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X-ray Diffraction from Buried Bi atomic wire formed on Si(001) — near the Bi LⅢ Absorption Edge

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X-ray diffraction measurement (the 'X-ray obvious-at-a-glance analysis') of Bi atomic wire after burial in an epitaxial Si layer was performed near the Bi LⅢ absorption edge; X-ray diffraction patterns from buried one-dimensional structure were obtained, and their intensities changed drastically near the absorption edge. This gives evidence that the buried one-dimensional structure contains Bi atoms.

Key words: X-ray diffraction, atomic wire, silicon, bismuth, anomalous dispersion

1. INTRODUCTION

Recently many efforts have been made to discover and develop non-lithographic bottom-up techniques for nanometer-scale devices and interconnections. Miki *et al.* have reported that Bi atomic wires 1.5 nm wide and up to several hundred nanometers long are formed on Si(001) surface when a Bi-covered Si(001) surface is annealed at around 590℃ [1]. In a previous paper [3] we showed by the X-ray diffraction (the 'X-ray obvious-at-a-glance analysis' method, which is a rapid method for evaluation of surface and interface structures [2]) that the one-dimensional structure remains even after burial in an epitaxial Si layer. In this paper results of X-ray diffraction measurements of the buried one-dimensional structure near the Bi LⅢ absorption edge (13.426 keV) are shown; drastic change in the X-ray diffraction intensity was observed near the absorption edge. This gives evidence that the buried one-dimensional structure contains Bi atoms.

2. EXPERIMENT

The sample was prepared in the same manner as described in the previous paper [3]. The X-ray diffraction measurement was performed in air at the undulator beamline BL13XU, SPring-8 [4]. The experimental geometry is shown schematically in the upper figure of Fig. 1 (a). An optical system was used, including a pair of slits to limit the beam size to 0.1 mm × 0.1 mm, a sample, a direct-beam stopper, and a flat X-ray imaging-plate (IP) detector with a pixel size of 50 μm × 50 μm to record diffraction. The distance of the sample to the imaging-plate detector was 235 mm. X-ray beams with photon energies around the Bi L Ⅲ absorption edge (13.42 keV) were incident on the sample at an angle of 0.21°.

3. RESULTS AND DISCUSSION

We recorded X-ray patterns diffracted from the samples at some azimuth angles ϕ around the surface normal. We define $\phi = 0°$ as the incident X-ray beam is parallel to the [110] direction, which corresponds to the $[100]_S$ direction if two primitive lattice vectors are taken to be parallel to the surface. A one-dimensional structure gives rise to sheets perpendicular to itself after diffraction; these are imaged as segmented streaks because of the intersection of the sheets with the Ewald sphere. The lower figure of Fig. 1 (a) shows an example of X-ray diffraction pattern experimentally obtained at $\phi = -1.5°$; streaks from the diffraction sheets appeared, which is evidence that a 1D structure remained in the sample even after burial in the epitaxial Si layer [3]. The three streaks indicated by arrows the figure correspond to diffraction sheets of $k = -1/2$, $k = 0$, and $k = 1/2$, where we use standard notation of $h\ k\ l$ to indicate a point in reciprocal space that is defined by the surface unit cell. This shows that the buried 1D structure has a superstructure along the wire, the periodicity of which is two times as large as the length of the primitive vector of the Si(001) surface [3].

Figures 1 (b) and (c) show dependence of X-ray diffraction intensity along zeroth-order and the fractional-order streaks on X-ray energy around the absorption edge of Bi LⅢ. Here we binned the image over 50 pixels in the vertical direction (parallel to the streaks) to discriminate background clearly, and then obtained the intensities by subtracting the background and integrating the signal in the horizontal direction. In Fig. 1 (c), results at $\phi = -1.5°$ (an asymmetric case) are shown since the fractional order streak was more clearly discriminated from the background at $\phi = -1.5°$ than $\phi = 0°$. In the case of the zeroth-order

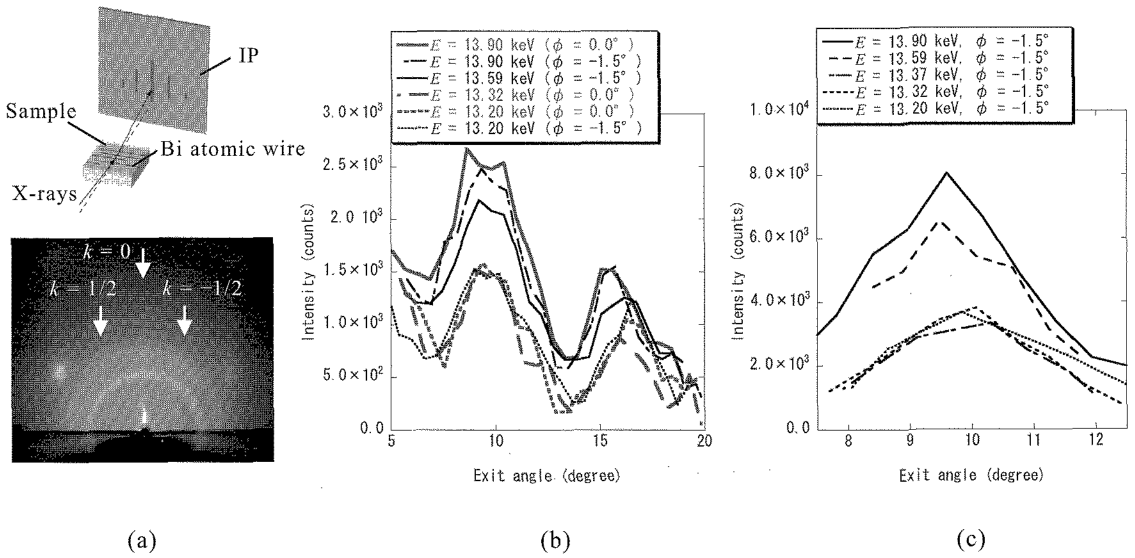

Fig. 1 (a) Upper figure: schematic diagram of experimental geometry at the azimuth angle ϕ = 0°; lower figure: X-ray diffraction patterns from the Si epilayer cap/Bi wires/Si(001) substrate sample at ϕ = −1.5°. (b) Dependence of intensity along the k = 0 streak on the X-ray energy. (c) Dependence of intensity along the k = 1/2 streak on the X-ray energy.

streak, the background could be subtracted at both ϕ = −1.5° and ϕ = 0°. As seen in the figures, the intensities of the streaks changed drastically around the absorption edge. These results give evidence that buried one-dimensional superstructure contains Bi atoms.

It has been reported that the structure of the Bi atomic wire on a clean Si surface (before burial) comprises a double core of seven-membered rings of silicon, and has a superstructure with the same two-by periodicity along the wire as that of the buried one-dimensional structure presented here [5]. If an epitaxial Si layer is grown on it and the structure before burial is not destroyed, a large 'tunnel' with many dangling bonds should be introduced. Recently it has been reported that, from both of tight binding and density functional theory (DFT), there is a more energetically favorable structure for the buried one-dimensional wire, which contains Bi dimers along the wire [3]. The results presented here support the proposed structure model.

The intensities in Figs. 1 (b) and (c) seem to show a step-like change near the absorption edge. From a rough calculation (using a finite number of atoms) of the intensity for the energetically favorable structure, it was shown that the step-like change is attributed to the imaginary part of the atomic scattering factor of Bi atom rather than the real part. The intensities in the figures are higher on the high-energy side of the absorption edge than that on the low-energy side. This was also reproduced by the rough calculation, although the difference of the intensity is somewhat smaller than the results of the experiment. Higher precision measurement with a higher energy resolution around the absorption edge will allow us not only more quantitative analysis of long-range order structure but local structure analysis around the Bi atoms forming the one-dimensional structure using the diffraction anomalous fine structure (DAFS) technique.

4. SUMMARY

X-ray diffraction measurement (the 'X-ray obvious-at-a-glance analysis') of Bi atomic wires after burial in an epitaxial Si layer was performed near the Bi LⅢ absorption edge. Streak patterns from a buried one-dimensional superstructure with two-by periodicity along the wire were observed. From dependence of the intensity along the zeroth-order and fractional-order streaks on the X-ray energy near the absorption edge, it was shown that the buried one-dimensional superstructure contains Bi atoms.

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