An Angle-Resolved Photoelectron Study of Charge-Density Wave in In/Cu(001)

Takeshi NAKAGAWA, and Tetsuya ARUGA*
Department of Chemistry, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

It has been anticipated that metal surfaces do not exhibit properties characteristic of low dimenstional electron system. However, we recently have shown that a structural phase transition is induced by the Fermi surface nesting of a surface resonance band in In/Cu(001) at the coverage of 0.5 ML [1]. In this report we report on the observation of surface charge density wave in another phase, c(4x4), of In/Cu(001) at In coverage of 0.63 ML. The c(4x4) phase transforms reversibly to the p(2x2) phase around 450 K upon heating. The change of the electronic structure in the phase transition was studied using angle-resolved photoelectron spectroscopy (ARPES).

ARPES experiment was done at BL-7B. All specra shown were taken with the photon energy of 22.8 eV and the total energy resolution was 150 meV.

The electronic structure of the high temperature phase, p(2x2), along $\bar{X}\bar{M}$ is shown in Fig. 1 (a). The surface resonance band (S_1) is observed, which disperses toward the Fermi level and crosses E_F at 0.5 $\bar{X}\bar{M}$. The crossing point is in agreement with the zone boundary of p(2x2). The shape of the Fermi surface is square-like, which is preferable for the nesting.

Upon cooling down the p(2x2) phase undergoes a reversible phase transition to the c(4x4) phase. The spectra of the c(4x4) along $\bar{X}\bar{M}$ is shown in Fig. 1(b). While the S_1 band crossing E_F is still observed, a new surface resonance band (S_2) appears. The S_2 band turns back to the higher binding energy without crossing EF.

The S_2 band is present in the low temperature phase and the S_2 band has a / 500 meV energy gap relative to E_F, which suggests that the Fermi surface nesting is the origin of the phase transition.

The existence of the metallic S_1 band even in the low temperature phase, c(4x4), is clearly observed. The reason for the existence of the metallic S_1 band at the low temperature phase can be explaned by one-dimensional nesting. In the case of one-dimensional nesting, one side of the square-like Fermi surface is nested with the opposite side, but the other sides are not nested. Thus the gap opening occures in one direction. Since in the case of the c(4x4) surface domains are rotated by $\pi/2$ with each other, both the S_1 band, which crosses E_F, and the folded-back S_2 band are observed. The c(4x4) surface as observed by STM lacks four-fold symmetry and belongs to *pmm* space group, which supports the one dimensional nesting mechanism.

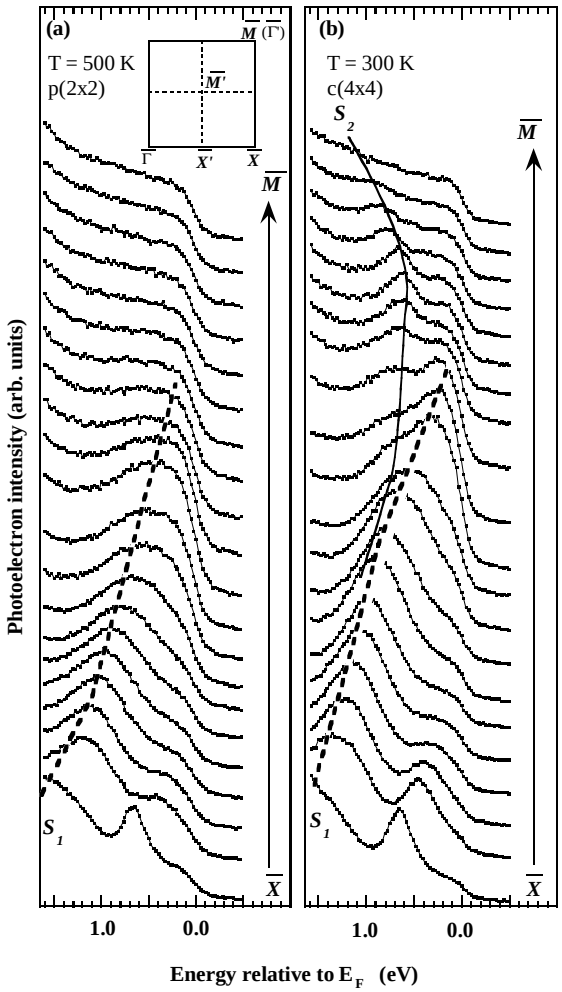

Figure 1. ARPES spectra for (a) the p(2x2) and (b) the c(4x4) phases. Also shown is the Brillouin zone for 1x1 (solid lines) and p(2x2) (dashed lines).

References

[1] T. Nakagawa, G. Boishin, H. Fujioka, H. W. Yeom, I. Matsuda, M. Nishijima, N. Takagi, and T. Aruga, Phys. Rev. Lett. 86, 854 (2001); T. Nakagawa, S. Mitsushima, H. Okuyam, M. Nishijima, and T. Aruga, to be published.
* aruga@kuchem.kyoto-u.ac.jp