Electronic structure of iron silicides grown on Si(001)

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Introduction

Iron silicides grown on silicon substrates have attracted much attention as a promising candidate for optoelectronic applications in Si technology [1]. Formation process of β-FeSi$_2$ and other metastable phases on Si(001) have been studied using scanning tunnelling microscopy (STM) [2,3], low-energy electron diffraction (LEED)[3], reflection high-energy electron diffraction (RHEED) [3] and valence-band photoelectron spectroscopy (PES) [4,5]. Recently, phase diagram for iron silicides grown by solid phase epitaxy (SPE) has been investigated in detail. However, relation between the electronic structure and the structure of the thin films at various coverages and annealing temperatures has not been well established. In the present work, we mainly investigated correspondence between the valence state and Si 2p core-level, and band dispersion of the valence state.

Experimental

PES measurements were performed at BL-18A of the Photon Factory at the Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK-PF). Si(001) samples (*n*-type, 1.0-10.0 Ω cm) were flashed at 1000 K for several times, and showed clean Si(001)2x1 at room temperature (RT), as confirmed by LEED. The iron (99.995%) was deposited on the clean surfaces at RT using an e-beam evaporator.

Results and discussion

Figure 1 and 2 show the photoelectron spectra of the Si 2p core level at the thickness of 0.75 ML and 1.5 ML, respectively. At 0.75 ML, peak shift towards higher binding energy side is observed after iron deposition at RT. The energy shift is continued upon annealing up to 970 K. The line shape almost recovers to that obtained just after iron deposition by annealing to 1170 K. In the valence spectra, a broad structure changes to a sharp structure with a single peak at 0.8-0.9 eV. This feature indicates that dangling bond state is recovered through silicidation process to form agglomerated islands. Therefore, it is found that valence band structure and core-level structure are closely related with each other.

In the valence band spectra at 1.5 ML, two distinct peak structures are formed at 0.60 and 2.15 eV and a weak shoulder at 3.45 eV above the annealing temperature of 570 K. To our knowledge, there appear no other previous works reporting the double peak structure in the valence state. We also observed clear band dispersion of these states. The surface structure corresponding to these states may be two-dimensionally well-ordered structure because it should have band dispersion. We could not observe any indications of the band dispersion at other experimental conditions. Possible candidate is the c(2x2) structure observed by LEED and STM [3]. In the Si 2p spectra, we observed a component at -0.55 eV, corresponding to the formation of the double peak structure. This low-binding energy component in the Si 2p state was only observed at 1.5 ML.

In order to clarify further the electronic structure of the iron silicide, we now plan to investigate the iron silicide especially with the c(2x2) structure, which is known to exhibit very flat surface and may have clear band dispersion. Flat surface should give us opportunity to use it as a template for organic molecules to realize opto-electronic devices.

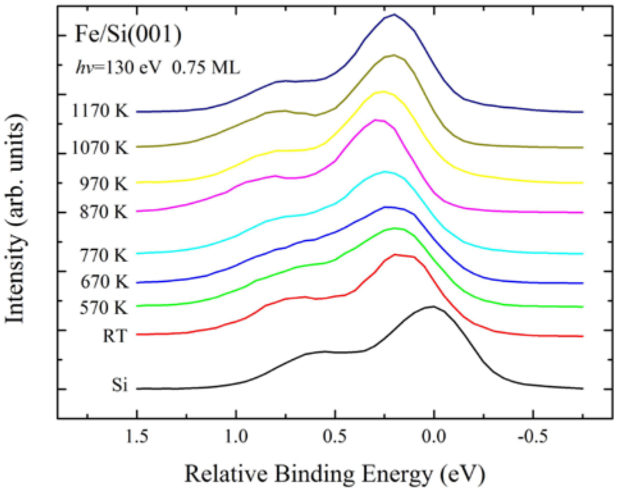

Fig. 1 Si 2p core level PES spectra of the clean Si surface Fe deposited surface at the coverage of 0.75 ML at RT, subsequently annealed to 570-1170 K. All the PES measurements were performed at RT.

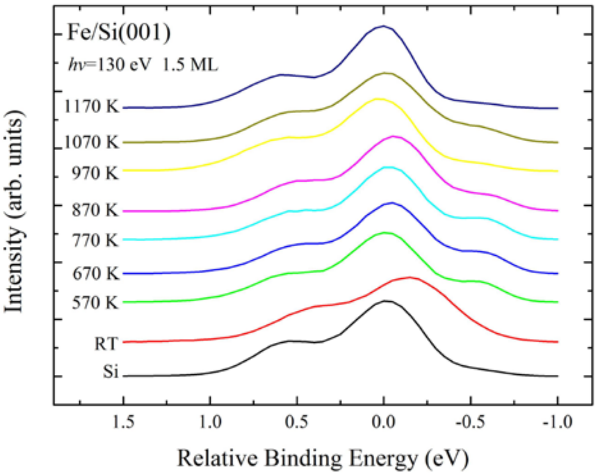

Fig. 2 Si 2p core level PES spectra of the clean Si surface Fe deposited surface at the coverage of 1.5 ML at RT, subsequently annealed to 570-1170 K. All the PES measurements were performed at RT.

References

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