Formation process of β-$FeSi_2$ on Si (111) substrate studied by means of SR-XPS

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Introduction

Recently, semiconducting iron silicide, β-$FeSi_2$ has attracted lots of attention because of its direct band gap of 0.85 eV [1]. From this reason, formation processes of β-$FeSi_2$ on Si substrates have widely been investigated. However, the reaction mechanisms between Fe and Si are not yet clearly understood.

In the present study, we study the formation mechanisms of β-$FeSi_2$ on Si (111) surface during solid-phase epitaxy (SPE) process by means of XPS using synchrotron radiation (SR-XPS).

Experimental

All the experiments were done at the beam-line 13C of the Photon Factory. The XPS spectra were recorded with a hemispherical electron analyzer (PHI 1600C).

The substrate used was a Si wafer oriented with [111] direction. Fe was deposited with a thickness of 1.0 nm at room temperature. After the Fe deposition, the substrate was stepwise annealed for 15 min at 523 K, 723 K, and 973 K.

Results and discussion

Figure 1 shows changes in the Fe/Si atomic ratios with the annealing temperature as a function of excitation energies. The atomic ratios were calculated from the peak intensities and photo-ionization cross-sections of Fe 3p and Si 2p spectra. After Fe deposition at room temperature (a), the Fe/Si ratio is rapidly increased with decreasing the excitation energy. This indicates the formation of a thin Fe layer on Si (111). With rising annealing temperature, the Fe/Si ratios become small indicating the compositional changes by the annealing.

To investigate the Fe/Si depth distribution in detail, two sets of simulation were performed. In the model 1, a Fe over-layer with a thickness of t homogeneously covers the Si surface. In the model 2, an over-layer with a thickness of t and a Fe/(Fe+Si) atomic ratio of a_0 homogeneously covers another layer with a Fe/(Fe+Si) atomic ratio of a_1. The Fe/Si atomic ratio at each excitation energy (hν) can be given by the following equations:

$$\left[\frac{Fe}{Si}\right]_{h\nu} = \frac{\int_0^{\infty} \exp(-z/\lambda_{Fe}\sin\theta)dz}{\int_0^{\infty} \exp(-z/\lambda_{Fe}\sin\theta)\exp(-(z-t)/\lambda_{Si}\sin\theta)dz} \quad \text{(Model 1)}$$

$$\left[\frac{Fe}{Si}\right]_{h\nu} = \frac{\int_0^{t} a_0 \exp(-z/\lambda_{Fe}\sin\theta)dz + \int_t^{\infty} a_1 \exp(-z/\lambda_{Fe}\sin\theta)dz}{\int_0^{t}(1-a_0)\exp(-z/\lambda_{Si}\sin\theta)dz + \int_t^{\infty}(1-a_1)\exp(-z/\lambda_{Si}\sin\theta)dz} \quad \text{(Model 2)}$$

The details of simulation are described elsewhere [2].

The experimentally obtained profile for the smple before annealing is well fitted by a simulated profile using the Model 1 with t = *1.07 nm*. On the other hand, the profile of the sample after annealing at 523 K was fitted by simulation using Model 2 and a_0 = *0.9*, a_1 = *0.1* and t = *0.34 nm*. This result indicates that the substrate surface is covered by a thin Fe-rich layer and that Si diffused into the Fe layer.

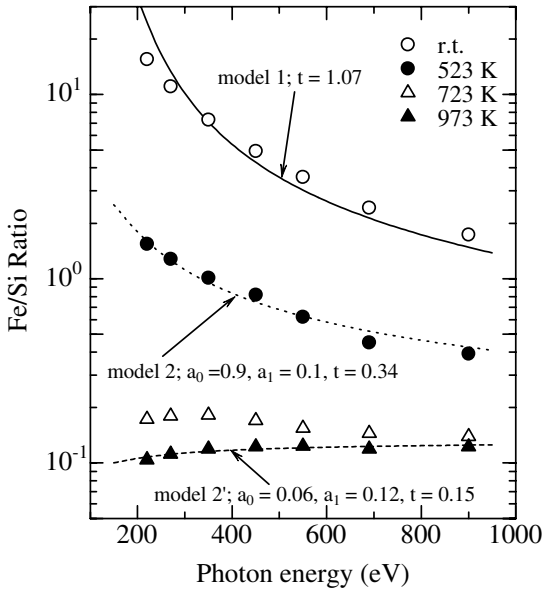

Fig. 1 Changes in the Fe, Si atomic ratios during SPE process recorded with different excitation energies

After annealing at 723 K, the Fe/Si atomic ratios become almost independent of the excitation energies. This indicates the chemical composition is even from the surface to the largest analysis depth. The results of Fe 2p and valence-band spectra suggest the formation of β-$FeSi_2$. However, the obtained Fe/Si atomic ratio, *0.2* is relatively small compared with the stoichiometric atomic ratio of β-$FeSi_2$ *(0.33)*. This may be attributed to the aggregation of β-$FeSi_2$ on the surface.

After annealing at 973 K, the simulated profile using a parameter set of a_0 = *0.06*, a_1 = *0.12* and t = *0.15 nm* can be compared with the experimental data. This result clearly suggest the formation of thin Si layer at topmost of the surface.

References

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