

Thesis Summary

High-resolution angle-resolved photoemission study of oxygen adsorbed
Fe/MgO(001)

(高分解能角度分解光電子分光による酸素吸着した Fe/MgO(001)の研究)

Name: ZHENG MINGTIAN

The metal–oxide interface is one of the most extensively investigated topics in the surface science the strong bonding at the surface between adsorbed oxygen and metal substrate atoms significantly modifies the crystallographic and electronic structures. The $p(1\times 1)$ oxygen adsorbed ferromagnetic Fe(001) surface, one of the prototypical systems for the metal-oxide interface, has attracted the interests of researchers from different fields and has been extensively studied for decades.

Previous theoretical and experimental studies have revealed the microscopic structure, the bonding nature, the electronic states of Fe(001)- $p(1\times 1)$ -O surface. However, in our point of view, detailed understanding of electron correlation as well as $p-d$ hybridization of the Fe(001)- $p(1\times 1)$ -O surface is far from satisfactory. the question remains how the band dispersions of surface states near Fermi edge (E_F) are modified by the effect of oxygen adsorbed on the Fe(001) surface. This detailed knowledge of the surface electronic structure of Fe-O bonding, which to our knowledge has not been clearly identified previously. The Fermi surfaces including surface states of both Fe(001) and Fe(001)- $p(1\times 1)$ -O surfaces near E_F also are still unclear due to the lack of experimental results from photoemission investigation.

Angle-resolved photoemission spectroscopy (ARPES) is one of the powerful experimental methods to investigate the surface electronic states, it is a surface-sensitive probe that can directly measure the band dispersions of the samples. Recent *state-of-the-art* high resolution ARPES systems make it possible to reveal detailed electron structures of solids that are directly related to the physical properties of solids, besides observing a complete image of band dispersions and Fermi surfaces, based on the quantitative analyses of spectral features, one can determine, in principle, respective magnitudes of the *electron-phonon* and *electron-electron* interactions at any point on the Fermi surface.

In this thesis, we have investigated surface- and bulk-derived electronic states near E_F of both Fe(001) and Fe(001)- $p(1\times 1)$ -O surfaces by utilizing linear-polarization-dependent high-resolution ARPES measurements combined with *state-of-the-art* DFT calculations. The polarization-dependent ARPES measurement had been performed at HiSOR BL-1. The Fe(001) and Fe(001)- $p(1\times 1)$ -O samples had been prepared *in-situ* by using electron beam evaporator in the preparation chamber of HiSOR BL-1 endstation. All of the ARPES measurement had been done at the photon energies from $h\nu=30$ eV to 80 eV for enhanced surface sensitivity.

We have presented detailed band dispersions of both Fe(001) and Fe(001)- $p(1\times 1)$ -O close to E_F . In the results of Fe(001), we have experimentally observed the d_{xz+yz} surface state of Fe crossing E_F at $k_{\parallel}=0.6 \text{ \AA}^{-1}$ along the $\bar{\Gamma}-\bar{X}$ lines. After oxygen adsorption, the Fe d_{xz+yz} surface state disappeared, new oxygen-induced bands appeared close to E_F , the linewidth of the bands became narrower and the Fermi surfaces were modified by the oxygen adsorption.

To clarify the orbital origins of the surface derived states in Fe(001)- $p(1\times 1)$ -O, DFT calculations for a 41 monolayer (ML) thick Fe(001) slab covered with a $p(1\times 1)$ -O layer on both surfaces have been done. Comparing the experimental ARPES results of Fe(001)- $p(1\times 1)$ -O with the DFT calculations, we have clarified the orbital origins of each band and found effective mass enhancement due to electron correlation. We have found the strong $p-d$ hybridization between the Fe d_{xy} and $d_{x^2-y^2}$ orbitals and O p_x and p_y orbitals in the first layer, and in the second Fe layer, the $d_{3z^2-r^2}$ orbital has a strong vertical bonding with the O p_z orbital. The existence of the $p-d$ hybridization between the Fe $d_{(x+y)z}$ and O p_z orbitals had also been confirmed.

We have also found the existence of charge transfer between Fe and adsorbed O atoms near the surface region as well as momentum dependent Fermi surface deformation. The electron-like bands I-V near the $\bar{\Gamma}$ point were shifted to a higher energy compared with the DFT calculations, while the energy of band XII was shifted downwards. The theoretical k_F values for the electronlike Fermi surfaces around the $\bar{\Gamma}$ point are larger (especially along the $\bar{\Gamma}-\bar{X}$ line) than the observed k_F values.

Those results provided a complete view of the electronic states of Fe(001) and Fe(001)- $p(1\times 1)$ -O, enhanced our understanding of the prototypical system of oxygen-metal interface, that could help us to develop advantageous applications based on the oxygen-metal interface such as magnetic tunnel junction and spin-detector.