27A/2010G658

Surface chemical states of $FeSi_2$ and Mg_2Si crystals studied by XPS and XAS

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Introduction

Semi-conducting silicides are extensively investigated for using as silicon-based electronic devices. Among silicides, β-$FeSi_2$ and Mg_2Si are candidates as high performance thermo-electronic devices. Recently, large crystalline β-$FeSi_2$ and Mg_2Si have been synthesized [1,2]. Since then, it is expected to use crystalline β-$FeSi_2$ and Mg_2Si as the substrate for homoepitaxial growth of films. In order to fabricate homoepitaxial films with excellent quality, well-controlled surface of the substrate as well as optimized growth conditions are necessary.

In the present study, a combination of X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) is applied to clarify surface chemical states of β-$FeSi_2$, and Mg_2Si crystals.

Experimental

The β-$FeSi_2$ and Mg_2Si crystals with several millimeters in width were used in this work. The fabrication procedures were described in previous papers [1,2].

The XPS and XAS measurements were performed at the beam line 27A [3]. In the XPS measurement, excitation X-ray energies were set at 2700, 3000 and 3300 eV. The Si K-edge XAS spectra were obtained using total electron and partial electron yield (TEY and PEY) modes.

Results and Discussion

The XPS measurement showed the formation of SiO_2 in the β-$FeSi_2$ and that of SiO_2 and MgO in the Mg_2Si crystals. With decreasing excitation X-ray energy, the peak area ratio of oxide to silicide increased significantly. This implies that these oxide layers were formed on the surface of the β-$FeSi_2$ and Mg_2Si crystals.

Figure 1 shows the Si K-edge XAS spectra of the β-$FeSi_2$ crystal measured with TEY and PEY modes. The spectrum obtained with the TEY mode is in good agreement with that shown in a previous paper [3]. The peaks at about 1845 and 1848 are assigned to SiO and SiO_2, respectively. No significant changes were observed in the spectrum obtained with the PEY mode.

The Si K-edge XAS spectra of the Mg_2Si crystal were shown in Fig. 2. Four peaks at 1841 and 1843, 1845 and 1848 eV are observed in the spectrum obtained with the TEY mode. In the spectrum obtained with the PEY mode, a dominant peak assigned to SiO was observed. This is presumably due to the formation of SiO on the top of the surface of the Mg_2Si crystal. The formation of SiO on the Mg_2Si crystal was not observed in the Si 1s XPS spectra, which would be due to the lack of surface sensitivity.

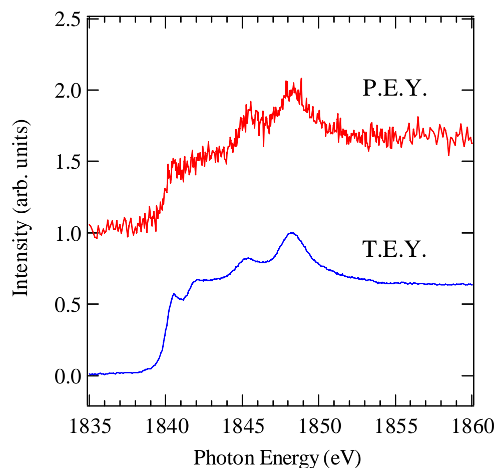

Fig.1. Si K-edge XAS spectra of a β-$FeSi_2$ crystal measured with PEY and TEY modes.

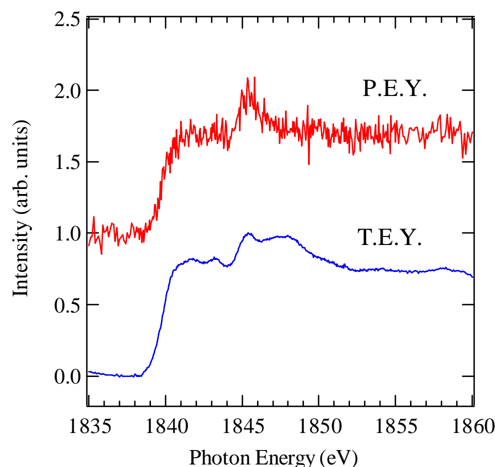

Fig.2. Si K-edge XAS spectra of a Mg_2Si crystal measured with PEY and TEY modes.

References

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