# Cubic SiC Surface Structure Studied by X-Ray Diffraction

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**Abstract.** In this paper, we use Grazing-Incidence X-ray Diffraction (GIXRD) to determine the atomic structure of the Si-rich 3C-SiC(001)3x2 surface reconstruction. Up to 5 models have been proposed in the past for this surface reconstruction, based on structural and non-structural experimental techniques and theoretical calculations. Until now, no clear evidence for a unique model had been given. Our GIXRD experiments allow to exclude all models except one. The results are in qualitative agreement with the Two Asymmetric Adlayer Dimer (TAAD) model proposed on the basis of ab-initio calculations: the reconstruction is made of 3 Si planes, the topmost layer consisting of Si-Si dimer rows with the dimers being perpendicular to the rows. However the data also reveal significant differences in atomic positions with the TAAD model. In particular we find alternately long and short Si dimers (ALSD) in the second reconstructed plane leading to the tilt of the topmost Si dimers. This further explains why the dimers are all tilted in the same direction with no buckling contrary to the Si or Ge (001) surfaces .

Silicon carbide is a wide band-gap semiconductor with a gap ranging from 2.4 to 3.3 eV depending on the polytype. It is a promising material for applications in electronics as it has exceptional physical properties for high temperature, high voltage high power and high frequency applications. Among all polytypes, 3C-SiC is the only cubic polytype and has the zinc-blende structure. The 3C-SiC(001) surface shows a great variety of reconstructions from Si-rich 3x2 to C-terminated c(2x2) reconstructions. The Si-rich 3C-SiC(001)3x2 surface reconstruction is of particular interest for several reasons. First because it involves at least 2 Si adlayers on top of a full carbon plane which has no equivalent in Si or Ge (001) cases. Next, the 3C-SiC(001)3x2 surface is particularly sensitive to $O_2$ : $10^3$ times more reactive to $O_2$ than Si surfaces. Finally, this surface is also of interest because it is the "substrate" for the Si atomic lines [1]. To understand the 3C-SiC(001)3x2 properties, the knowledge of the surface structure at atomic scale is necessary. 5 models have been proposed based on experimental (structural and non structural) techniques and theoretical calculations (Fig. 1). The proposed models include i) the double dimer row model-DDRM with a surface terminated by a 2/3 Si monolayer (ML) [2, 3, 4], ii) the single dimer row model-SDRM with 2/3 ML of Si [5], iii) the alternate dimer row model -ADRM predicted theoretically and having a 2x3 periodicity with 1/3 Si ML coverage and asymmetric dimers [6], iv) another ADRM having a 3x2 surface array and asymmetric dimers as established by atom-resolved STM [7], v) a two adlayer asymmetric dimer model -TAADM (TAADM = ADRM 2x3 + DDRM) predicted by ab-initio pseudopotential total energy and

grand canonical potential calculations [8]. The TAADM was apparently supported by other calculations of the reflectance anisotropy spectroscopy (RAS) [9]. However, the calculated RAS spectrum [10] for the DDRM [2, 3, 4] is also close to the experimental one [10]. Thus, no real insight could be drawn from these optical studies [6,7].

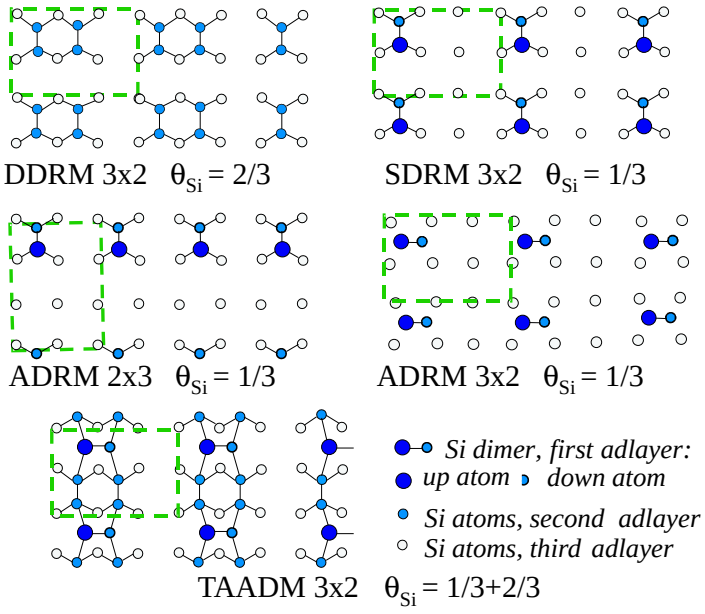


**Fig. 1.** Schematic top view of the 5 proposed models for the 3C-SiC(001) 3x2 surface reconstruction. a) DDRM [2, 3, 4], b) SDRM [5], c) ADRM 2x3 [6], d) ADRM 3x2 [7], e) TAADM [8].

In this context, we perform Grazing Incidence X-ray Diffraction experiments to accurately determine the atomic structure of the 3C-SiC(001)3x2 surface reconstruction. The experiments were carried out at ESRF-Grenoble using a 12keV X-ray beam on the French CRG-IF (BM32) beamline. The base pressure is $3.10^{-11}$ torr during all measurements resulting in the ability to maintain a very high surface quality during all measurements. As there is no high-quality 3C-SiC bulk crystals, we use 1 $\mu$m 3C-SiC thin film grown on Si which obliges us to work below the critical angle ($\alpha_i = 0.176^o$) at low photon energy (12 keV) to limitate the penetration depth of the beam. In consequence this experimental constraints limit the part of the reciprocal space which can be observed and make the measurements particularly challenging. We measured two complete sets of data (measured from two distinct 3x2 surfaces) which turned out to be in very good agreement. For each set we measure 78 inequivalent in-plane and 276 out-of plane reflections along 8 inequivalent rods and 168 reflections along 5 inequivalent crystal truncation rods (CTR). First, we look at the in-plane measured intensities (i-e for l=0). Comparison between experimental and theoretical $|F_{hk}|$ structure factors leads to last-square residual weight $\chi^2$ values given in Tab. 1. All model yields a high $\chi^2$ value except the TAAD model for which $\chi^2$=6.

| | DDRM 3x2 | SDRM 3x2 | ADRM 2x3 | ADRM 3x2 | TAADM 3x2 |
|---|---|---|---|---|---|
| $\chi^2$ | 14 | 21 | 21 | 21 | 6 |

**Table 1.** Stuctural $\chi^2$ factor for the different proposed models for the 3C-SiC 3x2 reconstruction.

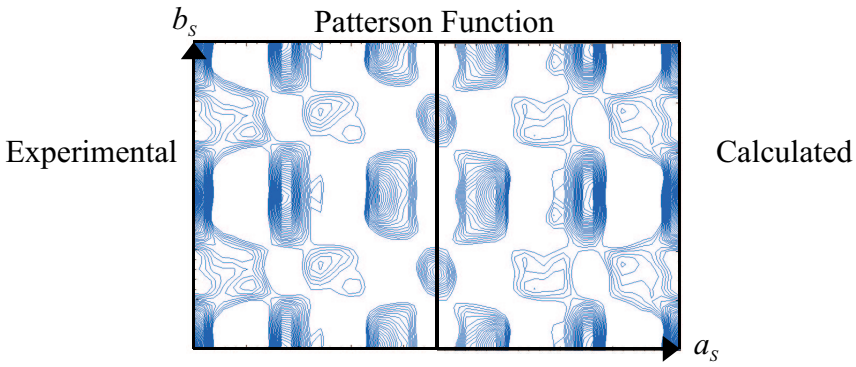


**Fig. 2.** Experimental (left) and calculated (right) Patterson contour map for the 3x2 reconstruction.

We now focus on the TAAD model and look at both in-plane and out-of-plane data. From intensity modulation along the rods, we deduce a 1.7 $\mathring{A}$ thickness for the reconstruction which is consistent with a reconstruction involving 3 Si planes. In-plane and out-of-plane atomic positions refinement by least-square residuals minimization on $\chi^2$ leads to $\chi^2$ values of 0.7 and 1.1 respectively. The experimental and calculated Patterson function maps are given as an example in Fig. 2. The fit of CTR gives a $\chi^2$ value of 1.8. It shows that the Si atoms in the $3^{rd}$ plane ($1^{st}$ atomic plane laying on the C plane) are only slightly deviated from bulk positions. From all these measured intensities (in-plane, along surface and crystal truncation rods), we deduce a structural model for the 3C-SiC(001)3x2 surface reconstruction.

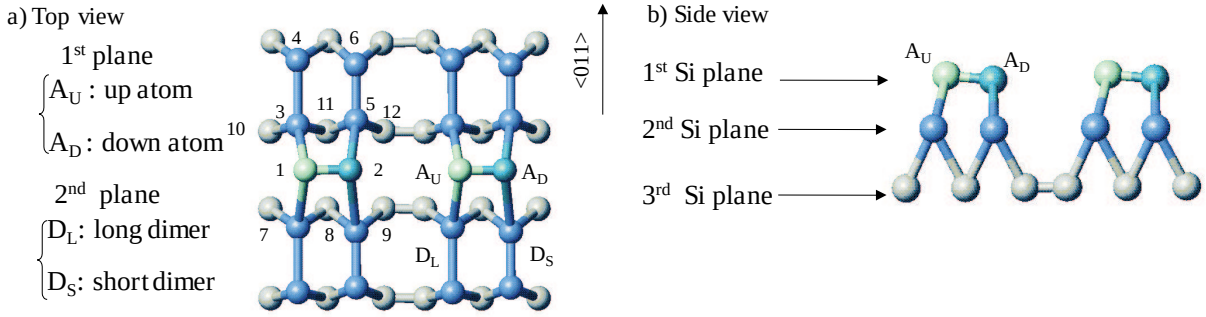


**Fig. 3.** a) top and b) side views of the 3C-SiC(001) 3x2 reconstruction showing the asymmetric dimers in the first reconstructed plane and the ALS dimers in the second plane.

This model is in good qualitative agreement with the TAADM proposed by Lu et al. [8], in particular we find in the top most layer dimer rows made of Si-Si dimers perpendicular to the rows and all tilted in the same direction. However it also reveals important differences especially for the atomic positions in the second reconstructed plane. Indeed, in this plane, we find that the dimers do not have the same length but are alternating long and short dimers (ALSD) with lengths of 2.55$\mathring{A}$ and 2.24 $\mathring{A}$ respectively. This alternately long and short dimers (ALSD) are bonded on both side to the $A_U$ and $A_D$ atoms of the top asymmetric dimer. This alternately feature results from surface stress. In the case of the Si-terminated c(4x2) surface the surface would be made of alternately up and down dimers (AUDD) reducing surface stress. For the 3C-SiC(001)3x2 reconstruction, there are two additional planes on the top of the Si terminated surface. Then, the AUDD dimer organization can no longer take place. Instead the stress is transferred to the second Si plane (2/3 ML). In this plane, the constraint is relaxed by having alternately long and short dimers (ALSD). This ALS dimers in turn influence the topmost dimers which are then tilted, the up atoms being bonded to the long dimers and the

down atoms to the short dimers. This further explains why the topmost dimers are all tilted in the same direction (no buckling) as observed by STM [7].

In conclusion, we have determined the atomic structure of the 3C-SiC(001)3x2 surface reconstruction using GIXRD. Our measurements allow us to exclude all available models, the TAADM being the closest. Accurate atomic positions determination give some significant differences, especially for Si atoms in the second plane where we find alternately long and short dimers (ALSD). We explain this result in terms of surface stress transfer from the $3^{rd}$ Si atomic plane (just above the carbon plane) to the Si plane above. Most interestingly, these long and short dimers explain why the topmost dimers are tilted all in the same direction with no buckling contrary to the Si or Ge(001) cases.

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