Determination of (3x2) surface structure of cubic SiC(001): Experiments and calculations

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3C-SiC(001) exhibits a variety of Si-rich surface reconstructions, when prepared under adequate conditions [1]. These phases are of the general form [(2n+1)x2]. The (3x2) structure has the smallest unit cell of the series [2]. These systems have deserved attention during the last few years due to several reasons. First, these reconstructions exhibit long atomic chains forming in some cases true nanowires on the surface [3-5]. Second, the atomic arrangement of the reconstructed surface is not known, and it involves several atomic layers subject to significant deformations. While different surface sensitive techniques have been applied to investigate the nature of the (3x2) reconstructions, there is almost no structural information on its atomic structure, besides the lateral atomic distribution as provided by STM [2].

In this communication we describe the structure of the 3C-SiC(001)-(3x2) surface reconstruction using the information provided by x-ray photoelectron diffraction (PED) [6]. The outgoing wave field in a photoemission experiment is diffracted by atoms in the vicinity of the emitter. This phenomenon is used in the PED technique. We refer the reader to Ref. [6] for more details. The experimental intensity modulations were compared in this work with the results of a suitable scattering formalism that simulates the measured PED by modeling the structure of the last atomic layers [7]. A spherical-wave multiple-scattering cluster formalism was used to reproduce the data and discern the correct surface structure of Si-rich 3C-SiC(001)-(3x2), obtained from a systematic search between the models proposed in the literature [2,8-12]. We used a cluster of more than 2000 atoms, with a mean-free-path dependent attenuation of the electron yield, calculated according to Ref. [13]. Simulated PED patterns were generated with emitters at symmetry-inequivalent sites in the first to seventh topmost interface layers. We have simulated two-domain samples, corresponding to 180º rotation. The Si and C muffin-tin scattering phase shifts were used. The quality of the surface model is judged on the basis of the agreement between theory and experiment, that is measured by the figure of merit R_1 [14]. R_1 also allows to know the sensitivity to the different parameters and to optimize the atomic structure. The surface model is modified until a good value of R_1 (< 0.04) is reached. Atoms in the layer underneath dimerize as well, with alternating long and short bond lengths. The long-and-short alternateness between dimer bond lengths explains the top dimmer asymmetry along one single direction. The dimerization takes place through lateral relaxation, without large vertical distortions. The third atomic layer is also dimerized, with a dimer bond length of (2.43 ± 0.10) Å. We conclude that STM and GIXRD experimental techniques and theoretical calculations converge in a unifying model for the 3C-SiC(001)-(3x2) surface.

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