

Thickness dependence of electronic band structures of Ni ultrathin films on Cu(001)

Sunghun Kim^{1,*}, Koichiro Yaji^{1,**}, Yasuo Takeichi¹, Ayumi Harasawa¹, and Akito Kakizaki¹
¹Institute for Solid State Physics, University of Tokyo, Kashiwa, 277-8581, Japan

1 Introduction

Ultrathin nickel (Ni) film on Cu(001) single crystal is one of the most famous systems which represents peculiar magnetic property as perpendicular magnetic anisotropy (PMA). The Ni films show PMA in a thickness range between 10 and 40 atomic monolayers (ML), while the easy axis of magnetization becomes the in-plane direction with respect to the film surface below and above this range [1, 2]. We note that not only the magnetic property but also the electronic structures of Ni/Cu(001) should be investigated in order to clarify the physical origin of the magnetic anisotropy transition (MAT). Former theoretical studies show that the electronic structure of Ni single layer is very different from that of bulk Ni [3, 4]. On the other hand, three-dimensional like Fermi surface was reported at 1.2 ML of Ni/Cu(001) [5]. Also different result at a single monolayer has been traced by using angle-resolved photoelectron spectroscopy (ARPES) [6]. This motivates to clarify thickness dependence of electronic structure near the Fermi level, furthermore to find the evidence for MAT on Ni/Cu(001).

2 Experiment

A disk-shaped ($t = 1$ mm) Cu single crystal with [001] direction normal to the surface has been used for growing the Ni films. The mechanically and electrochemically polished Cu(001) substrate was cleaned by several cycles of Ar⁺ ion sputtering at 1 keV and annealing up to 830 K for 10 minutes in ultra-high vacuum (UHV) chamber. The clean surface of Cu(001) was checked by low-energy electron diffraction (LEED), Auger electron spectroscopy (AES) and ARPES. Ni was deposited on Cu(001) *in situ* at room temperature. The pressure in the UHV chamber was kept below 8×10^{-10} mbar during the deposition. The thickness of the film was controlled by observing the intensity oscillation of reflection high-energy electron diffraction (RHEED) as shown in Fig. 1. The ARPES spectra were measured with a hemispherical electron energy analyzer (VG SCIENTA SES-100) and synchrotron radiation provided at the BL-18A in Photon Factory. Sample temperature was set to 60 K during the ARPES measurements.

3 Results and Discussion

Figure 2(a) shows photoelectron spectra of each Ni film taken with normal emission. Ni *d*-states are appeared around 0.8 eV on 2.5 ML-Ni film. These states clearly split into two with increasing the thickness, where the peak positions are marked with A and B. The peak positions of A and B were plotted as a function of film thickness as shown in Fig. 2(b). Binding energy shift can be found with increasing the thickness up to 7 ML. This behavior agrees the result reported by Pampuch *et al.* [6].

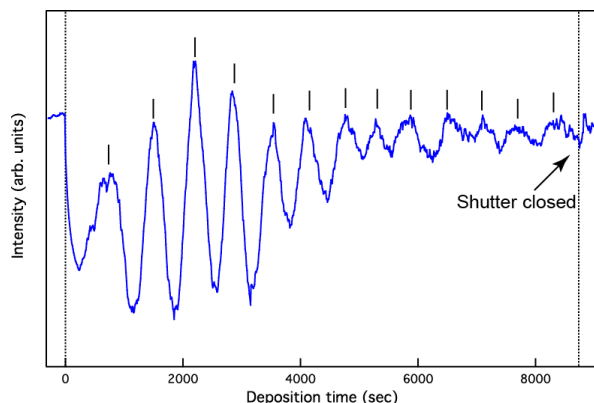


Fig. 1: RHEED intensity oscillation with Ni deposition.

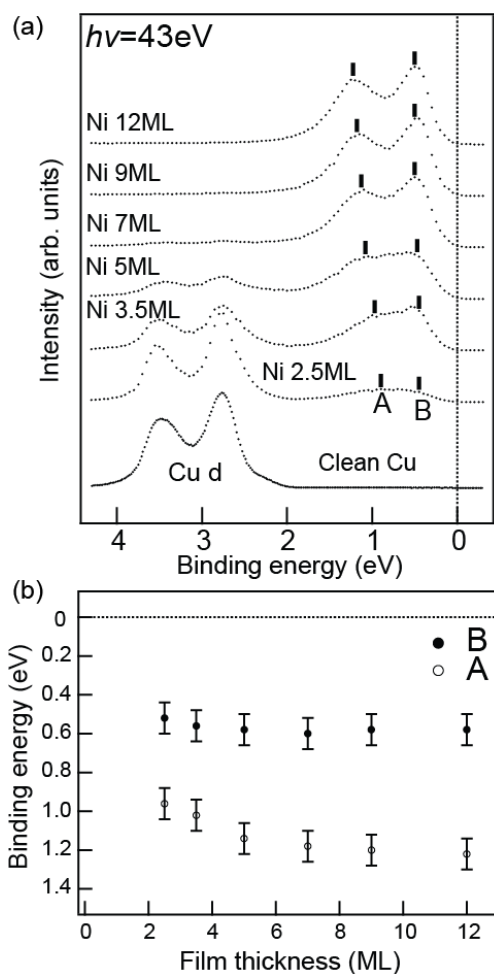


Fig. 2: (a) Photoelectron spectra in normal emission. (b) Peak positions of A and B as a function of thickness.

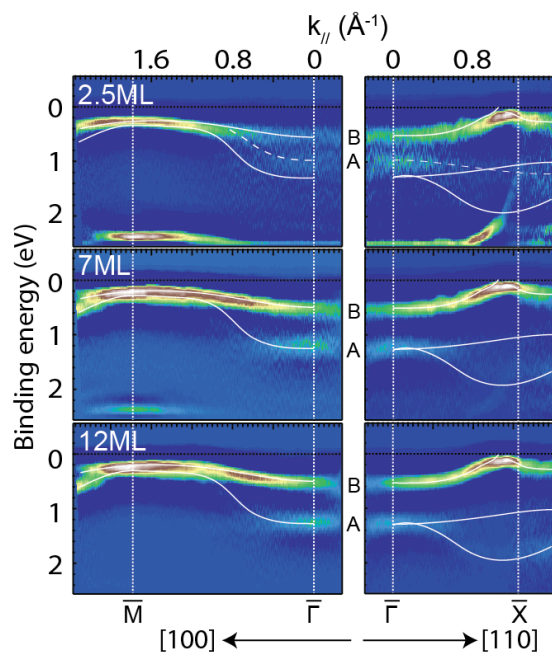


Fig. 3: In-plane band structure of 2.5, 7 and 12 ML Ni/Cu(001)

Figure 3 shows the band structures of 2.5, 7 and 12 ML Ni/Cu(001) taken with the in-plane directions i.e. Γ -M and Γ -X. White solid curves represent the typical band structures of 12 ML Ni, and dashed curves follow that of 2.5 ML Ni, for guides to see. It is found that the shape of the upper band, named B, for 2.5 ML is similar to those for 7 and 12 ML. On the other hand, the shape of the lower band (A) for 2.5 ML is obviously different from those of the other two films along both Γ -M and Γ -X. The band structure of 7 ML Ni is similar to that of 12 ML Ni that exhibits the bulk-like band structure. Note that the 7ML- and 12 ML-Ni show the in-plane magnetic anisotropy and PMA, respectively. However we found no critical change of the band structures.

It is generally known that the PMA appears with decreasing the thickness of films, in which magneto-elastic anisotropy caused by lattice mismatch is considered for the reason. However, the Ni/Cu(001) system shows again the in-plane magnetic anisotropy with decreasing the thickness (less than 6~8 ML-Ni). Although the present results show no direct hints for MAT in this system, magneto-crystalline anisotropy is still convincing for the reason that causes MAT, because this is a direct consequence of spin-orbit coupling reflecting electronic structure.

In summary, we have investigated the band structures of Ni/Cu(001) ultrathin films by ARPES. We found the thickness dependence of the band structures between the 2.5 ML- and 7 ML. On the other hand, no difference of the band structures was found at the critical thickness of MAT. In the future, we would investigate the spin-dependent band structures of Ni/Cu(001) in order to

clarify the physical origin of MAT, where spin- and angle-resolved photoelectron spectroscopy can be good technique.

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* kimsh@issp.u-tokyo.ac.jp

** yaji@issp.u-tokyo.ac.jp