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Electronic and atomic structure of the 4H-SiC(1 $\bar{1}$ 0 2)-c(2 × 2) surface

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Abstract

The (1 $\bar{1}$ 0 2) orientated plane of hexagonal silicon carbide of the 4H polytype consists of a periodic arrangement of stripes with alternating bond configuration on a nanometer scale. The two stripe configurations of the bulk truncated surface have an atomic structure very close to the carbon-face SiC basal plane and the cubic SiC(1 0 0) surface, respectively. The structural and electronic properties of the c(2 × 2) reconstruction on the 4H-SiC(1 $\bar{1}$ 0 2) surface were investigated using photoemission spectroscopy (PES), scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). The core level photoemission spectra reveal two surface shifted Si2p components and one shifted C1s component in addition to the SiC bulk peaks. In accordance with the periodicity observed in LEED, atomically resolved STM micrographs show a c(2 × 2) arrangement of bright features which are accounted as Si adatoms. The electronic structure of this SiC(1 $\bar{1}$ 0 2)-c(2 × 2) phase is experimentally determined by angle resolved PES studies of the valence band revealing four surface states. Based on the experimental observations and a comparison to similar phases on other SiC surfaces, a tentative surface model can be developed which consists of Si adatoms in so-called H3 sites on the basal-plane type stripes and carbon dimers in Si bridging configuration on the cubic stripes of the bulk truncated surface.

Keywords: Silicon carbide; Atomic structure; Surface relaxation and reconstruction; Single crystal surfaces; Semiconducting surfaces; Photoelectron spectroscopy; Scanning tunneling microscopy; Low-energy electron diffraction (LEED)

1. Introduction

Silicon carbide (SiC) is a wide band gap semiconductor with material properties, which make it a very good candidate for high power electronic devices operable under extreme condition such as high temperature, high voltage, high frequency and high power [1]. SiC is also considered to be a very promising material for biophysics applications due to its low weight, high strength, extreme hardness, wear and corrosion resistance and inertness [2,3]. In view of the noted electronic applications and the long needed control of epitaxial SiC growth its surface interactions are particular important. Consequentially, the atomic structure and electronic properties of SiC surfaces have been investigated for quite some time both experimentally and theoretically (see the recent reviews in Refs. [4–9]). Incidentally, the prospect to develop nanostructures and the possibility of biological applications are creating a strong complementary interest in SiC surfaces. In this respect, also non-basal plane surfaces of SiC have become more interesting lately [10–15]. Here the polytype dependent periodicity along the *c*-axis is automatically transferred to the surface. In particular, a surface orientation situated diagonally in the bulk unit cell of hexagonal SiC polytypes, i.e. approximately 62° tilted from the basal plane, possesses intriguing structural properties even in a simple bulk truncated termination. The (1 × 1) unit cell of such a 4H-SiC(1 $\bar{1}$ 0 2) surface contains two regions of different bond configuration, corresponding to alternating stripes of hexagonal type and cubic type surface atom configuration [14].

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Three well ordered phases can be prepared in ultra-high vacuum (UHV) on this $(1\bar{1}02)$ surface [15]. In a regime of Si-rich surface stoichiometry a (2×1) phase develops. A c(2×2) phase can be obtained at higher substrate temperature and the surface is found to be very close to SiC bulk stoichiometry. At even higher substrate temperature a (1×1) phase develops which is found to be carbon rich [15]. However, no detailed studies of these phases have been made up to now.

In the present work, a detailed study of the electronic properties of the 4H-SiC$(1\bar{1}02)$-c(2×2) surface is presented. Low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) are used to determine shape and structure of the surface unit cell. Core level and angle-resolved valence band photoemission spectroscopy (PES) provide information about the electronic structure of the surface. The experimental setup for the different methods is described in the following Section 2. The results are presented in Section 3, and in that section also a possible structural model for this surface is tentatively developed from the experimental findings. The work is concluded in Section 4.

2. Experiment

The photoemission studies were performed at two different beam lines at the MAX synchrotron radiation laboratory. Beam line I311 was mainly used for high resolution core level studies. It is equipped with a modified SX-700 monochromator [16] and an end station built up around a large hemispherical Scienta electron analyzer [17]. The endstation operates at a base pressure of about 1×10^{-10} mbar. Sample preparation was performed by means of a resistive sample heating setup and a resistively heated Si wafer for Si deposition whereby LEED can be used to control the development of the desired surface phase. The electron analyzer accepts a cone of angular width of $\pm 8°$. Normal electron emission and a photon incidence angle of 55° were chosen as the experimental geometry. A total energy resolution of better than 20, 100 and 300 meV at photon energies of 140, 330 and 600 eV, respectively, was selected in the studies of the Si2p and C1s core levels. The angle resolved valence band photoemission (ARPES) investigations were mainly performed at beam line 33. This beam line is equipped with a SGM monochromator [18] and an ARPES end station with the same preparation facilities attached. Here, an incidence angle of 45° was selected and the angular resolution was set to $\pm 2°$. A total energy resolution of less than 120 meV at photon energies from 14 to 40 eV was selected. For determining the surface states and their dispersion along the $\overline{\Gamma}$–$\overline{Y}$, $\overline{Y}$–$\overline{X}$ and $\overline{\Gamma}$–$\overline{X}$ directions (see next paragraph and Fig. 1b) the sample was oriented with LEED so that the angle (i.e. $k_{\|}$) was always scanned in the horizontal plane. In order to estimate broadening effects caused by the sample temperature, photoemission data were also collected at 100 K. However, since no significant differences were observed only room temperature data are presented below. The binding energies were referenced to the Fermi level determined from a Ta foil mounted on the sample holder. The STM and LEED studies were performed in a home-built UHV chamber equipped with a four-grid rear-view LEED optics and a Besocke type STM accessible by a home-built sample transfer [19]. Additionally, an Auger electron spectroscopy (AES) system was available to check the surface composition. In this chamber the samples were heated by electron bombardment. For Si deposition an

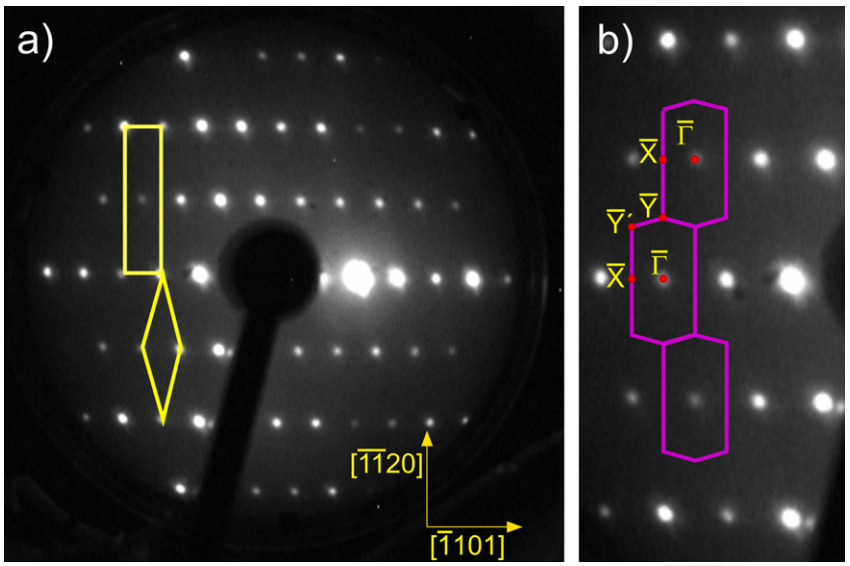

Fig. 1. LEED pattern obtained from the c(2×2) reconstructed 4H-SiC$(1\bar{1}02)$ surface at (a) 84 eV with the primitive $\begin{pmatrix} 1/2 & 1/2 \\ -1/2 & 1/2 \end{pmatrix}$ reciprocal unit cell and a (1×1) cell with the centered spot as well as the main crystal directions indicated. (b) A magnified pattern at the same energy with the corresponding surface Brillouin zone and the high symmetry points indicated.