Electronic structure of $NbSe_3$ from angular resolved photoemission spectroscopy

M. Sing[1], J. Schäfer[2,3], S. W. Schmidt[4], S. A. Kellar[5], R. E. Thorne[6], Z.-X. Shen[5], S. Hüfner[4], R. Claessen[1], S. D. Kevan[3]

[1]Universität Augsburg, Experimentalphysik II, D-86135 Augsburg, Germany
[2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
[3]Department of Physics, University of Oregon, Eugene, Oregon 97403, USA
[4]Fachbereich Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany
[5]Department of Physics, Applied Physics, and Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, California 94305, USA
[6]Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853-2501, USA

INTRODUCTION

Recently, quasi one-dimensional metallic systems have attracted much attention due to their extraordinary properties driven by their reduced dimensionality. Among these are the formations of charge and spin density waves (CDWs/SDWs), superconductivity, enhanced fluctuations and a dominant role of electron-correlation effects possibly leading to Luttinger liquid behavior in some of the systems in question. With this in mind we performed angular resolved photoemission measurements of the quasi-one-dimensional metal, $NbSe_3$, to gain insight into the (occupied part of the) $k_{||}$-resolved electronic structure near the Fermi energy as a function of temperature. The two known CDW-transitions in $NbSe_3$ at about 143 K and 45 K should be reflected by changes in the low-energy electronic-excitations as measured by photoemission spectroscopy.

EXPERIMENTAL

The needlelike shape of the $NbSe_3$ single crystals with typical dimensions of several centimeters in length and only 120 μm and 30 μm in width and height, respectively, demands special care in terms of sample preparation and instrumental specifications. To improve the signal-to-background ratio three or four fibres were mounted side by side then glued across the rim of a graphitized cup-like sample holder. The crystals were cleaved *in situ* at a pressure of 10^{-10} torr by knocking off a piece of W-foil attached to the top of the fibres. The instrumental demands for $k_{||}$-resolved measurements of such tiny crystals with small photoemission cross-sections at the Fermi energy, i.e. high photon flux, small spot size, parallel energy and angular detection are uniquely met by the beamline 10.0.1.1 and its HERS end station equipped with a SCIENTA 200 analyzer.

The spectra were taken at a photon energy of 21.2 eV (He I) which makes it possible to record band maps with a $k_{||}$-window of about 57% of the Γ-Z (1D) direction of the 1st Brillouin zone and an energy window of 1-2 eV within about 2hrs. Thus, most of the occupied part of the bands at E_F around the Γ-point are covered by a single "shot" in the angular mode. The total energy and angular resolution were chosen to be 13 meV and 0.3°, respectively.

RESULTS AND DISCUSSION

Figure 1 shows EDC-curves recorded at 300 K. A more convenient representation of the same data as a two-dimensional image intensity plot is depicted in Fig. 2 which can be interpreted directly in terms of a band map. The spectra are normalized to the higher order intensity above E_F, the $k_{||}$-axis was scaled such that according to band structure calculations [1] the bottom of the first two bands (see below) is situated at the Γ-point ($k_{||} = 0$).

In both figures one can clearly observe dispersing features in the vicinity of the Fermi level. There are two nearly-free electron-like bands discernible at *ca*. 250 and 500 meV, respectively. These are in good agreement with the above-cited LCAO band calculations.

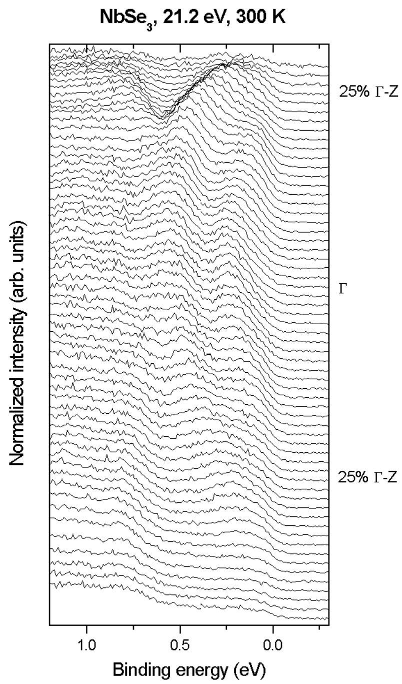

Fig. 1: EDCs along the 1D axis of $NbSe_3$ near E_F = 0 eV binding energy at 300 K.

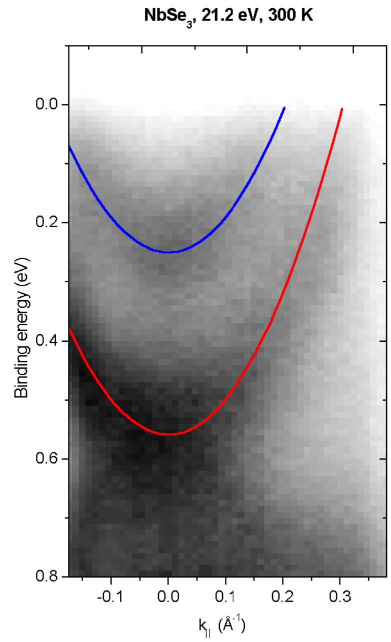

Fig. 2: Two-dimensional image intensity plot of the same spectra as shown in Fig. 1.

From the curvature of the two bands near E_F one can estimate an effective electron mass near one for both bands. We determine the Fermi vectors to be at about 0.2 and 0.3 Å^{-1}, which is also in fair agreement with the band calculations. Similar measurements at temperatures of 30 K, 100 K, and 200 K (not shown) basically exhibit the same features and so far give no hint of changes in the electronic structure when passing through the two CDW transitions. We note, however, that the surfaces prepared here are not sufficiently characterized to rule out a defect or adsorbate induced suppression of the Peierls distortion near the surface. While certainly more work is required here, these first experiments give proof that the high performance of this beamline and its end station is excellently suited for this demanding experiment.

REFERENCES

[1] D. W. Bullett, J. Phys. C: Solid State Phys. **12**, 277 (1979).

This work was supported by the Deutsche Forschungsgemeinschaft under DFG CL 124/3-1 and Sonderforschungsbereich (SFB) 277, and by the U.S. Department of energy's Office of Basic Energy Science, Division of Material Science through grant DE-FG03-96ER45594.

Principal investigator: S. D. Kevan, Department of Physics, University of Oregon, Eugene, Oregon 97403, USA. Email: kevan@oregon.uoregon.edu. Telephone: 541-346-4742.