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Investigation of surface structure related features in the multiple-scattering simulations of photoelectron diffraction of 3C–SiC(0 0 1)-$c(4 \times 2)$

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Abstract

In this paper we have conducted a systematic study of the photoelectron diffraction (PED) effects from the 3C–SiC(0 0 1)-$c(4 \times 2)$ surface by means of multiple-scattering calculations. Two models have been proposed to describe this surface: alternately up and down dimers (AUDD) [P. Soukiassian, F. Semond, L. Douillard, A. Mayne, G. Djuradin, L. Pizzagalli, C. Joachim, Phys. Rev. Lett. 78 (1997) 907], based on the scanning tunneling microscopy data, and missing-row asymmetric-dimer (MRAD) [W. Lu, P. Krüger, J. Pollmann, Phys. Rev. Lett. 81 (1998) 2292], based on the total energy pseudopotential calculations. By calculating PED patterns from different emitters in these two models, we show that the surface structure induced features are visible even in total emission diffraction patterns. For the overall diffractogram a scatterer properties of the first layer under the surface become crucial due to the backscattering at low kinetic energies. This layer is Si-layer in the MRAD model, but C-layer in the AUDD model. While this causes clear differences between the diffraction patterns of the AUDD and the MRAD models, it is shown to diminish the differences between the PED patterns of the AUDD and the other models which consist of only one monolayer of Si on top.

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1. Introduction

The studies of SiC have been triggered by its more desirable properties for the applications, but nevertheless similar structure and reconstructions as the ones of the Si surfaces. SiC is being widely implemented in the short-wavelength optoelectronic devices (green, blue and violet diodes, ultraviolet photodetectors), transistors and transistor memory cells [1]. Interface formation between SiC and other materials, which is highly relevant for the applications, depends primarily on the properties of the silicon–carbides surface reconstruction. And several different reconstructions can be obtained on the 3C–SiC(0 0 1) (3C stands for the cubic SiC polytype) surface by diminishing the Si/C ratio: (1×1), (3×2), (5×2), $c(4 \times 2)$, $c(2 \times 2)$. Another surface reconstruction, (2×1), is shown to be a defective phase of $c(4 \times 2)$ [2,3], enabling the only known reversible surface phase transition $c(4 \times 2) \leftrightarrow (2 \times 1)$ in a semiconducting compound [2].

The similarity of the (2×1) reconstructions on 3C–SiC(0 0 1) and on Si(1 0 0) has made 3C–SiC(0 0 1) very popular for surface studies. However, the $c(4 \times 2)$ reconstruction of the Si(0 0 1) surface is not similar to the one of the 3C–SiC(0 0 1). This reconstruction has thus been intensively studied and two structural models have been proposed to describe it: the alternately up and down dimers (AUDD) [4] and the missing-row asymmetric-dimer

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(MRAD) [5] models. The latter was based on total energy pseudopotential calculations and some comparison with the available scanning tunneling microscopy (STM)-data. It suggests that on top of the surface Si-layer another 0.5 ML of Si exists and forms asymmetric dimers. The AUDD model was based on the STM measurements and supported later by core-level investigations [6] and the observations of the reversible phase transition from the $c(4\times2)$ to the (2×1) surface [2,3]. Within this model the surface is terminated by a single Si-layer which forms rows of symmetric dimers that are displaced vertically alternating up and down.

Until now many different proofs have been shown in favor of one or the other model describing the $c(4\times2)$ surface. There are four independent experimental studies supporting the AUDD model: STM data [4], core-level spectroscopy [6], STM and ARUPS [2], hydrogenation studies [7]. The MRAD is supported by pseudopotential calculations [5], early core-level studies [9] and the same STM data, as the AUDD [4].

In the present paper, we report structural investigation of the 3C–SiC(0 0 1)-$c(4\times2)$ surface by means of a powerful surface structure investigation method—multiple-scattering calculations of the PED angular intensity distributions. In this way, we are in a position to determine the nature of the contributions from the two competing models of the 3C–SiC(0 0 1)-$c(4\times2)$ surface to the diffraction patterns or the photon energy scans. Our calculations reveal where the most prominent differences between the models can be seen in the PED patterns and what is causing them. The systematic study of the MRAD, the AUDD and some other models than AUDD with surface terminated by only one Si monolayer reveals the relationship between the backscattering dominated diffraction patterns and surface termination in terms of Si coverage.

2. Calculations

Whereas a PE-diffractogram at kinetic energies above 500 eV is a stereographic projection of the atomic positions (for review see Ref. [10]), at lower kinetic energies more isotropic electron scattering occurs, which requires multiple-scattering analysis methods [11,12]. But multiple-scattering effects are also restricted by the decrease of the inelastic mean-free path to only a few Å. We have used the free software MSCD developed by Chen and Van Hove [11] for the multiple-scattering calculations of the PED-patterns.

We have been running our calculations with Rehr–Albert approximation order 2 and multiple-scattering order 8 on a cluster with the radius 8 Å and depth 7 Å. The θ-range and step were 0–76 or 90°/2° and φ-range and step were 0–357°/3°. The incident angle of the light was 55° and polarization was linear, chosen with respect to our experimental study.

The bulk 3C–SiC(0 0 1) structure is zinc-blende. The lattice constants used for the presented calculations were experimental value of $a_0/\sqrt{2}=3.08$ [4] for the AUDD model and theoretical $a_0/\sqrt{2}=3.068$ [13] for the MRAD model. This difference turned out to be irrelevant. Clusters containing ~100 atoms have been used for the calculations presented in this paper in order to minimize the time of the calculations. This was necessary because the extension of our systematic study required some 150 calculations. Larger cluster has been used for some selected calculations (217 instead of 90 atoms; not shown) and they reveal even more fine structure than the presented ones, but are consistent with all conclusions of this paper.

3. Results

Two structural models have been proposed to describe the 3C–SiC(0 0 1)-$c(4\times2)$ surface: the AUDD [4] and the MRAD [5] models. They are presented from top and side view in Fig. 1, with Si atoms in grey and C atoms shaded and a bit smaller. Only the Si atoms from the topmost layer are presented with black and white circles. Within the AUDD model the surface is terminated by a single Si-layer (Fig. 1b) which forms rows of symmetric dimers that are displaced vertically alternating up and down, as can be seen in Fig. 1a. The black dimers in Fig. 1a and b are 0.1 Å below the white ones [4]. A unit cell of the $c(4\times2)$ reconstruction is chosen in one of many possible ways and marked by a rhomb.

Contrary to the AUDD surface termination, the MRAD model suggests that on top of the surface Si-layer (grey circles in Fig. 1c marked 3–6 in Fig. 1d; this is the layer which consists of up and down dimers in the AUDD model) another 0.5 ML of Si exists and forms asymmetric dimers (black and white circles). This asymmetry refers to both unequal lateral displacements of the two dimer-atoms from the centrum of the underlying Si network (grey circles in Fig. 1c), but also to the differences in the z-position of these two atoms, z measuring the distance perpendicular to the surface, as can be seen in Fig. 1d. The black atoms in Fig. 1c and d are 0.544 Å below the white ones [5]. Despite these significant structural differences, both models have the same $c(4\times2)$ symmetry, which is also in the case of MRAD marked by one possible choice of a unit cell.

The numbers in Fig. 1b and d stand for inequivalent atoms used for the calculations and will be referred to in the following. The second and the third layer in the MRAD model as counted from the surface are having four inequivalent atoms each. This is because of the reconstruction induced small changes in the atomic positions of the underlying layers. If this is neglected, the last three layers in Figs. 1b and d are same.

In Fig. 2 we show multiple-scattering simulations of the PED using the MRAD model of the 3C–SiC(0 0 1)-$c(4\times2)$ surface at the kinetic energy of a Si 2p core level excited with the photon energy of 200 eV. In PED, the emitted photoelectron wave from a chosen core-level (Si 2p) scatters at the surrounding atoms and interferes with the directly emitted wave to give an interference pattern as a