

Electronic structure of iron silicides grown on Si(001)

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Introduction

Iron silicides grown on silicon substrate have attracted much attention as a promising candidate for optoelectronic applications in Si technology [1]. Among various iron silicides, β -FeSi₂ is of great importance because it has a semiconducting phase with a band gap of about 0.8 eV in the energy range of optical fibre communication [2]. Recently, formation processes of β -FeSi₂ and other phases have been intensively studied using scanning tunnelling microscopy (STM) [3,4], low-energy electron diffraction (LEED) [4], reflection high-energy electron diffraction (RHEED) [4], and valence-band photoelectron spectroscopy (PES) [5,6,7,8,9].

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. STM measurements were performed at National Institute for Materials Science (NIMS) in order to investigate relation between the valence electronic states and the surface structure.

Results and discussion

Figure 1 shows an STM image of the c(2x2) structure. There are several possibilities for the structure. The STS measurements showed that a band gap ($E_g=0.9$ eV) exists indicative of semiconducting β -FeSi₂[3], while the UPS and XRD study suggested metallic α -FeSi₂[9]. In the present work, we have checked the formation of the c(2x2) structure by LEED.

Figure 2 shows a valence photoelectron spectrum of Fe deposited and subsequently annealed Si(001) surface at the thickness of 1.5 ML and the annealing temperature of 670 K. Two distinct peak structures were observed at 0.7 and 2.3 eV. Formation of the band gap clearly indicates that a semiconducting phase is formed. We have previously reported details of the annealing temperature dependence of the valence states [10] and the Si 2p core levels [11]. Based on these results as well as the data in the literature, we deduced that the double peaks correspond to the β -FeSi₂ phase.

In the present work, we investigated dispersion of the double peaks, as shown in Fig. 3. We observed three components for which we tentatively assigned as the surface-derived states (S1, S2, S3), including the bulk states of the silicide islands. Band dispersion of the S1 state is similar to that of the surface state on the clean

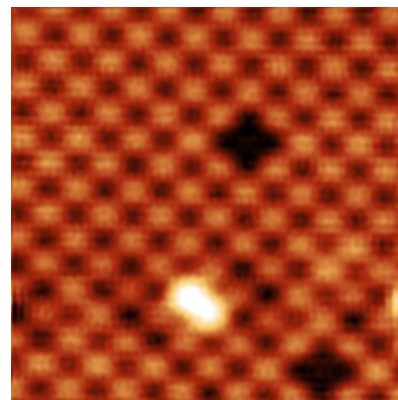


Fig. 1 An STM image of the c(2x2) structure.

Si(001) surface though the folding point is slightly different. It is possible that a clean surface area with a dimer row is partially contaminated with iron and produces this modified band. On the other hand, S2 and S3 are apparently originated from the iron silicide islands because no similar bands exist on the clean Si(001) surface. Our STM study showed that a flat and wide terrace with the $c(2 \times 2)$ structure is formed on top of the silicide islands. This high crystallinity of the silicide islands should be the origin of the formation of the band with a clear dispersion. So far, we could observe a clear dispersion only for the case of the double peaks. Thus, we expect that there should be a clear reason to hinder the formation of well-crystallized islands with large lateral size. In fact, small islands are likely to be formed in the case of the other phases [4].

It should be noted that our assignment of the observed $c(2 \times 2)$ structure to the β -FeSi₂ phase is still not well established. But, it is clear that there is a phase with the $c(2 \times 2)$ structure which is semiconducting and has a clear band dispersion. There remains an important question. Is it possible to confirm that there is one-to-one correspondence between the $c(2 \times 2)$ structure and the β -FeSi₂ phase?. If the metallic α -FeSi₂ could also have the $c(2 \times 2)$ structure as suggested by Ref. [9], it should be possible to observe a band dispersion which is different from that in the present case. In particular, there should be a band which crosses the Fermi level. We hope to confirm this point in our future work.

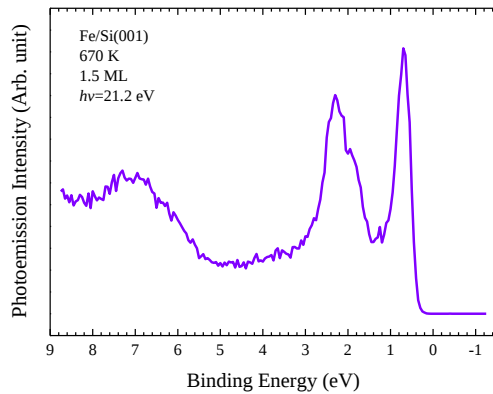


Fig. 2 UPS spectrum of Fe/Si(001).

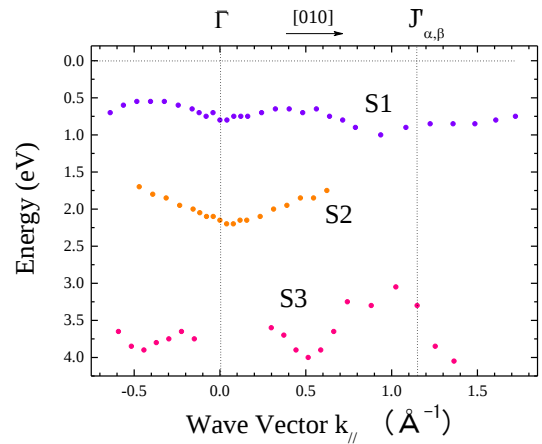


Fig. 3 Band structure of Fe/Si(001).

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