Study of unoccupied electronic states of solids by means of inverse-photoemission spectroscopy

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The various physical properties of solids, e.g. electrical, thermal and magnetic properties, originate from electrons in solids. Thus it is important to clarify the electronic states of solids for understanding their physical properties. Among many experimental techniques, photoemission spectroscopy (PES), that has made remarkable progress with the development of synchrotron radiation instrumentation, is the powerful method to prove occupied electronic states below the Fermi level (E_F). At the Hiroshima Synchrotron Radiation Center (HiSOR) of Hiroshima University, high resolution PES in VUV and SX regions is available for investigating the Fermi surface, band dispersion and total or partial density of states of solids. As a reversal mode of PES, on the other hand, inverse-photoemission spectroscopy (IPES) is the powerful method to directly investigate unoccupied electronic states. With a combination of PES and IPES, we can investigate electronic states of solids over the valence and conduction bands.

In the IPES process, a monochromatic electron beam is injected into samples, where the electrons couple with the free electron states well above E_F. Then the electrons decay into the lower unoccupied states and hence photons are emitted, which gives direct information of unoccupied states [1]. The IPES spectrometer that detects photons with energy ranges of 10-100 eV is working at the HiSOR. In my talk, I will introduce HiSOR activities and then, present about specific resent researches of IPES measurements for quasi-2D material, 1T-TaS_2.

The 1T-TaS_2, has three charge density wave (CDW) phases; incommensurate (IC) phase in the temperature range between 600 and 350 K, nearly commensurate (NC) phase with a hexagonal array of commensurate domains with typical size of 70 Å, and commensurate (C) phase with $\sqrt{13}\times\sqrt{13}$ superlattice below 180 K [2]. The phase transition from IC to C phase is accompanied by a transition from metal to insulator. From the photoemission spectroscopy (PES) study of valence bands of 1T-TaS_2, band reconstruction due to the $\sqrt{13}\times\sqrt{13}$ superlattice and energy gap of ~100 meV in the C phase have been observed [3]. In this study, we have investigated unoccupied band structure in ΓM and ΓK directions for the IC phase (380 K) and C phase (100 K) of 1T-TaS_2 by means of angle-resolved IPES (ARIPES). We have successfully observed the clear unoccupied band dispersion in both IC and C phase of 1T-TaS_2. In the IC phase, a continuous band from Γ to M, which can be attributed to the Ta d_{xy} and $d_{x^2-y^2}$ states, exists near E_F. In the C phase, we found the evidence of band folding. The single continuous band from Γ to M splits up into two bands around M point due to the reconstructed $\sqrt{13}\times\sqrt{13}$ Brillouin zone. In comparison of the ARIPES spectra around Γ point of IC phase with those of C phase, we observed an energy gap of ~100 meV at E_F in the C phase. This energy gap size is identical with that derived from the PES result [3].

References

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