Structural analysis of surface superstructures and atomic layer materials using by 2DMAT on supercomputer system at ISSP

Akari TAKAYAMA

Department of Physics,

Waseda University, Ohkubo, Shinjuku-ku, Tokyo 169-8555

In our research, we use supercomputers for structural analysis in terms of determining the structure of materials. Since structure and physical properties are closely related, it is essential to know the exact structure in order to correctly understand the physical properties. Generally, surface and interface structures are complicated than bulk crystal due to structural relaxation and structural reconstruction at surface and interface. For instance, structure of epitaxial graphene growth on SiC is still controversial due to the underlying-buffer layer with a long-period ($6\sqrt{3}\times6\sqrt{3}$-R30°). Also the $\sqrt{3}\times\sqrt{3}$-Pb/Si(111) surface superstructure, which is known to undergo a structural phase transition at T = 86 K, forms a "mosaic" structure, thus its detailed structure is fully understood. In this study, we investigated the structure of graphene on SiC including a buffer layer and Pb/Si(111) surface superstructure by using total reflection high-energy positron diffraction (TRHEPD) method. For structure analysis, we used "2DMAT" [1], an open source framework for 2D material structure analysis, which is included as standard software in ISSP's supercomputer. Using massive parallel computer simulations on supercomputer is very useful for structure analysis of large periodic structure and surface superstructure with lattice reconstruction because they require many variables for analysis.

Figure 1 shows the rocking curve under the one-beam condition obtained from the experiment (circles) and from calculation (solid line) for 0-BL graphene (buffer layer) of SiC(0001). From the fitting calculation for this rocking curve, we determined the buckling structure of buffer layer and found that our determined structure corresponds well with the structural model proposed by Lima *et al*. [2]. Moreover, the ratio of bounding and free-standing regions with/from substrate were determined to be 22 % and 78 %, respectively, in this sample. The ratio is consistent with previous studies [3, 4].

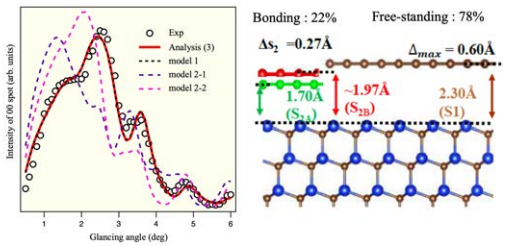

Fig. 1: Structure analysis results of buffer layer on SiC.

Figure 2 shows the rocking curve under the one-beam condition obtained from the experiment (circles) and from calculation (solid line) for mosaic phase of √3×√3-Pb/Si(111). We have succeeded in determining the structure of the mosaic phase by analyzing the Pb occupancy as a variable. In addition, no noticeable changes in the rocking curves were observed at low (T = 13 K) and room temperatures. This suggests that the phase transition in this structure is caused by soft phonons [5].

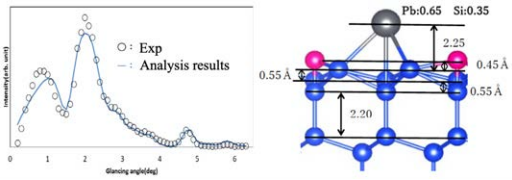

Fig. 2: Structure analysis results of mosaic phase of Pb/Si(111).

References

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