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Determination of the structure of the clean and oxidized SiC (0001)-3×3 surface reconstruction by surface x-ray diffraction

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Introduction

Silicon Carbide (SiC) is a wide band gap semiconductor that has a number of possible applications in replacing Silicon in electronic devices such as power devices. One of the problems that must be solved to make SiC-based devices really competitive with Si-based ones is the insufficient quality of the SiO_2-SiC interface.

In this work, we have studied the initial oxidation of the 4H-SiC (0001) 3×3 surface reconstruction with surface x-ray diffraction. First the structure of the clean 3×3 surface was accurately determined. Then the structural changes due to low oxygen exposures at room temperature were investigated.

Experiment

The experiment was performed with the six-circle diffractometer equipped with an ultra-high vacuum chamber that is installed at BL 15B2. The 3×3 surface reconstruction was prepared by depositing at room temperature several nanometer Si on the surface of a 4H-SiC (0001) sample, then heating the sample to about 1075ºC for 1 min. This resulted in a sharp 3×3 RHEED pattern. The surface was exposed to about 30 L of oxygen at room temperature.

The surface structure was determined by fitting the intensities calculated from model structures to those determined from measurements of in-plane and out-of-plane intensities of fractional-order reflections, before and after the oxygen exposure.

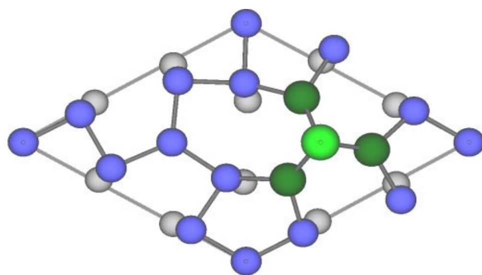

Fig. 1 Best fit positions for the clean 3×3 reconstruction.

Results

The model of Starke et. al. [1] best fitted the diffraction data from the clean 3×3 surface. This model consists of a Si tetramer (light and dark green atoms) placed on top of a Si adlayer (blue atoms) on the Si terminated (0001) surface (grey atoms). The atomic positions could be determined accurately from the experimental data. Fig. 1 shows the best fit atomic positions for this model.

Two models have been proposed for the adsorption site for oxygen on the 3×3 surface: adsorption at the Si adlayer between the Si tetramers on the surface [2] and adsorption between the top-most atom of the Si tetramer (light green) and the other Si tetramer atoms (dark green) [3].

By comparing the in-plane Patterson maps for the clean and the oxidized surface, it was seen that changes occur mainly at interatomic vectors that are associated with the Si tetramer atoms. A model with three oxygen atoms (red) placed between the top-most Si atom and the other Si tetramer atoms gives a good fit to the in-plane experimental intensities (Fig. 2). Only the atoms of the Si tetramer move with respect to the clean surface, the atoms in the adlayer and below stay almost at the same positions.

References

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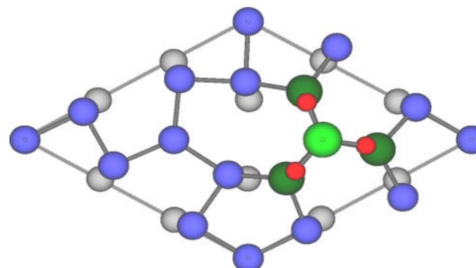

Fig. 2 Best fit positions for the oxidized 3×3 surface.