Structural Study of SiC(0001)3×3 Surface by Surface X-Ray Diffraction

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Introduction

Silicon carbide (SiC) is anticipated as a material suitable for electronic devices, such as high-power, high-temperature, high frequency devices due to its wide band gap, high electron mobility and stability at high temperature. The SiC(0001)3×3 surface is one of the most extensively discussed surfaces since discovery. The atomic arrangement of the 3×3 surface has been explained by several structure models.

In this work, we studied the 3×3 reconstructed structure by a surface X-ray diffraction.

Results and Discussion

We measured a total 117 different reflections, of which 40 were non-equivalent. The measured intensity profiles have a Lorentzian line shape and the integrated intensities are obtained from curve fitting. We made a Patterson map as shown in Fig. 1 using the observed structure factors.

Several structure models for the 3×3 structure as shown in Fig. 2 have been proposed in many investigations by various techniques. The expected Patterson maps from the model are shown in Fig. 3. Compared with the Patterson map obtained from experiment as shown in Fig. 1, the Patterson maps (a) and (b) in Fig. 3 differ greatly from the experimental one as shown in Fig. 1.

In conclusion, we found the Patterson maps of Kulakov model and Starke model are relatively in good agreement with the experimental one, although there are still some discrepancies.

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