Reconstruction of the Si-terminated β-SiC(100) surface

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Abstract

We have determined the atomic structure of the c(4 × 2) reconstructed Si-terminated β-SiC(100) surface by comparing experimental height profiles with theoretical ones calculated with the scanning tunneling microscopy (STM)–elastic scattering quantum chemistry (ESQC) method. A large number of possible atomic configurations are considered. We found that the better fit between experiments and theory is obtained if half of the Si dimers have their altitude lowered by 0.1 Å. Consequently, we conclude that the c(4 × 2) reconstruction is caused by alternative up and down dimers within the dimer rows, the lower dimers being not visible in the STM images. © 1998 Elsevier Science S.A.

Keywords: β-SiC(100) surface; elastic scattering quantum chemistry method; Atomic configurations

1. Introduction

Cubic silicon carbide (β-SiC) is an interesting semiconductor material because of its unique properties: a strong potential for use in high temperature and high power electronic devices [1]. Therefore, the characterisation of the structure of β-SiC surfaces is of major interest.

The Si terminated (001) surface of β-SiC has been widely studied during the last decade. Experimentally, low energy electron diffraction (LEED) and energy loss spectroscopy measurements by Kaplan [2] have shown that the surface reconstructs in p(2 × 1) or c(4 × 2) patterns. He concluded that the c(4 × 2) reconstruction is favoured over the p(2 × 1) if the surface roughness is small. This opinion is supported by medium energy ion scattering and LEED measurements by Hara et al. [3]. In a more recent study, Powers et al. [4] have found that their LEED results agreed favourably with a buckled silicon dimer model, the dimer length being 2.31 Å.

However, theoretically, the results are still far from having a complete agreement regarding the determination of the atomic structure of the surface. The first calculation of the dimer bond length has been made by Yan et al. [5] using firstly the empirical Tersoff potential, then the Carr–Parinello method [6]. They found respectively a dimer bond length of 2.46 Å and 2.26 Å, in a relative good agreement with the deduced experimental value [4]. However, ab initio calculations [7,8] concluded that the dimer bond length is about 2.75 Å. Moreover, in a recent Carr–Parinello study, Catellani et al. [9] have found another different value (2.58 Å). The large spectrum of calculated values reveals that the energy minimum should be flat and that the required precision to correctly determine the atomic configuration is beyond the scope of these models.

In this work, we used an alternative way of determining the atomic structure of the β-SiC (001) surface. Scanning tunneling microscopy (STM) images of several different atomic configurations are calculated with the elastic scattering quantum chemistry (ESQC) method [10]. Comparing these theoretical images with high resolution STM images of β-SiC (001) surfaces showing c(4 × 2) reconstructions allowed us to indirectly determine the atomic structure of the surface. We showed that the best fit is obtained for a dimer row model with alternative up and down dimers (AUDD) within a row.

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2. Model

The ESQC method [10] is an unique tool to calculate the current variation due to a defect embedded in a periodic chain. Its property makes it particularly suitable to perform surface STM image calculations, the defect being composed of the STM junction, the tip and the relaxed part of the surface. Constant current mode is simulated by continuously adjusting the tip to surface distance to keep the tunneling current constant.

In this work, the tip body and the bulk substrate are modelled by four layer cells, which are periodically repeated in the lateral directions. Complete surface scans have been realised with 4×2 atoms per layer of the unit cell, bigger cells containing 2×8 or 4×4 atoms being used on some chosen positions to confirm that the used 4×2 cell is large enough to avoid size effects. Calculations take into account all the valence electronic structure of the Si (3s 3p) and C (2s 2p) atoms. The atomic orbitals are Slater orbitals with parameters chosen to correctly reproduce the band structure of β-SiC [11].

The STM tip is modelled by a single Si atom, because the experimental STM tip is very sharp and it is usually considered that it is atom-like ended by one Si atom coming from the surface during the approach. The reconstructed surface is represented by 4×2 Si atoms (or more for bigger periodic cells), arranged in order to reproduce several structural models. In this way, only the atomic relaxation of the layer atoms is considered. We think that the small shifts occurring in the subsurface layers would have no influence on the calculated images.

3. Results

The Fig. 1 shows a STM image of the c(4×2) reconstruction of the β-SiC (001) surface. The experimental procedure used to obtain such high-quality surfaces is described elsewhere [12]. As remarked previously by Soukiassian et al. [12], each spot represents a Si dimer. We measured the distance between two successive spots along the XX′ and YY′ directions (Fig. 1) and found, respectively, $4a$ and $2a$, a being the lattice parameter ($a = 3.08$ Å) of the unreconstructed β-SiC (001) surface. Consequently, as one spot counts as two Si atoms, the surface coverage θ would be only $1/2$ ML, what would disagree with previous studies of this surface [3,13] concluding in a surface coverage of 1 ML.

In order to determine the right atomic structure, STM–ESQC calculated STM height profiles of different surface atomic configurations are compared with the experiments. The experimental conditions are used in the calculations, i.e., scans are calculated for a tunneling current of 0.2 nA. Fig. 2 shows a symbolic picture of the unit cell used in most of the calculations. First, we investigated wether the
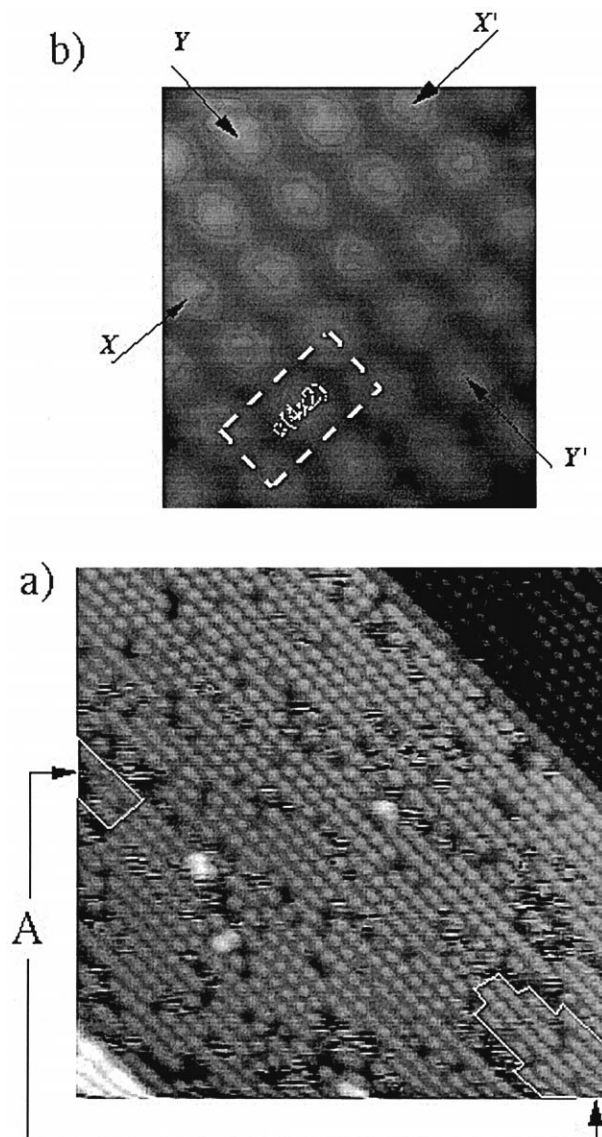

Fig. 1. (a) β-SiC(100)-c(4×2) surface 200 Å × 200 Å STM topograph (filled electronic states). Examples of area having lower corrugations are labeled A. The sample bias was $V = -3$ V with a 0.2 nA tunneling current. (b) Details of an area showing the c(4×2) unit cell.

dimers B are no visible in the STM image because their heights Z above the surface is decreased ($Z_B < Z_A$). We assume that the dimer length is 2.73 Å and $Z_A = 1.08$ Å, as given by ab initio calculations [8]. The Fig. 3 shows both experimental and theoretical scans. It appears that a
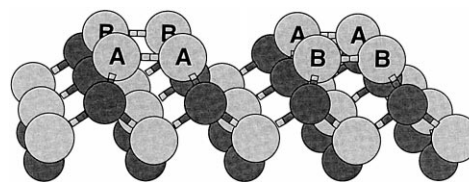

Fig. 2. Picture of the atomic configuration used for the calculations. Light (dark) grey circles represent the Si (C) atoms.
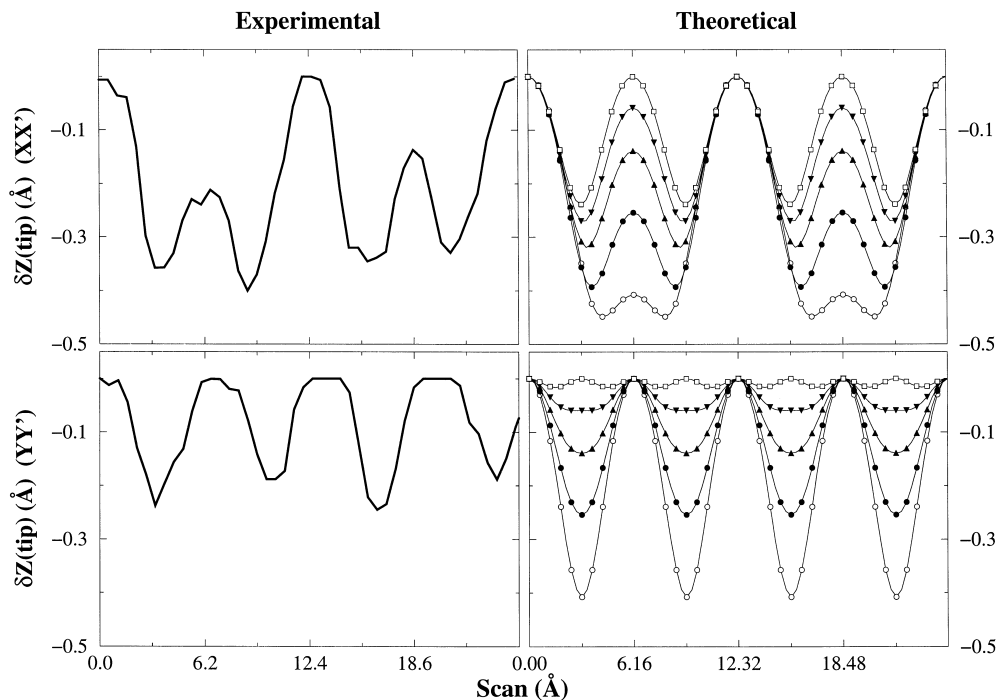
Experimental   **Theoretical**

Fig. 3. Experimental (left part) and theoretical (right part) height profiles along the XX′ and YY′ directions. (i) Open squares: $\delta z = z_A - z_B = 0$ Å (A and B defined in Fig. 2); (ii) filled triangles down: $\delta z = 0.02$ Å; (iii) filled triangles up: $\delta z = 0.05$ Å; (iv) filled circles: $\delta z = 0.1$ Å; (v) open circles: no B dimers ($\theta = 1/2$).

surface configuration where only A dimers are present ($\theta = 1/2$) is not suited to reproduce the experimental profiles. However, if dimers B are slightly lowered on the

surface by an amount of approximately 0.1 Å, both features and calculated contrasts are in excellent agreement with the experiment. If the height difference between

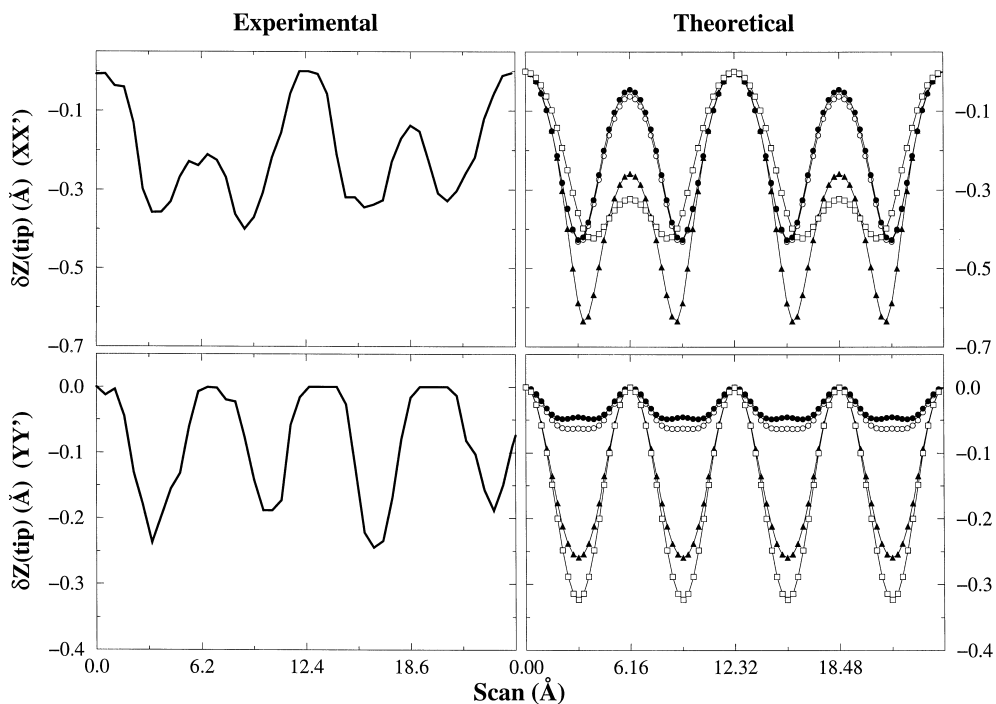**Experimental**   **Theoretical**

Fig. 4. Experimental (left part) and theoretical (right part) height profiles along the XX′ and YY′ directions. (i) Filled triangles up: $\delta z = z_A - z_B = 0.23$ Å, $d_A = 2.5$ Å and $d_B = 2.27$ Å (d is the dimer bond length); (ii) open circles: $\delta z = 0.05$ Å, $d_A = 2.53$ Å and $d_B = 2.48$ Å; (iii) filled circles: $\delta z = 0.1$ Å, $d_A = 2.56$ Å and $d_B = 2.48$ Å; (iv) open squares: SiC alloy for the surface layer (dimer A is a silicon dimer, whereas dimer B is a carbon dimer).

dimers A and B is much more reduced (0.02 Å), we observe a strong reduction of the contrast which would produce a loss of resolution within a dimer row. Such behaviour exists in regions marked by A on the Fig. 1, these regions being located in high defects density environment. So defects prevent the formation of the AUDD configuration within the row. This picture is in agreement with the observation that the $c(4 \times 2)$ reconstruction can only be obtained if the surface roughness is small [2,3]. Finally, if dimers A and B are located at the same altitude above the surface, the corrugation becomes very small along the YY′ direction and the dimer are not resolved within a row.

Even if the experimental scans are correctly reproduced with the AUDD model, different configurations must be explored to ensure that this agreement is not fortuitous and cannot be obtained with other solutions. In Fig. 4, we report the scans obtained for atomic configuration where the lengths and heights of the dimers are given by different preliminary ab initio results. [1] The tested configurations are not able to account for the experimental contrasts. Finally, we considered the improbable possibility that carbon atoms are present in the surface layer. In this case, we suppose that the dimer B is composed of two carbon atoms. The B dimer length is now 1.36 Å and the dimer is located 0.6 Å above the underlayer. This configuration yields correct qualitative features, but the contrast is too small.

In conclusion, we have investigated the atomic configuration of the β-SiC(100) surface which could be accountable for the $c(4 \times 2)$ reconstruction observed in STM images. The height profiles corresponding to several configurations are calculated with the STM–ESQC method, then compared to the experimental ones. We found a better agreement when the dimers have the same bond length and a height difference of 0.1 Å, resulting in the AUDD model.

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