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.

Experimental

Valence 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 shows the photoelectron spectra of the valence band at the thickness of 6 ML. On annealing to 570 K, two distinct peak structures appear at 0.60 and 2.15 eV and a weak shoulder at 3.45 eV. At the annealing temperature over 870 K, the peak at 2.15 eV is broadened and the shoulder at 3.45 eV is more pronounced. Figure 2 shows the photoelectron spectra of the valence band at the thickness of 9 ML. Only a broad feature is observed below the Fermi energy, consistent with the previous report [4]. At the annealing temperature of 870 K, a sharp peak appears at 0.75 eV. The peak position shifts to 0.80 eV above the annealing temperature of 1070 K.

At the coverage of 6 ML, no LEED spot was observed below the annealing temperature of 570 K [3]. The phase diagram proposed based on the STM measurements combined with LEED and RHEED shows no difference in the structure between RT and at 570 K. However, the electronic structure changes drastically by annealing even though the clear LEED spot was not observed. The line shape of the Si 2p core level slightly changes by annealing at 570 K (not shown here). Hence, weak silicidation process should occur at the interface of Ti/Si(001). The distribution of the islands formed by Fe deposition does not change significantly. The broadening of the peak at 2.15 eV over the annealing temperature of 870 K corresponds to the formation of the two-dimensional (2D) c(2x2) islands [3]. At the coverage of 9 ML, no LEED spot was observed below the annealing temperature of 670 K [3]. The valence band feature is broadened by annealing up to 770 K while no distinct peak structure was not observed in contrast to the case of 6 ML. The sharp peak observed above the annealing temperature of 870 K corresponds to the three-dimensional (3D) layered islands [3].

The present results suggest that the 2D islands and the 3D island can be well identified from the valence band features. It is reasonable that the c(2x2) structure indicative of the 2D islands produces a distinct peak at 2.15 eV at the coverage of 6 ML.

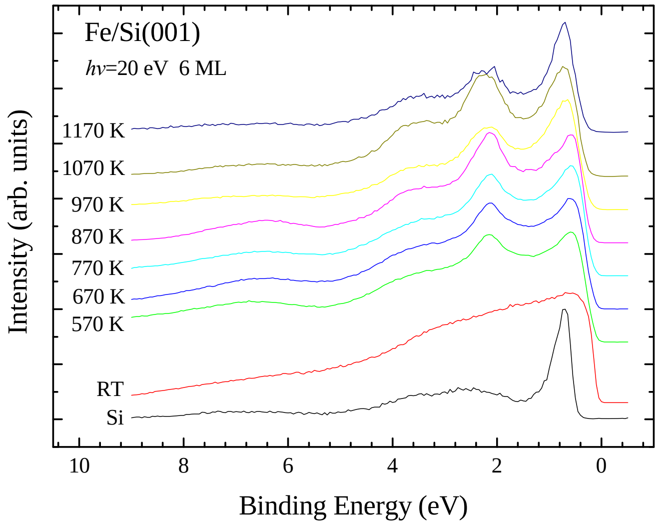

Fig. 1 Valence PES spectra of the clean Si surface and Fe deposited surface at the coverage of 6 ML at RT, subsequently annealed to 570-1170 K. All the PES measurements were performed at RT.

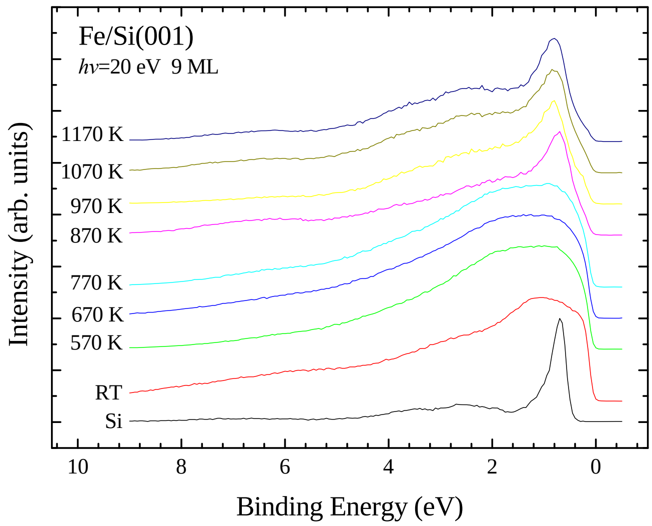

Fig. 2 Valence PES spectra of the clean Si surface and Fe deposited surface at the coverage of 9 ML at RT, subsequently annealed to 570-1170 K. All the PES measurements were performed at RT.

References

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