

Structure and Spin-Polarized Electronic Properties of Ultrathin Fe Films on Pd(001)

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Magnetism of ultrathin 3d metal films have attracted much attention not only for application to the devices, but for understanding the fundamental aspects of evolution/annihilation of itinerant ferromagnetism. In the ultrathin films, lattice mismatch between the film and the substrate causes a structural deformation of the film, and the hybridization of the electronic states at the interface can modify the electronic properties of the film. Therefore, such films show various magnetic properties unlike the bulk material [1]. Fe films on Pd(001) is reported to have strained structure and to show the various magnetic properties dependent on the film thickness [2, 3]. The lattice constant of Pd(001) ($a = 3.89 \text{ \AA}$) is the intermediate value between that of fcc-Fe ($a = 3.59 \text{ \AA}$) and bcc-Fe ($\sqrt{2}a = 4.06 \text{ \AA}$). Moreover, since the Fermi level of Pd lie near the 4d valence bands, the hybridization between Pd 4d and Fe 3d states is predicted to play an important role on the magnetism at the initial stages of the film growth [4]. While the magnetic properties of Fe/Pd(001) is widely reported, the electronic properties of the film is less understood. Therefore, we have investigated the structure and spin-polarized electronic properties of Fe/Pd(001) to clarify the role of them in the magnetism of the film.

The clean surface of the Pd(001) substrate was obtained by repeated cycles of Ar^+ sputtering and annealing at 880 K. Fe was deposited onto the substrate in the rate of 0.2 monolayer (ML) per minutes. The deposition rate was cross-checked by the quartz crystal microbalance and the observation of RHEED oscillation. The substrate temperature during the deposition was carefully set to the room temperature to avoid the possible intermixing at the interface [3]. Observed RHEED oscillation indicates the layer-by-layer growth of the Fe film. X-ray photoelectron diffraction (XPD) was performed to observe the thickness dependence of the structure of the film. The electronic properties were investigated by (spin- and) angle-resolved photoelectron spectroscopy (ARPES/SARPES). XPD and ARPES measurement was performed at BL-18A in KEK-PF. SARPES was performed at BL-19A equipped with electron spin polarimeter utilizing very-low-energy electron diffraction (VLEED) [5].

Figure 1 shows the results of XPD experiment using Al $K\alpha$ ($h\nu = 1486.6 \text{ eV}$) as the excitation source. Fe $2p_{3/2}$ core-level peak intensity of each thickness are plotted against the emission angles. For the spectrum noted "clean," Pd $3p_{3/2}$ peak was measured to check that the adequate diffraction pattern can be obtained. All the peaks found in clean Pd are the forward focusing peaks from fcc(001) surface. For the films less than 3 ML, it is difficult to find a clear feature since the diffraction peaks can be observed when the scatterer is in front of the emitter in the forward focusing mode. From 3 to 12 ML, one can find the peaks moving away from the normal to the surface (0 degree) with increasing the film thickness. This tendency

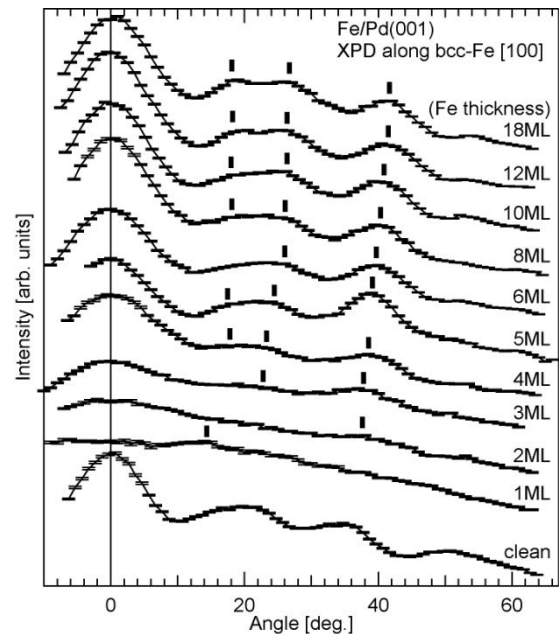


Fig. 1. XPD results along bcc-Fe[100] of Fe films on Pd(001).

can be explained by the structural relaxation from body-centered-tetragonal (bct) structure to bcc structure; At the initial stages of the film growth, Fe atoms are adsorbed on the hollow site of Pd(001) surface. Since the lattice constant of Pd is 4.2 % less than that of bcc-Fe, lateral spacing of the film is reduced while the interlayer spacing is expanded. By increasing the film thickness, continuous relaxation progresses until bcc-Fe(001) structure recovers. Peaks found in 18 ML are the scattering peaks of unconstrained bcc-Fe. Since no obvious difference can be found between the data of 12 and 18 ML, the relaxation is likely finished at 12 ML.

Figure 2 shows the band structure of bct-Fe film on Pd(001) along the momentum perpendicular to the plane. The color scale mapping shows the 2nd derivative of normal emission ARPES spectra of 6 ML Fe film. Features found in the band mapping is fairly different from that of well-known band structure of bcc-Fe. Red (black) lines show the calculated majority (minority) band structure of bct-Fe. The experimentally obtained band structure represents the Fe 3d bands of bct-Fe, which is split-off by the loss of the symmetry compared to the bcc-Fe. Red (black) triangles show the peak position of majority- (minority-) spin states obtained by SARPES of 8ML Fe/Pd(001). Spin-resolved measurements well support the explanation mentioned above.

Since the experimentally obtained SARPES spectra of 18 ML Fe/Pd(001) (not shown here) is indistinguishable from that of Fe(001), thick Fe films on Pd(001) have mostly the same character as bulk bcc-Fe in the point of both structure and electronic properties. By SARPES measurements, Curie temperature of the 8 ML Fe film was found to be far above the room temperature. Therefore, such modification of the structure and electronic properties in the intermediate thickness range is too small to induce a major change in the magnetism of the film. On the other hand, the relationship between the electronic properties and the magnetism of Fe films less than 3 ML is still not clear. Further observations would be performed to answer this question.

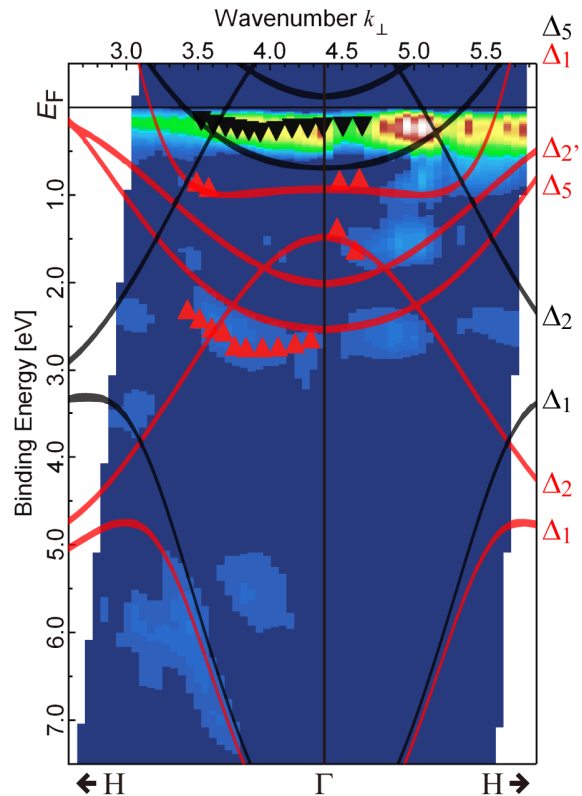


Fig. 2. The band structure of the bct-Fe film on Pd(001). The color scale mapping shows the results obtained by normal emission ARPES. Red (black) lines show the calculated majority (minority) band structure of bct-Fe. Red (black) triangles represents the peaks found in the SARPES spectra.

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