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Homoepitaxial film on β-$FeSi_2$ single crystal 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-$FeSi_2$ having a band gap of 0.85 eV is a candidate as a promising semiconductor. Recently, large single crystalline β-$FeSi_2$ has synthesized by solution growth using Ga solvent [1]. Since then, it is expected to use crystalline β-$FeSi_2$ as a substrate for homoepitaxial growth of β-$FeSi_2$ 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 a β-$FeSi_2$ single crystal and a homoepitaxial β-$FeSi_2$ film.

Experimental

The β-$FeSi_2$ single crystals with several millimeters in width were synthesized with the temperature-gradient solution method using Ga-solvent. The single crystals were annealed at 900°C in ultra high vacuum to remove native oxide layers. Homoepitaxial films were then grown on the crystals at a substrate temperature of 700°C by molecular beam epitaxy.

The XPS and XAS measurements were performed at beam lines 13C and 27A [2]. The Si 2p XPS spectra were measured at the beam line 13C. In the XPS measurement, excitation X-ray energies were set at 389, 650 and 970 eV. The Si K-edge XAS spectra were obtained at the beam line 27A.

Results and Discussion

Figure 1 shows the Si 2p XPS spectra of the β-$FeSi_2$ single crystal and the homoepitaxial film. The spectra were measured with the excitation X-ray energies ranging from 389 to 970 eV to perform depth profiling. Four peaks are observed in all spectra. The peaks at about 103 and 101 eV assigned to SiO_2 and SiO_{2-X} increase with decreasing excitation energy. The two peaks at lower binding energies correspond to the Si $2p_{3/2}$ and $2p_{1/2}$ peaks of $FeSi_2$. The simulation of the surface oxide layers suggests that the thicknesses are estimated to be 1.0 nm and 0.8 nm for the single crystal and the homoepitaxial film, respectively.

Figure 2 shows the Si K-edge XAS spectra of the β-$FeSi_2$ single crystal and the homoepitaxial film. Four peaks at 1839.4 and 1840.8, 1844.3 and 1847.1 eV are observed in these spectra. The spectrum of the homoepitaxial film is similar to that of the single crystal, meaning that a homogeneous β-$FeSi_2$ film can be obtained in this condition. However, slight increases of the peaks at 1840.8 and 1844.3 eV in the spectrum of the homoepitaxial film suggest the presence of other chemical states such as FeSi. This would be due to the inappropriate substrate temperature during epitaxial growth. Therefore, further studies on optimized substrate temperature are necessary to obtain homoepitaxial films with single phase.

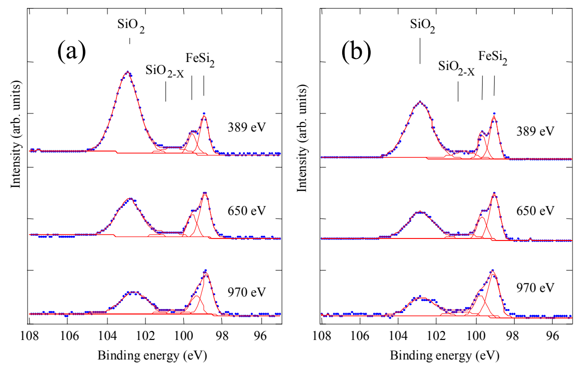

Fig.1. Si 2p XPS spectra of (a) a β-$FeSi_2$ single crystal and (b) a homoepitaxial film measured with the excitation energies ranging from 389 to 970 eV.

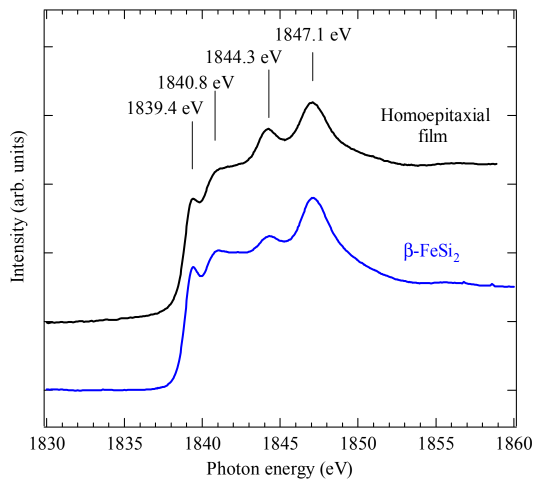

Fig.2. Si K-edge XAS spectra of a β-$FeSi_2$ single crystal and a homoepitaxial film.

References

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