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Non-destructive depth profiling for the surface of β-$FeSi_2$ thin films 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. We have used an ion-beam sputtering deposition (IBSD) method for fabrication of β-$FeSi_2$ films, obtaining highly-oriented β-$FeSi_2$ films [1]. In order to optimize the deposition condition, the knowledge of surface chemical states of fabricated films is considerably important.

In the present study, a combination of XPS and XAS is applied to clarify surface chemical states of the β-$FeSi_2$ films fabricated by the IBSD method. The differences in the chemical states of the films fabricated at substrate temperatures of 873, 973 and 1173 K are investigated.

Experimental

The iron silicide films were deposited on Si(100) substrates by the IBSD method. The substrate temperatures were kept at 873, 973 and 1173 K during deposition.

The XPS and XAS measurements were performed at beam lines 13C and 27A. The Si 2p XPS and Fe L-edge XAS spectra were measured at the beam line 13C. In the XPS measurement, excitation X-ray energies were set at 254, 389, 505, 650, 775 and 970 eV. The Fe L-edge XAS spectra were obtained by dividing the signals from the samples recorded on a channeltron in the total-electron-yield mode. 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 β-$FeSi_2$ films fabricated at substrate temperatures of 973 K. The spectra were measured with the excitation X-ray energy ranging from 254 to 970 eV to perform depth profiling. Four peaks are observed in all spectra. The peaks at about 103 and 101 eV are assigned to SiO_2 and SiO_{2-X}, respectively. The two peaks at lower binding energies correspond to the Si $2p_{3/2}$ and $2p_{1/2}$ peaks of $FeSi_2$ and/or Si. A simulation of surface oxide layers suggests that the formation of SiO_2 at the upper layer and SiO_{2-X} at the lower layer of surface oxides.

Figure 2 shows the Fe L-edge XPS spectra of the β-$FeSi_2$ films fabricated at substrate temperatures of 873, 973 and 1173 K, respectively. Two peaks at 707.3 and 708.3 eV are observed in the spectra of the samples fabricated at 873 and 973 K. The peak at 708.3 eV is assigned to β-$FeSi_2$ [2]. This peak is shifted to higher energy in the spectrum of the samples fabricated at 1173 K The shift to higher energy suggests the formation of metallic α-$FeSi_2$, which gives a peak at 709.3 eV [2]. The relative intensity of the peak at 707.3 eV in the spectrum of the sample fabricated at 873 K is slightly larger than that at 973 K. This peak is probably due to the decomposition of the $FeSi_2$ structure by preferential oxidation of Si. The spectrum of the sample fabricated at 1173 K has a peak with lower energy. At higher temperature over 1173 K, $FeSi_2$ allows the formation of α and ε phases. Therefore, this peak can be attributed to the ε phase, i.e., an FeSi structure. These results indicate that the combination of XPS and XAS is a powerful tool to elucidate the surface chemical states of thin films.

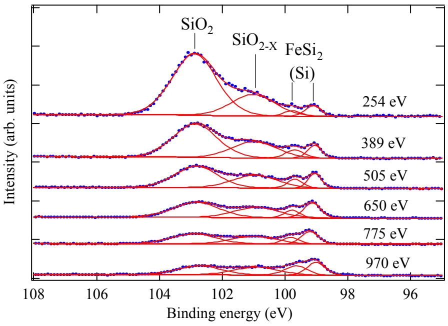

Fig.1 The Si 2p XPS spectra of the β-$FeSi_2$ film fabricated at 973 K.

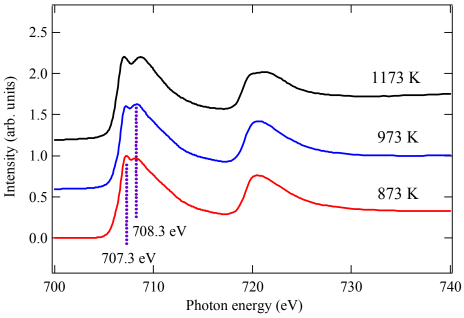

Fig.2 The Fe L-edge XAS spectra of the β-$FeSi_2$ films fabricated at 873, 973 and 1173 K, respectively.

References

[1] H. Yamamoto *et al.*, *Thin Solid Films* **461**, 99 (2004).
[2] F. Sirotti *et al., Phys. Rev.* **B 48**, 8299 (1993).

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