| ESRF | **Experiment title:**<br>Determination of the atomic structure of the surface reconstructions and atomic Si lines on 3C-SiC(100). | **Experiment number**:<br>32-3-45 |
|---|---|---|
| **Beamline**:<br>BM32 | **Date of experiment**:<br>From: 05/12/00 to: 12/12/00 | **Date of report**:<br>28/02/01 |
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We investigated the 3C-SiC(100) 3x2 (Si-rich) surface reconstruction by GIXRD at the BM32 line.

Previous test experiments had been performed in 1997 on a (100) SiC surface, but no results could be extracted from the data due to three main experimental troubles : the 4° miscut of the SiC film, and the presence of several different surface reconstructions due to a strong temperature gradient when preparing the surface by direct current heating, but most importantly, the presence of many additional scattering rods emanating from the high density of stacking fault in the 3 μm-thick SiC layer.

Since then, the growth method has been improved resulting in a very low density of stacking faults below the surface. In addition, we got rid of the other problems by choosing a sample wihout miscut (sample "on") and by mouting with special care the electrical contacts of the sample in order to achieve an homogenous heating – less than 30°C difference through the 2 cm sample. This required preliminary experimental tests prior to the beam time.

The excellent vacuum (very low $10^{-11}$ Torr) in the experimental chamber during the beam time allowed to prepare a stable 3x2 reconstruction which could be analysed for the whole set of measurements without any significant contamination. The first X-ray diffraction measurements confirmed the Si-rich nature of this surface, and exhibited diffraction peaks unambiguously characteristic of a clean 3x2 structure. We could perform systematic measurements of the diffracted intensities in the surface plane, and out of plane along the reconstruction rods and the truncated bulk rods.

We derived the in-plane experimental structure factors, and we compared them to the theoritical structure factors, given by the different existing models of this reconstruction. Obviously most of these models do not fit at all to the experimental data, and therefore can already be eliminated. However, one model gives a satisfactory agreement with the experiment, but the precise positions must be improved by fitting procedure.

We already obtained the in-plane positions, with an aggreement factor $\chi^2$ of 0.9. The comparison between experimental and theoritical structure factors is illustrated by the figure included below.

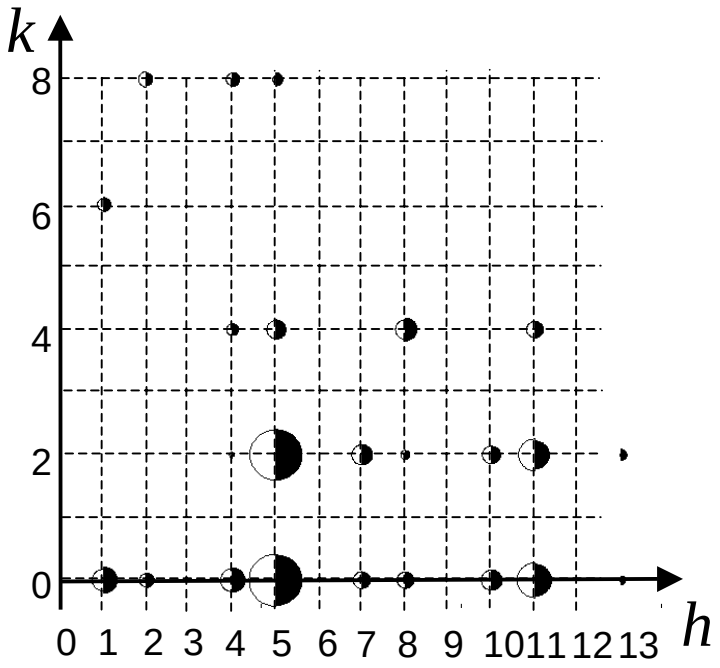


Figure : In-plane diffraction pattern of the 3x2 SiC(001) reconstruction, after application of the p2mm symmetry. The agreement is excellent between calculated (empty half circles) and experimental (half disks) structure factors. Only the intensity with even k were fitted because the diffraction peaks with odd k were two wide to be satisfactorily integrated, due to stacking-fault disorder along this direction.

Beside this result was confirmed by second set of measurements that was performed on another 3x2 SiC(100) reconstruction prepared on the same sample, with the same agreement.

Now, we are improving the out of plane positions of the atoms that participate to the reconstruction by working on the reconstruction rods. We obtained some preliminary satisfactory results that still have to be improved. Furthermore, we have to deduce from the truncation rods the bonding of the reconstruction planes with the underlaying SiC bulk.

So, thanks to good experimental conditions, and in peculiar the possibility of preparing the surface before the beam time, we obtained data of excellent quality and we are in the position to provide a complete structural model of the 3C-SiC(100) 3x2 surface and sub-surface, which was under debate since several years. It should be achieved in a few weeks and soon submitted to publication.