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Ta 5d Band Symmetry of 1*T*-$TaS_{1.2}Se_{0.8}$ in Commensurate CDW Phase

Yoshihiro AIURA*[1], Izumi HASE[1], Hiroshi BANDO[1], Kazutoshi YAGI-WATANABE[1], Kenichi OZAWA[2], Takeshi IWASE[3], Yoshikazu NISHIHARA[3]
[1]AIST, Tsukuba, Ibaraki 305-8568, Japan
[2]Department of Chemistry and Materials Science, Tokyo Institute of Technology, Meguro-ku, Tokyo 152-0033, Japan
[3]Faculty of Science, Ibaraki University, Mito, Ibaraki 310-8512, Japan

Introduction

In this report, we show a polarization-dependent ARPES study on 1T-$TaS_{1.2}Se_{0.8}$ in the CDW phase [1]. Clear polarization effects of the ARPES spectra are shown for the first time in a layered transition metal dichalcogenide. By comparison with the ARPES spectra, the conventional band and our empirical model calculations, we conclude that the electronic structure of 1T-$TaS_{1.2}Se_{0.8}$ in the commensurate CDW phase is mainly governed by the unreconstructed crystal potential, rather than the CDW-related potential.

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). The sample goniometer used here provides independent polar, azimuth and tilt rotations of the sample (R-Dec Co. Ltd., *i* GONIO LT) [2]. The radiation was linearly polarized in the horizontal plane of incidence. Only photoelectrons emitted in the plane defined by the light beam and the surface normal were observed. The analysis of the ARPES spectra is based on a symmetry selection rule using polarized light. The emission angle of the photoelectron measured from the surface normal was varied by rotating the energy analyzer horizontally or vertically. The azimuth angle was varied by rotating the samples about the surface normal.

Results and Discussion

In order to study the effect of symmetry on the ARPES spectra, we measured azimuth dispersion spectra for the fixed momenta of 0.70π, 0.89π and 1.08π using p-polarized light and s-polarized light, as shown in Figs. 1 (c) and (d). Each azimuth scan has been carried out along one of the arcs shown in Fig. 1 (a). The azimuth spectra show significant polarization effects for light along the high symmetry line ΓM. Particularly, the spectral weight around the M point, which is clearly shown in the case using p-polarized light, is drastically reduced with s-polarized light, as also shown in the energy distribution curves (EDCs) of Fig. 1 (b).

The polarization dependence of the ARPES spectra was well interpreted in terms of the single-particle spectral function by the model calculation [3]. We showed that polarization-dependent ARPES method gives crucial information for understanding the electronic structure of quasi-two-dimensional transition-metal dichalcogenides.

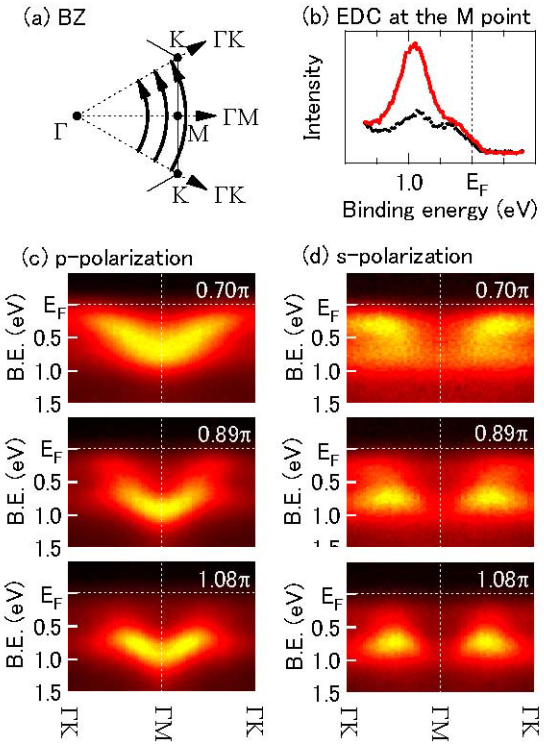

FIG. 1 (a) Sketch of the arcs where spectra have been taken with fixed momenta of 0.70π, 0.89π and 1.08π. (b) EDC spectra at the M point using p-polarized light (solid curve) and s-polarized light (dotted curves). Azimuth dispersion spectra for the fixed momenta of 0.70π, 0.89π and 1.08π using (c) p-polarized light and (d) s-polarized light. Spectra start in the ΓK direction and end in the next ΓK direction via the ΓM direction. All spectra were taken at hν=40 eV and T=300 K

References

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* y.aiura@aist.go.jp