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Fermi surface and superconducting gap of $2H$-$NbSe_2$ using low-temperature ultrahigh-resolution angle-resolved photoemission spectroscopy

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Abstract

We have studied the Fermi surface (FS) and superconducting gap of $2H$-$NbSe_2$, using angle-resolved photoemission spectroscopy with an energy resolution of 2.2 meV and an angle resolution of $\pm 0.13°$. We succeeded in distinguishing all FS sheets predicted from band calculations and found that the observed hexagonal Fermi surface nesting vector centered at the Γ point is larger than the CDW nesting vector reported from neutron diffraction measurements. Furthermore, a superconducting gap at one FS sheet is successfully observed.

Keywords: Fermi surface; Superconducting gap; ARPES

1. Introduction

2H-$NbSe_2$ is a quasi-two-dimensional superconductor ($T_c = 7.2$ K) exhibiting an incommensurate charge density wave (CDW) transition at $T_{CDW} \sim 35$ K. To understand these properties, it is crucial to know the accurate Fermi surface (FS) topology and to directly observe momentum (k)-dependent superconducting gap. For the FS topology, recent angle-resolved photoemission spectroscopy (ARPES) showed a FS of hexagonal shape in the Brillouin zone center and a second sheet centered about K(H), and reported the CDW nesting vector corresponds to the hexagonal FS nesting vector [1]. However, the study could not resolve multiple FS sheets and the pancake-like sheet at the Γ point, predicted from band calculations [2]. On the other hand, the superconducting gap of $2H$-$NbSe_2$ has not been reported from any PES study due to the limitations of energy resolution and sample temperature. In this paper, we report the detailed FS topology and superconducting gap of $2H$-$NbSe_2$ studied by ultrahigh-resolution (energy and angular) ARPES.

2. Experimental

The present work has been carried out with an ultrahigh-resolution photoemission spectrometer built at ISSP, using a monochromatic He I source, a Scienta SES2002 analyzer, and a newly designed thermally shielded sample holder with a flowing liquid He cryostat. We set the energy resolution 4.8 meV for the FS mapping and 2.2 meV for observing the superconducting gap with the angle resolution of $\pm 0.13°$. Clean (0 0 0 1) surfaces were obtained by cleaving 2H-$NbSe_2$ single crystals in-situ. The Fermi level (E_F) is determined from the Fermi edge of a gold film and its accuracy is better than ± 0.05 meV.

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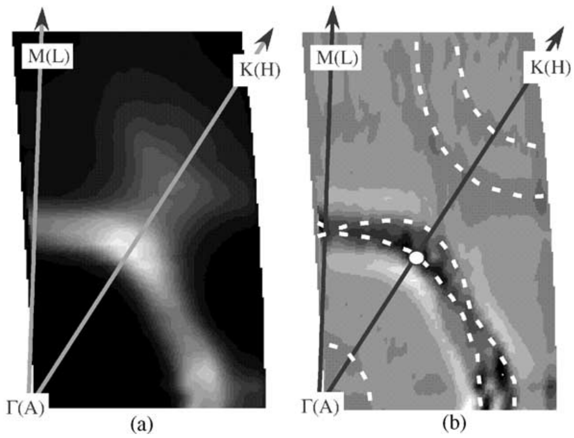

Fig. 1. Fermi surface of $2H$-$NbSe_2$ determined from present ARPE study (angular resolution: $\pm0.13°$): (a) Photoemission intensity map. (b) Two-dimensional second derivertive intensity map. Dotted lines are guide to the eyes, corresponding to each FS sheet.

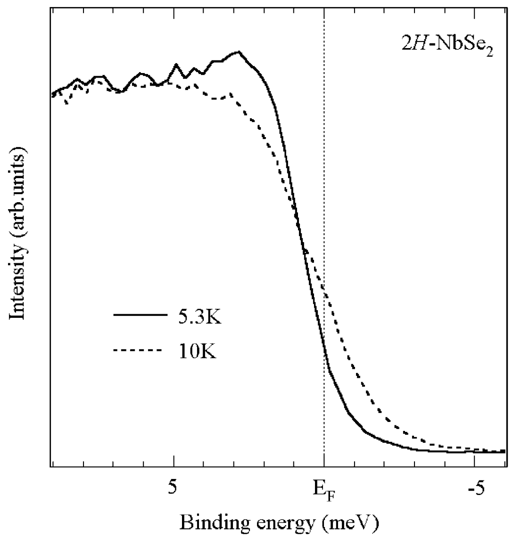

Fig. 2. Temperature dependence of ultrahigh-resolution ARPE spectra of superconducting states (5.3 K, solid line) and normal states (10 K, dotted line) measured at the open circle in the Fig. 1b.

3. Results and discussion

Fig. 1a shows an intensity map of ARPE spectra of $2H$-$NbSe_2$ single crystal (0 0 0 1) with an energy window set below and above 5 meV from E_F. The appearance of the intensity map is quite similar to that reported by Straub et al. [1]. However, since we could resolve two peaks in the momentum distribution curves (not shown) at E_F for the hexagonal FS, we took a second derivertive of intensity map to resolve these bands. As shown in Fig. 1b, we succeeded to resolve its double-walled nature for the cylindrical FS sheets both at the Γ point and the K point. Furthermore, we observe that there is a region around the Γ point where color is darker than its surround, suggesting an existence of another FS sheet. These observations are consistent with the prediction from the band calculations (2 cylindrical at Γ, 2 cylindrical at K, and 1 pancake-like sheets close to Γ) [2]. From the present result, we found the observed hexagonal Fermi surface nesting vector centered at the Γ point is larger than the CDW nesting vector (0.688 $Å^{-1}$) reported from neutron diffraction measurements [3]. This implies the CDW nesting vector exists at other place in the Brillouin zone.

Fig. 2 shows the photoemission spectra at 5.3 and 10 K across the superconducting transition $T_c = 7.2$ K. The measurement point in the Brillouin zone is shown with an open circle in Fig. 1b. We clearly observed the opening of a superconducting gap as a shift of the midpoint of the leading edge (0.65 ± 0.05 meV). To our best knowledge, this is the first observation of superconducting gap of $2H$-$NbSe_2$ using ARPES.

4. Conclusion

From a detailed mapping of FS of $2H$-$NbSe_2$, we succeeded in observing all of the FS sheets predicted from band calculations, and also found the hexagonal FS nesting vector cannot be related to the CDW nesting vector. In addition, we could observe the superconducting gap at a selected point on one FS sheets, showing the potential of ARPES for studying anisotropy of the superconducting gap.

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