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X-ray Diffraction of Bismuth nanoparticles

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Introduction

Bismuth atoms are covalently bonded and form layer structure in rhombohedral Bi. Raman scattering and transmission-electron microscopy (TEM) studies show that Bi nanoparticles dispersed in thin films exhibit a transformation from nanocrystalline rhombohedral structures to smaller amorphous particles at a thickness of 0.8 nm with decreasing size [1].

Amorphization is a key issue of the phase transition, but it has not been confirmed by methods of TEM and so on. In the present study we report results of x-ray diffraction (XRD) to confirm the existence of the amorphous phase in the Bi nanoparticles.

Experimental

Bi layers (0.5 nm) and NaCl layers (11 nm) were deposited alternately onto a water-cooled alumina substrate from an alumina crucible. The Bi nanoparticles are isolated and dispersed within the NaCl matrix. The sample encapsulated in the capillary was annealed at 300 °C for a hour.

The XRD patterns were measured with synchrotron radiation at the BL-1B in the Photon Factory of High Energy Accelerator Research Organization KEK-PF. The X-ray energy used for the XRD measurements was 12.40keV. The XRD measurements of the as-deposited and the annealed samples were carried out at room temperature. Powder4 was used to estimate backgrounds of the XRD profiles [2].

Result and Discussion

Intensities are normalized by integrated intensities of NaCl (200) peaks which do not overlap with any other peaks. Almost peaks are assigned to the rhombohedral Bi and the cubic NaCl with few exceptions in the annealed sample. Background region of the annealed sample is magnified in Figure 1. Few broad peaks are observed around 2 and 3 Å-1 in the background profile.

If there are amorphous nanoparticles, they must contribute to the x-ray scattering. The background of the as-deposited sample consists of the diffractions from the amorphous nanoparticles and the glass of capillary, whereas that of the annealed sample consists only of diffraction from the glass of capillary. So the difference is due to the diffraction of the amorphous nanoparticles.

In order to estimate structure factor of the amorphous nanoparticles the difference is divided by atomic scattering factor of Bi [3]. Figure 2 shows the structure factor deduced roughly from the difference. The structure factor has peaks around 2 and 3 Å-1. The 20~30-nm-thick

films deposited onto the substrate at 4.2 K are amorphous, which structure factor has peaks at 2.1, 3.1 Å-1 and so on [4]. The profile of the amorphous nanoparticles has same feature of that of the $20 \sim 30$ -nm-thick films. The dip around 3 Å-1 may be come from the analytical or the experimental problem, that is, there are strong peaks of NaCl. Absolute values of the curves are not accurate at this stage, since the peaks overlap with those of the crystalline NaCl. The structure factor of the nanoparticles implies that the Bi nanoparticles contain the amorphous phase. The amorphous phase is stable up to the room temperature, whereas the 20 ~ 30-nm-thick films crystallize at 20 K.

References

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Fig.1: The raw and background data are shown in red and blue lines, respectively.



Fig.2: The structure factor of the amorphous nanoparticles.