. On nominally C-terminated (000 $\bar{1}$) surfaces, single steps are always present and hydrogen must be considered passivating the surface.

1 Introduction

Silicon carbide is one of the most promising semiconductor materials due to its unique physical and crystallographic properties allowing high power and high frequency devices operable in high temperature environments [1]. Unfortunately, the difficulties in growing SiC material of sufficient crystalline and electronic quality have so far hampered its development for commercially available devices. It is apparent that the atomic structure and morphology of the surface influences the growing polytype as well as the incorporation of defects. So, the detailed knowledge

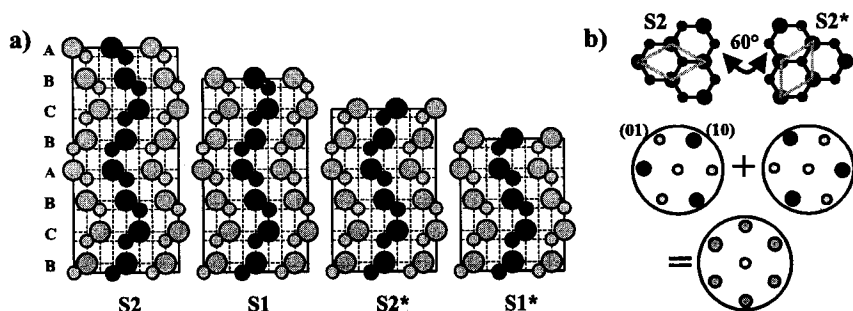


Fig. 1. (a) Cross sectional view of the 4H-SiC polytype. The different surface terminations are labeled according to the depth of the orientation change of the periodic bilayer stacking sequence (S2=ABCBA, S1=BCBAB, S2*=CBABC, S1*=BABCB). (b) The inevitable presence of two domains rotated by 60° on hexagonal polytypes causes a six-fold symmetric LEED pattern.

of the surface structure of different polytypes may be the first step to understand and control the surface properties and growth of SiC. The widely used growth plane for all polytypes is a hexagonal bilayer consisting of Si and C atoms on alternating positions in tetrahedral bond coordination [2]. The different polytypes are distinguished by the periodically repeated stacking sequence of bilayers along the *c*-axis of the crystal where linear stacking or a 60° rotated orientation of subsequent bilayers are allowed. So, for the surface region of a specific polytype, different stacking terminations are feasible. As many truncations with different stacking sequences below the surface edge must be considered, as there are bilayers contained in the 3-dimensional unit cell (Fig. 1a). Their analysis as well as the determination of the atomic geometry and passivation of the hexagonal planes using low-energy electron diffraction (LEED) are addressed in the present study for three different polytypes.

2 Experimental and Theoretical Techniques

The samples of the hexagonal polytypes used (4H- and 6H-SiC) were either bulk grown Lely type samples or homoepitaxial layers grown by chemical vapour deposition (CVD) on top of Lely type substrates. Several methods of *ex situ* preparation were applied including oxidation and hydrogen etching. Also, samples treated with *aqua regia* and as grown samples have been investigated. After the initial treatment, all samples were cleaned from organic and metallic contaminations. Afterwards, the oxide (either artificially produced or natural grown) was removed by concentrated and/or buffered HF [3]. The cubic sample used was a heteroepitaxial 3C-SiC film grown on Si(111) which was just briefly dipped in HF accounting for the fragility of the SiC film. All freshly prepared samples were immediately transferred into ultra-high vacuum (UHV) to limit recontamination of the sample surfaces. No further *in situ* treatment was necessary, i.e. all samples showed sharp LEED-patterns with low background. Auger electron spectroscopy (AES) was used to identify possible contamination. The atomic surface structures were analysed using *quantitative* LEED. In all cases, we observed a (1×1)-periodicity of the diffraction pattern directly corresponding to the lateral periodicity of a hexagonal SiC bilayer. For quantitative LEED, the diffraction intensities versus energy (I(E)-spectra) were measured using a TV camera and an automated data acquisition system [4]. The atomic positions within the first surface layers were determined by calculation of I(E)-spectra for plausible surface structure models using a full dynamical theory [5] and varying the model parameters. The best-fit model was identified by minimizing the Pendry R-factor [6] comparing experimental and theoretical data ($R_p=0$ for ideal agreement).

3 Results

3.1 Polarity and Polytype Determination

The first step to identify the layer stacking sequence is to determine the polytype and the polarity of the SiC crystal. As the diffraction intensities in LEED depend strongly on the chemical nature of the scatterers and their sequence along the direction of incidence, the two polarities of the hexagonal SiC surfaces exhibit completely different I(E)-spectra (Fig. 2a). So, a distinction concerning the polarity can be made without a quantitative LEED-analysis by comparing the experimental I(E)-spectra with those of known cases (*fingerprinting*). The distinction between hexagonal and cubic SiC samples can also be easily achieved using the symmetry of their LEED-patterns when the incident electron beam is aligned normal to the sample surface. A single domain of a specific layer stacking always exhibits three-fold surface symmetry and results in a three-fold symmetric diffraction pattern. For 3C-SiC this is the case, as only linear

stacking occurs [2, 3]. For hexagonal polytype surfaces symmetry-related stacking terminations only rotated by 60° with respect to each other are simultaneously present and give rise to a six-fold symmetric diffraction pattern due to superposition (Fig. 1b). In the course of our work we found characteristic features in the I(E)-spectra seemingly indicating instantly whether the sample is 4H- or 6H-SiC. Yet, we found that such characteristics can also be caused by other effects like different stacking termination ratios or adsorbates. So, at this point, one has to launch quantitative LEED-analyses to determine these parameters safely.

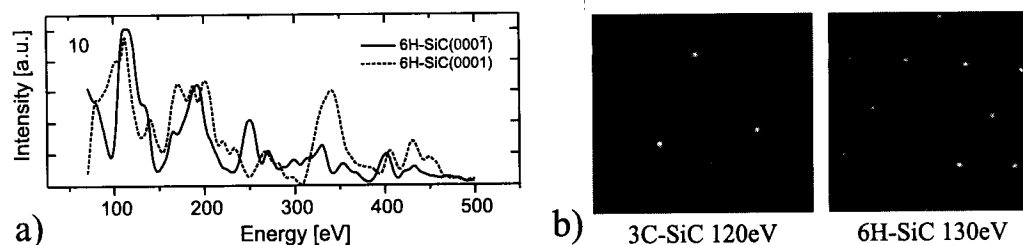


Fig. 2. Experimental fingerprinting: (a) 6H-SiC(0001) (Si-terminated) and 6H-SiC(0001) (C-terminated). (b) 3C- and 6H-LEED patterns exhibiting different symmetry.

3.2 Polarity Dependent Step Bunching

A detailed LEED structure analysis for each sample was carried out allowing for different surface stacking sequences, layer spacings and possible ad-species (details can be found in refs. [3, 7]). In the case of the 4H-polytype, two different surface stacking terminations (S2-, S1-domain) have to be considered and for the 6H-polytype a total of three domains (S3, S2, S1) [7]. On the nominally Si-terminated (0001) surface the LEED intensity analyses reveal a domination of one stacking sequence: S2 on 4H- and S3 on 6H-samples (best-fit models cf. Tab. 1). However, in some cases on 6H-SiC we observed an equally distributed domain mixing. Nevertheless, a linearly surface stacking is preferred for both polytypes in agreement with transmission electron microscopy (TEM) studies of CVD grown films [8]. This predomination of one domain implies a step bunching mechanism on the Si-terminated surfaces, which gives rise to the formation of steps with polytype-specific height (and multiples thereof), namely two bilayers on 4H- and three bilayers on 6H-SiC. A schematic side view of the 4H-SiC stacking domains is shown in Fig. 1. The relationship between termination preference and step structure is evident. On all nominally C-terminated 4H- and 6H-SiC(0001) samples, an equally weighted mixture of all possible stacking structures was found (best-fit models cf. Tab. 1). Therefore, in this case the step heights are evenly distributed and no polytype dependence can be found.

3.3 Polarity Dependent Surface Passivation

The second part of the LEED study is related to the surface passivation established during the *ex situ* chemical preparation. For the SiC(0001) surfaces, the ad-species oxygen on top of the topmost silicon atoms was found with different surface coverages (cf. Tab. 1). This oxygen obviously represents hydroxyl species which were detected by vibrational analysis of a 6H-SiC(0001) sample using high-resolution energy electron loss spectroscopy (HREELS) [9]. Although we found different step morphologies and adatom coverages for both crystal faces, the first substrate layer spacings are always close to the SiC bulk values for the Si- as well as for the C-terminated surface (cf. Tab. 1). Total energy calculations [10] found a significant

Table 1. Best-fit values for termination domain mixing percentages (4H[S2:S1], 6H[S3:S2:S1]), layer distances, adatom coverages and bond lengths together with best-fit Pendry R-factor (R_P). [SiC bulk values: 0.63Å (bilayer thickness), 1.89Å (bilayer distance)]

sample	domain weight	first bilayer thickness	first bilayer distance	adatom coverage	adatom bond length	R_P
3C-SiC(111)	untwinned	0.63Å	1.86Å	50% oxygen	1.61Å	0.18
4H-SiC(0001)	4 : 1	0.63Å	1.87Å	60% oxygen	1.65Å	0.15
	2 : 1	0.64Å	1.82Å	-	-	0.35
6H-SiC(0001)	8 : 1 : 1	0.58Å	1.91Å	80% oxygen	1.66Å	0.13
	1 : 1 : 1	0.63Å	1.87Å	-	-	0.25
4H-SiC(000 $\bar{1}$)	1 : 1	0.60Å	1.90Å	-	-	0.28
6H-SiC(000 $\bar{1}$)	1 : 1 : 1	0.60Å	1.91Å	100% hydrogen	1.02Å	0.18

contraction of the topmost bilayer when dangling hybrids are present at the surface. So, as the results of the LEED structure analysis represent the average height of saturated *and* unsaturated ordered surface areas, one has to conclude that the dangling bonds are completely saturated for all investigated samples. Indeed, for the SiC(000 $\bar{1}$) samples no molecular termination containing oxygen could be found by AES and so, due to the bonding geometry of the first substrate layer, a dangling bond saturation with a hydrogen atom must be considered. Unfortunately, the scattering power of hydrogen for electrons is too low for its identification in the LEED analysis [3].

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