High-resolution angle-resolved photoemission study of kish graphite

Y. Miura[1], K. Shimada[2], H. Negishi[3], S. Negishi[2], H. Shiozawa[2], M. Higashiguchi[1], N. Tobita[1], X.Y. Chui[1], Y. Aiura[4], H. Namatame[2], M. Taniguchi[1]

[1]*Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*
[2]*Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan*
[3]*Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima 739-8530, Japan*
[4]*National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan*

Abstract

A high-resolution angle-resolved photoemission study of kish graphite using synchrotron radiation (hν=32 eV) has been conducted. We have directly observed a small Fermi surface (k_F<~0.05Å^{-1}) centered at the K point, and determined the π band group velocities along the K-M and K-Γ directions.

Keywords: Kish graphite, Fermi surface, angle-resolved photoemission spectroscopy

Kish graphite is one of the most typical layered materials and has attracted much interest for novel and unusual physical properties by intercalation of atoms and molecules. The graphite intercalation compound (GIC) is considered as one of the candidates for the multi-functional materials. As a host material of GIC, it is important to elucidate the Fermi surface (FS) of kish graphite. According to the band-structure calculation [1], a hexagonal graphite has an electron pocket at the K point and a hole pocket at the H point [1]. Although angle-resolved photoemission spectroscopy (ARPES) studies on graphite have been done extensively so far [2,3], the electron/hole FS has not been directly observed since the size of the FSs are very small (k_F<0.045 Å^{-1}) [1] compared with the conventional momentum resolution (Δk~0.1 Å^{-1})[2,3]. Moreover, we should tune the incident photon energy to detect the K or H points. Owing to recent rapid development of high-resolution ARPES with synchrotron radiation (ΔE~5-10 meV, Δk~0.01 Å^{-1}), one can access to the small FSs of kish graphite.

In the present paper, we report a high-resolution ARPES study on the FS at the K point of kish graphite. With improved angular and energy resolutions, we could mapped the small FS at the K point and examine the π band dispersion along the K-M and K-Γ directions.

ARPES experiments were conducted on the linear undulator beamline of a compact electron-storage ring (HiSOR) at Hiroshima University with a high-resolution hemispherical electron-energy analyzer (ESCA200, SCIENTA) [4]. Total energy resolution was set at ΔE=11 meV and angular resolution at Δθ=0.3° ($\Delta k_{//}$=0.014Å^{-1}). Clean surface of kish graphite was obtained by annealing at 1300 K in the ultrahigh vacuum. In order to perform the FS mapping, we used a low-temperature goniometer (R-Dec Co. Ltd., iGONIO LT). The sample temperature was set at 40 K during measurements. The inner potential was assumed to be V_0=14.5 eV [2]. In order to examine the FS at the K point, we set the photon energy at hν=32 eV. The polarization vector of the incident radiation is parallel to the Γ-K-M direction.

Fig. 1(a) exhibits the Brillouin zone (BZ) of kish graphite in the ΓKM plane. Shaded region in Fig. 1(a) indicates the area examined by ARPES. Fig. 1(b) shows an intensity plot of the Fermi surface at the K point in a linear grey scale. White portion corresponds to the strongest spectral intensity. We added spectral intensity for the energy range from the binding energy E_B=-15 meV up to +15 meV [5]. In order to evaluate Fermi wave number k_F, we fitted the FS intensity along the white dashed line in Fig. 1(b) with a Gaussian. We evaluated k_F<~0.05 $Å^{-1}$ based on the half-width half-maximum of Gaussian, which shows reasonable agreement with the magnitudes of the electron pocket along the Γ-K direction (k_F~0.045$Å^{-1}$) given by the band-structure calculation [1].

Fig. 2(a) exhibits an intensity plot of the energy-band dispersion along the dashed line in Fig. 1(b). In order to exclude the finite temperature effect near the Fermi level (E_F), we have divided each of the energy distribution curves by the Fermi-Dirac distribution function. One can recognize the spectral intensity along the K-Γ direction is strong compared with that along the K-M direction, indicating significant transition-matrix-element effect. In order to determine band positions, we fitted momentum distribution curves (MDCs) with two Lorentzians on a linear background as shown in Fig. 2(b). Dots in Fig. 2(a) display obtained peak positions.

At the K point, we could not clearly resolve the detailed band positions corresponding to the electron pocket due to broad spectral features for E_B<20 meV. An examination of the K point with different excitation energy may provide us further information of the matrix-element effect on the line width.

By the gradient of the energy-band dispersion, the group velocities (*v*s) of the π band along the K-M and K-Γ directions are *v*= $(8.2\pm0.4)\times10^5$ m/s and $(6.8\pm0.2)\times10^5$ m/s, respectively. The group velocity along the K-M direction is larger than that along the K-Γ direction, in agreement with the anisotropy of the FS [1].

In conclusion, we have observed the FS (k_F<~0.05 $Å^{-1}$) of kish graphite at the K point by means of high-resolution ARPES. The anisotropic π band group velocity along the K-M and K-Γ are determined.

This work was partly supported by a Grant-in-Aid for COE Research (13CE2002) by MEXT of Japan. We thank N-BARD, Hiroshima Univ. for liquid He. The experiments have been done under the approval of HSRC (accept No. 04-A-1).

References

[1] J.-C. Charlier et al. Phys. Rev. B **44** (1991) 13237;
J.-C. Charlier et al. Phys. Rev. B **43** (1991) 4579.

[2] A.R. Law et al. Phys. Rev. B **34** (1986) 4289.

[3] C. Heske et al. Phys. Rev. B **59** (1999) 4680.

[4] K. Shimada et al., Surf. Rev. Lett. **9** (2002) 529.

[5] Th. Straub et al., Phys. Rev. B **55** (1997) 13473.

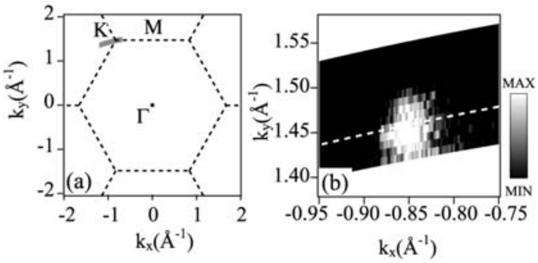

Fig.1. (a) Brillouin zone of kish graphite in the ΓKM plane. (b) Intensity plot of the FS of kish graphite determined by ARPES.

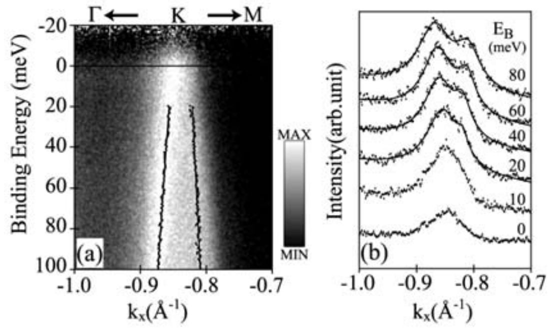

Fig.2. (a) Intensity plot exhibiting the energy-band dispersion along the white dotted line in Fig.1(b). Black dots represent band positions, and black lines fitting curves. (b) MDCs for E_B=0-80 meV.