[III~3] [초청]

Formation β-$FeSi_2$ and the electronic structures of the Fe/Si(111) interface studied by LEED and SRUPS

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1. Introduction

The realization of heteroepitaxial growth of semiconducting silicide on Si is of great importance for possible applications in optoelectronic devices. β-$FeSi_2$ is one of the candidates for such materials because it is a *p*-type semiconductor with a band gap of about 0.85 eV. Many efforts have been made to study the growth, electrical and optical properties of this material, however, the details of the electronic structures are not understood well. We report here the formation of epi-β-$FeSi_2$/Si(111) and the electronic structure at the Fe/Si(111) interface which were studied by the synchrotron radiation photoemission spectroscopy(SRPES) and the low energy electron diffraction(LEED) at Pohang light source(PLS).

2. Experimentals

The experiments were carried out in the UHV chamber equipped with rear-view LEED and SRPES at 2B1 beam line of PLS. Phosporous doped Si(111) wafer of 0.3×2.2×30mm was used as the substrate. After loading the wafer into the UHV chamber, the system was baked out for ~24 hour and then the pressure of the system reached to 3~5×10^{-11}Torr. Atomically clean Si(111)-7x7 surface was well developed after the wafer was resistively heated upto ~1200℃ by flowing dc current to the wafer. Fe was deposited by resistively heating the W-filament on which high purity Fe-wire was wrapped, and we monitored the LEED pattern and the PES spectra after each deposition. Two sets of samples were prepared : (1) deposition of Fe on Si(111)-7x7 surface at room temperature followed by *in situ* annealing at 680℃, and (2) deposition of Fe on Si(111) at 680℃.

3. Results

(1) LEED results

For RT deposition, the Si(111)-7x7 reconstructed pattern changed to 1x1 pattern when the deposoted Fe was 3Å and this pattern changed to a 3-fold Fe(111) at 5Å. The Fe(111) pattern was remained up until the Fe thickness was about 55Å. The β-$FeSi_2$(111) + Si(111)-7x7 pattern was obtained after *in situ* annealing the Fe(55Å)/Si(111) sample at

~700℃ for 10min.

The same β-$FeSi_2$(111) + Si(111)-7x7 pattern was obtained after 22Å Fe was deposited on the Si(111) substrate which was mainteined at ~700℃. The LEED results indicate that β-$FeSi_2$ can be grown epitaxially on Si(111)-7x7 substrate by either SPE or RDE method.

(2) SRPES results

The Si-2p core level and the valence band PES spectra for the Si(111)-7x7 surface and the Fe-3p core level and the valence band PES spectra for Fe(55Å)/Si(111) were used as reference for Si and Fe, respectively.

The Fe thickness dependence of the binding energy of the Si-2p and Fe-3p core level showed that the growth mode of Fe on Si(111)-7x7 at room temperature was a layer-by-layer growth. When β-$FeSi_2$ is formed, however, the Si-2p core level is shifted ~1eV to the lower binding side and Fe-3p core level is shifted ~1eV to the higher binding side. The same results of the chemical shift were also obtained from the RDE samples. The Fe thickness dependence of the valence band spectra indicated that the valence band emission is the weighted average of the Si and Fe density of state. The valence band spectra of the β-$FeSi_2$ was a characteristic one which was not the weighted average of Fe and Si valence band. Same spectra for the β-$FeSi_2$ valence band spectra was obtained from the RDE-grown sample.

4. Conclusion

Epitaxial films of β-$FeSi_2$ can be grown on Si(111) subatrate by either SPE or RDE in ultra high vacuum condition. The core level of Si-2p and Fe-3p are shifted upon β-$FeSi_2$ formation. A characteristic shape of the valence band for the β-$FeSi_2$ was obtained.