Investigation on the β -$FeSi_2$ formation mechanisms on Si (111) substrate by means of SR-XPS

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Introduction

Semiconducting iron silicide, β-$FeSi_2$ has recently attracted lots of interests because of its small direct band gap of 0.85 eV [1]. For the understanding of iron silicide formation mechanisms, it is essential to investigate the compositional variations during silicide formation process because the control of iron diffusion in silicon is a key factor in this process.

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 photoelectron take-off angle was 54.7° relative to the surface normal. The substrate used was Si wafer oriented [111] direction. The Fe was deposited 20 Å at room temperature. After the Fe deposition, the substrate was stepwise annealed to 473 K, 673 K, and 973 K for 15 minutes.

Results and discussion

Figure 1 shows changes in the Fe and Si atomic ratios during SPE process recorded with different excitation energies as a function of annealing temperature. The atomic ratios were calculated from the peak intensities and photo-ionization cross-sections of Fe 3p and Si 2p spectra. After the Fe deposition at room temperature, the atomic ratio of Fe rapidly increases with decreasing the excitation energy. With rising annealing temperature, the atomic ratios of Fe were gradually decreased. From these results, it is speculated that the surface Fe layer was formed by the Fe deposition and that the deposited Fe gradually diffused into the bulk during the subsequent annealing. These speculations were confirmed by the comparison with the simulation using inelastic mean free path (IMFP) of photoelectron inside the thin films [2].

Figure 2 shows valence band photoemission spectra recorded during SPE process. In the spectra recorded after the Fe deposition, a sharp Fermi edge is observed. However, the edge structure becomes broad by the annealing at 473 K. This change was attributed to the formation of β-$FeSi_2$ on the substrate. In the Fe 2p spectrum, a small new feature which is assigned to a plasmon loss feature due to silicide formation is observed. This change confirms the above discussion on the changes in the valence-band spectra. After annealing at 973 K, the signal from β-$FeSi_2$ can not be discriminated from the background. This may be attributed to the diffusion of Fe into Si.

The above results revealed the Fe diffusion and reaction behavior. These results provide important information on the iron silicide formation mechanisms during the SPE process.

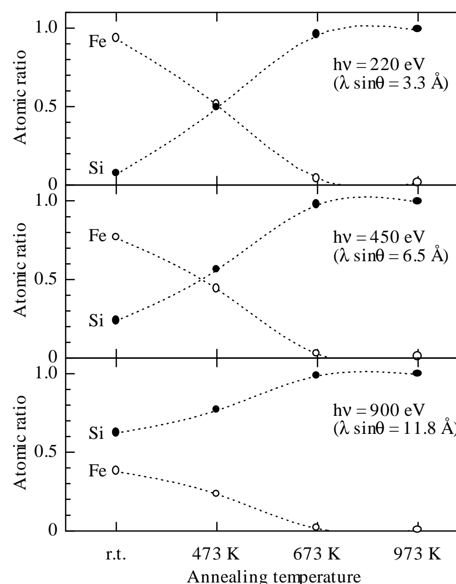

Fig. 1 Changes in the Fe, Si atomic ratios during SPE process recorded with different excitation energies.

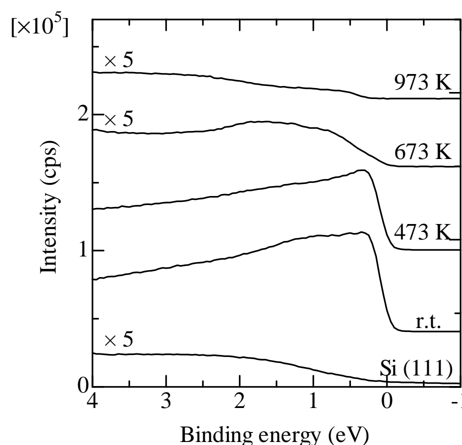

Fig. 2 Changes in the valence band photoemission spectra during SPE process.

References

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