

Experimental verification of buckled structure of silicene on a Ag(111) surface using TRHEPD

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1 Introduction

Silicene, silicon version of graphene, is attracting increasing attention as a new functional material for a future electronic device because of its possibility of intriguing properties such as Dirac cone. The theoretical calculations demonstrated that the shape of the Dirac cone depends considerably on the buckling in the silicene and the spacing between the silicene and the underlying substrate. Recently, the synthesis of a silicene on a Ag(111) surface was successfully reported [1]. While the buckled structure of the silicene was predicted by the theoretical calculations due to the strong sp^3 -bonding character, it was not verified experimentally.

Total-reflection high-energy positron diffraction (TRHEPD) is a surface-sensitive tool for the determination of topmost surface structures [2]. Recently, the quality of the positron beam was drastically improved through the installation of the brightness enhancement system. In this study, the structure of the silicene on the Ag(111) surface was determined by this technique [3].

2 Experiment

To fabricate crystalline Ag thin film, Ag atoms of 20 monolayers were deposited on the Si(111)-(7×7) surface at 130 K and subsequently annealed up to room temperature. The silicene was made by depositing one bilayer Si atoms on the Ag(111) surface at 520 K. Weak $\sqrt{13}\times\sqrt{13}$ spots were observed in addition to the 4×4 spots resulting from the formation of the silicene. The fraction of the $\sqrt{13}\times\sqrt{13}$ domains was estimated to be less than 5 %. Thus, the $\sqrt{13}\times\sqrt{13}$ domains hardly affect the structure analysis of the silicene.

Experiments were carried out at the Slow Positron Facility of Institute of Materials Structure Science, KEK. The intense positron beam was generated from the pair creation through the bremsstrahlung radiation using a dedicated linac. A highly parallel and monochromatic intense positron beam was produced using a transmission-type brightness enhancement system. The beam was then accelerated to 10 keV. The rocking curve was measured by rotating the sample at a step of 0.1° .

3 Results and Discussion

Figure 1 shows the TRHEPD rocking curves of the specular spot from the silicene on the Ag(111) surface. The incident azimuth is 13° away from the $[11\bar{2}]$ direction (one-beam condition). Under the one-beam

condition, the TRHEPD intensities depend mainly on the surface-normal components of the atomic positions and its atomic density at each layer. To determine the atomic positions of the silicene, the rocking curves were calculated on the basis of the dynamical diffraction theory. The magnitude of the buckling in the silicene and the spacing between the silicene and the Ag substrate were varied so as to minimize the difference between the measured and the calculated curves.

The solid line in Fig. 1 represents the calculated curve using the optimum structure parameters; it reproduces the measured curve very well. As a result, the magnitude of the buckling in the silicene was determined to be 0.83 \AA . The spacing between the lower layer of the silicene and the first layer of the Ag substrate was determined to be 2.17 \AA . These values were consistent with the theoretical calculations within an uncertainty of $\pm 0.05 \text{ \AA}$. Thus, the buckled structure of the silicene on the Ag(111) surface was verified experimentally, which is in contrast to a planer structure of graphene.

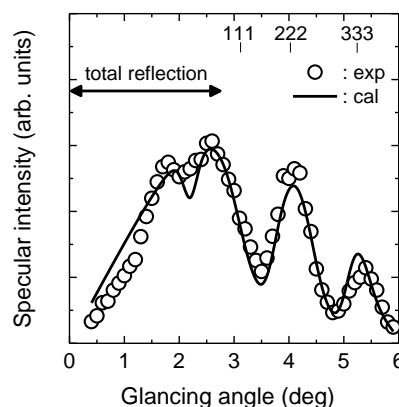


Fig. 1: TRHEPD rocking curves of the specular spots from the silicene on the Ag(111) surface at room temperature. The open circles indicate the experimental curve. The solid line shows the calculated curve using the optimum structure parameters.

References

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