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Structural Analysis of Bismuth Nanowire by X-ray Standing Wave Method

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1. Introduction

Atomically perfect nanowire with bismuth atoms has attracted much interest in recent years [1-5]. The Bi wire was found to be qualitatively different from other atomic wires that are formed by many group-III and -V elements at the initial stage of epitaxial growth on Si (001) [6] because the Bi wire has some characteristic features (free of kinks or defects, a narrow width of 1nm is kept for several hundreds of nm, the wires appear to be embedded within the surface).

The Bi wire is made in a selective desorption process of Bi from the Si(001) surface [1]. Since the formation of the perfect atomic wire is a self-assembling process in the Si(001) surface, this system might play a role of template in the pursuit of fabrication techniques for electronic nanodevices. The formation mechanism itself is also an important part of interest from scientific viewpoint, because a precursor surface of Bi monolayer is well known with specific superstructures [7].

STM analysis recently revealed some electronic and structural characteristics of the Bi wire [1-3], while the relative atomic arrangement around Bi atoms was reported on the x-ray photoelectron diffraction (XPD) result [4]. However, detailed structure with atomic coordinates is still not clear. A main part of difficulty of the analysis is the fact that the Bi wires lie into the Si(001) surface.

X-ray standing wave (XSW) method, which is powerful to structural analysis of small amount of dopant at surface or interface [8], is suitable for this perfect, dilute, and embedded system. In this paper, we present a structural analysis of the Bi nanowire by the XSW method where the three-dimensional site of Bi atoms has been estimated relative to the Si bulk crystal. We propose a new model of atomic structure of the nanowire.

2. Experiments

A vicinal Si(001) wafer (4 degrees from the surface normal toward the [110] direction) was used to produce a single domain of Bi lines. After STM observation of the perfect lines, the surface was capped with amorphous Si of 20 monolayers thick by electron beam deposition at room temperature, to provide for an open-air condition in synchrotron radiation (SR) facilities.

The XSW method is based on to excite selectively a specific element and to control the x-ray wave field intensity in the substrate crystal under diffracting condition. Since the spatial controllability of the wave field is precise in about 0.001 nm, atomic site information of the element can be derived from an angular dependence of the fluorescence yield. The analysis gives an average absolute atomic site of Bi with respect to the substrate Si lattice plane.

The experiments were carried out at the undulator station (BL09XU) of the SPring-8 and the vertical wiggler station (BL14B) of the Photon Factory (PF) at KEK. The incident photon energy was kept at 16.5 KeV for Bi L-excitation. The L α fluorescence yield spectra from the Bi atoms were obtained using a solid state detector (SSD). The XSW yield profile was taken for both the Si 004 and Si 115 reflections by scanning angle of the Si crystal in the vicinity of the Bragg reflection. At each angular step, a reflected x-ray intensity and Bi L α fluorescence yield were recorded.

3. Results and Discussions

Fig.1 illustrates the measured 004 and 115 reflectivities (filled circles) and the corresponding Bi L α normalized fluorescence yields (open circles).

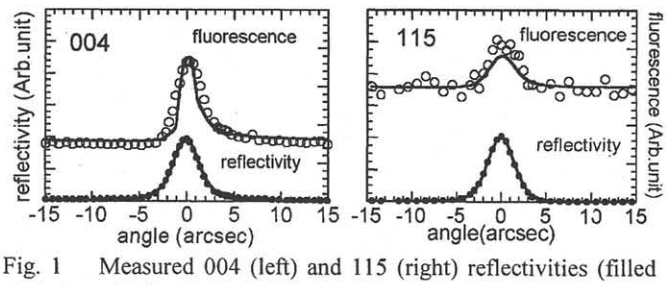

Fig. 1 Measured 004 (left) and 115 (right) reflectivities (filled circles) and the corresponding Bi L α normalized fluorescence yields (open circles). The solid lines are best fits to the data.

The solid lines are the best fits calculated using dynamical diffraction theory. For each reflection, XSW results are represented by two independent fitting parameters: the average atomic position d_{hkl} and the

coherent fraction Fc. dhkl is referred to the phase of x-ray standing wave, which has same periodicity as the (hkl) diffracting net planes. The coherent fraction Fc represents the spread of distribution of the atoms around the coherent position for selectively excited element.

dhkl and Fc for the 004 scan were d_{004} =0.26±0.04 Å, F_{004}=0.59±0.18, respectively. Then, the measured Bi height from the Si(004) bulklike atomic plane is 0.26 ±0.04Å with about 60% of coherence of the position. Considering that the Bi atoms are in a horizontal (parallel to the (004)) plane with the fixed d_{004} height, the measured d_{115} value is transformed to d_{110} within a horizontal plane by use of geometrical projection.

dhkl and Fc for the [110] axis were d_{110}=0.0±0.5Å, F_{110}=0.5±0.1, respectively. The larger error in the [110] results is attributed to the small yield of fluorescence for the 115 scan depending on the experimental condition. Though, the χ^2 fitting results denoted that the Bi atoms exist closed to the first Si(004) layer (i.e. in the Si-dimers layer), not in the second layer. Bi is difficult to be in the third or deeper layer because of a large atomic radius and the small relaxation around the Bi wires in STM images.

Fig.2 shows a proposed model of the wire structure and the Bi position that is allowed by the XSW results. The hutched area (top view) and the solid lines (side view) correspond to the allowed Bi atomic position.

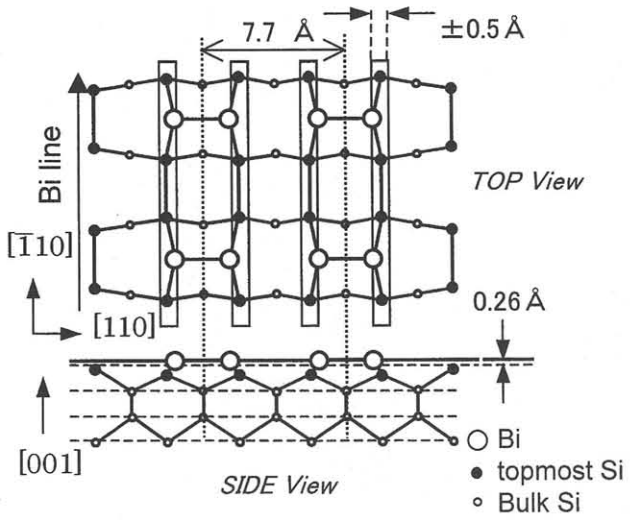

Fig.2 Derived Bi wire model and the Bi position that is allowed by the XSW analysis. The marked values (±0.5Å and 0.26Å) on atomic coordinates are results of the XSW analysis.

Considering other physical information on atomic bond and atomic valence number (2.89Å for Bi-Bi bond and 2.73-2.78Å for Bi-Si bond [5]), the model that satisfies most characteristics in other reports is as shown in Fig.2. Large open circles are Bi atoms, filled circles are Si-dimer atoms, and small open circles are other Si atoms in lower layers. Vertical dotted lines represent the bright twin peaks (7.7 Å apart) in the STM image [1-3]. There still remains a serious disagreement with the XPD result for the Bi-dimer bond direction [4]. It might be attributed only to an influence of the capping layers of amorphous Si, while a weak interaction between the Bi wires and the capping Si atoms was suggested in other report [9]. Our result implies a stronger effect of the capping layers than expected.

4. Conclusions

We analyzed the three-dimensional Bi atomic site inside the Bi nanowire within the Si (001) surface, using the XSW method. The Bi atomic site was estimated with respect to the Si substrate lattice, and a new model was proposed for structure of the Bi wire. From viewpoint of device fabrication, the analysis of one-dimensional system in a buried interface will play an important role with an availability of the XSW method. Particularly, the study of low dimensional systems needs highly brilliant x-rays of SR because of low signal rate from a small amount of dopant atoms.

Acknowledgments

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