1C/2002G174

Electronic structure of layered 1T-$TaSe_2$ in commensurate charge-density-wave phase studied by angle-resolved photoemission spectroscopy

Yoshihiro AURA*[1], Hiroshi BANDO[1], Riki KITAGAWA[2], Seiji MARUYAMA[2], Yoshikazu NISHIHARA[2], Koji HORIBA[3], Masaharu OSHIMA[3], Masashi NAKATAKE[4]
[1]AIST, Tsukuba, Ibaraki 305-8568, Japan [2]Ibaraki University, Mito, Ibaraki 310-8512, Japan
[3]University of Tokyo, Tokyo 113-8656, Japan [4]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan

Introduction

To elucidate the physical properties of the layered transition metal dichalcogenides, 1T-$TaSe_2$, it is a key point to understand the role of the electron-phonon coupling which is responsible for the occurrence of the charge-density-wave (CDW) and the subsequent electron correlation effects in the Ta 5d band, in the electronic structure. In the present report, we show a detailed angle-resolved photoemission (ARPES) study of the electronic structure of layered 1T-$TaSe_2$ in commensurate CDW phase.

Experimental

ARPES measurements were carried out at BL-1C of the Photon Factory (KEK, Tsukuba) using an electron spectrometer mounted on a two-axis goniometer (VG ARUPS10). A sample goniometer used here (*i* GONIO LT, R-Dec Co., Ltd.) provides independent polar, azimuth and tilt rotation of the sample [1]. All ARPES spectra were taken at the photon energy (hν) of 40 eV. The emission angle of the photoelectron measured from the surface normal (θ_e) can be varied by rotating the sample along the polar axis or by rotating the energy analyzer horizontally. To avoid polarization effects of the light reported previously, we rotated the energy analyzer and fixed the angle of incidence of the light (θ_I) to 45 º. The azimuth angle (φ_e) was varied by rotating the samples to the surface normal. The samples were cleaved *in situ* in ultra high vacuum. The base pressure in the system was about 1 x 10^{-9} Torr. The angular resolution and the energy resolution were 2 º and about 150 meV, respectively.

Results and Discussion

Figure 1 shows azimuthal dispersion plots of 1T-$TaSe_2$. Spectra were taken at 300 K. θ_e was set to 16 º. The azimuthal scan has been carried out along the circular trajectory, as shown in the top panel. The scan starts in the [ΓM] direction and covers a range of 360 º by the step of 2 º (middle panel). Periodical band structures are observed clearly reflecting the symmetry of the electronic structure. To show the detailed behavior of the band dispersion, the expanded view, which was taken in a range of 120 º by the step of 1 º, is also shown in the bottom panel. It is shown that the empirical band structure is asymmetrical to the M point. This asymmetrical behavior is possibly be caused by the formation of the CDW.

Our ARPES results indicate that not only the electron-phonon coupling which is responsible for the formation of the CDW but also the subsequent electron correlation effects in the Ta 5d band play an important role for the establishment of electronic structure of 1T-$TaSe_2$ in the commensurate CDW phase.

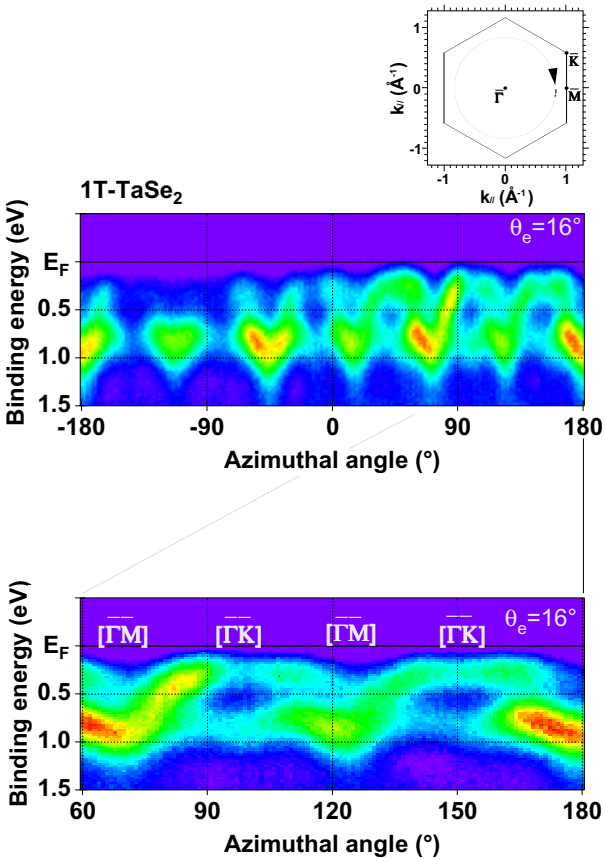

Figure 1 Azimuthal dispersion plots of 1T-$TaSe_2$. The azimuthal scan has been carried out along the circular trajectories (top panel). Spectra start starts in the [ΓM] direction and cover a range of 360 º by the step of 2 º (middle panel) and a range of 120 º by the step of 1 º (bottom panel).

References

[1] Y. Aiura, H. Bando, T. Miyamoto, A. Chiba, R. Kitagawa, S. Maruyama, Y. Nishihara, Rev. Sci. Instrum. (to be published, 1 June 2003).

* y.aiura@aist.go.jp