STRUCTURAL STUDY OF Si/Ge/Si(001) CRYSTAL BY A HOLOGRAPHIC METHOD USING X-RAY DIFFRACTION

Holography is a well-known technique to directly reconstruct an image of objects. In this technique, a detecting plate called a hologram is first created by using an interference effect between two waves: one is a reference wave coming directly from a light source to the detecting plate, while another is an object wave coming after once scattered by objects. In the second step, one can reconstruct the objects by illuminating the reference wave on the hologram. In the present work, we show a similar holographic method to reconstruct images of surface and interface atoms with an atomic resolution. Here we treat two-dimensionally ordered atoms on a substrate crystal. Hitherto similar attempts have been made as to two-dimensional structures projected on the surface [1]. In this work, however, we show the first experimental results of three-dimensional reconstructed images of surface atoms.

To analyze the structure of surface atoms on crystals, we usually measure integrated intensities for a number of diffraction spots. Then we compare the observed intensities with those calculated for possible models until we find a good model that attains a good agreement between those two intensities. In the present work, however, we could directly determine the structure of surface atoms from experimentally obtained intensities.

Figure 1 illustrates the principle of the present method. In this case the diffraction amplitude is divide dn two; one is a contribution from a surface layer to be determined, and the other is a contribution from a substrate crystal given by the sum of amplitudes from semi-infinite layers. In most cases one knows the structure of the substrate crystal, and can calculate the phase and modulus of the amplitude by crystal-truncation-rod scattering [2] based on the kinematical theory of X-ray diffraction. Thus we can regard the wave scattered from the substrate crystal as a reference wave. In this situation, we can reconstruct unknown surface atoms by a Fourier transform after proper normalization of the experimental data instead of illuminating a reference wave as in optical holography.

Figure 2 shows images of Ge atoms on Si(001) substrate crystal reconstructed from observed intensities. Here we used a sample in which a monolayer of Ge atoms are epitaxially grown on a clean Si(001) surface at 775 K. A few nanometers of an amorphous Si layer was further deposited on the sample at 295 K to withstand in the atmosphere. To reconstruct the images, we have obtained intensities about at 250 points, most of which are measured at points on the rod close to Bragg points.

Figure 3 shows a schematic illustration of the interface. Figure 2 corresponds to the hatched areas in Fig. 3. The result clearly shows that Ge atoms locate positions that Si atoms would

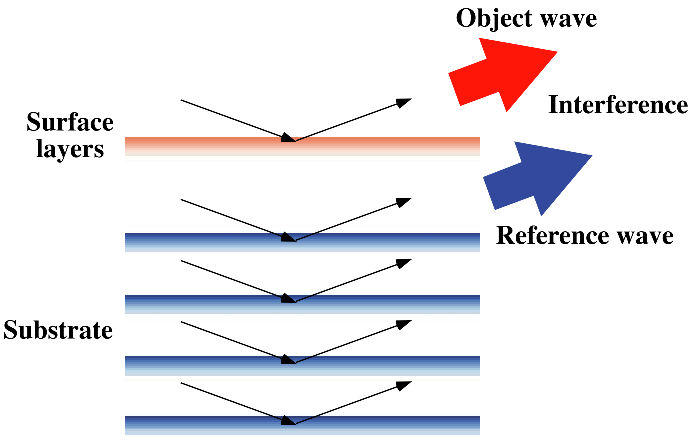

Fig. 1. Principle of the present method to reconstruct images of surface atoms using an interference effect.

otherwise occupy. The position of Ge atoms is slightly relaxed toward the surface, reflecting the difference in bond lengths between Ge and Si in crystals.

In regard to structural analysis of surfaces and interfaces, constructing an initial model is a most intricate task. However, once the initial structure is directly obtained from experimental data, one could easily refine the structure, with for instance, the use of conventional fitting procedures.

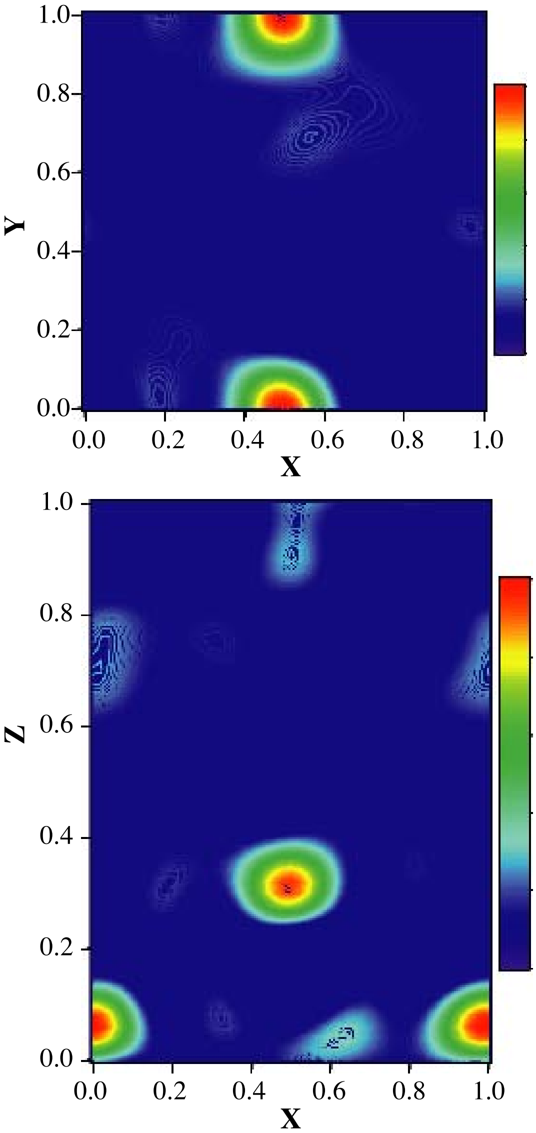

Fig. 2. Contour maps of Ge atoms on Si(001) substrate crystal at planes parallel (upper) and perpendicular (lower) to the surface. Rectangular regions correspond to the hatched areas in Fig. 3.

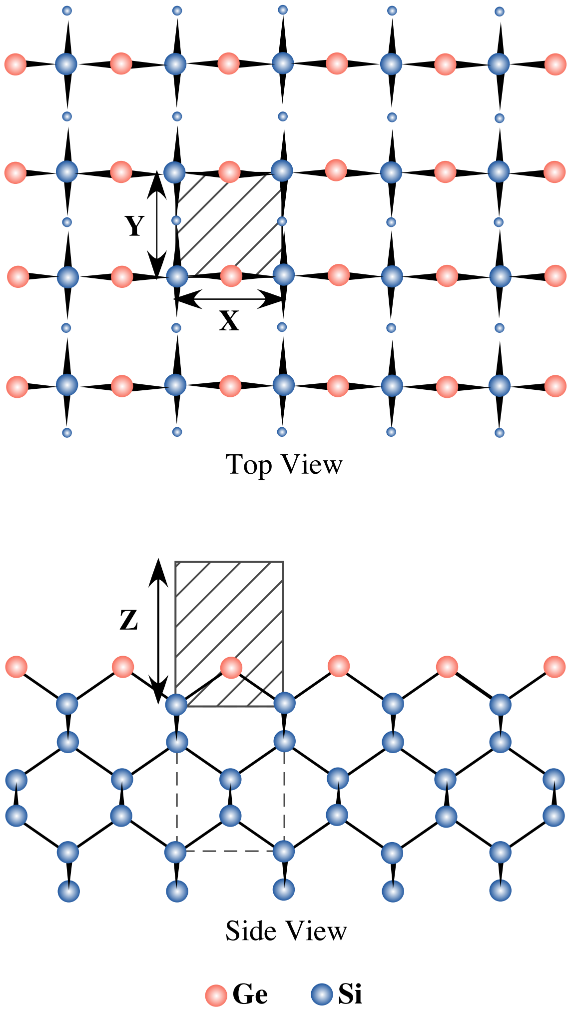

Fig. 3. Schematic illustration of reconstructed Ge atoms with respect to the Si(001) substrate crystal.

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