Journal of Physics and Chemistry of Solids 72 (2011) 562–564

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

Van Hove singularity as a possible origin of the bandwidth renormalization in layered superconductors

S.V. Borisenko [a,*], A.A. Kordyuk [a,b], V.B. Zabolotnyy [a], D.V. Evtushinsky [a], T.K. Kim [a], B. Büchner [a], A.N. Yaresko [c], V.D. Borisenko [d], H. Berger [e]

[a] Leibniz-Institute for Solid State Research, IFW-Dresden, D-01171 Dresden, Germany
[b] Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine
[c] Max-Planck-Institute for Solid State Research, D-70569 Stuttgart, Germany
[d] Vinnytsia State Technical University, 95 Khmelnytske Shose, 21021 Vinnytsia, Ukraine
[e] Institute of Physics of Complex Matter, EPFL, 1015 Lausanne, Switzerland

ARTICLE INFO

Available online 16 October 2010

ABSTRACT

We use angle-resolved photoemission spectroscopy to study bandwidth renormalization in layered superconductor 2H-$NbSe_2$. Renormalization of the conduction band in comparison with the very similar 2H-$TaSe_2$ is of the factor of two. We discuss the possibility that the Van Hove singularity could be responsible for this effect not only in dichalcogenides but also in pnictides.

Novel pnictide superconductors are characterized by anomalous renormalization of the conduction band. In all studied families, including "1111" [1,2], "122" [3,4], "11" [5,6] and "111" [7], the renormalization factor was found to vary from 2 to 3. In the latter case the agreement with band structure calculations taking into account the renormalized energy scale was remarkable, without applying any momentum or band-dependent energy shifts. We have recently argued that the possible reason for such a strong renormalization could be related to the presence of the Van Hove singularity close to the Fermi level [7]. In order to check this possibility in simpler compounds we initiated the present study. We have selected two well-known reference compounds 2H-$TaSe_2$ and 2H-$NbSe_2$, where the saddle point Van Hove singularities are located above and below the Fermi level, respectively.

Angle-resolved photoemission (ARPES) experiments have been carried out using synchrotron radiation from the BESSY storage ring. The overall energy resolution was set to ~10 meV at $h\nu = 50$ eV. All single crystals have been cleaved in UHV, exposing the mirror-like surfaces. The band structure has been calculated for the experimental crystal structures using the LMTO method in the atomic sphere approximation.

The low-energy electronic structure of both compounds is formed mostly by two bands [8] that support two sets of the Fermi surfaces (Fig. 1). The first band crosses the Fermi level twice, resulting in the inner Γ- and K-hole-like Fermi surfaces. The second band behaves in a similar way to that of 2H-$NbSe_2$, giving rise to outer hole-like Γ- and K-Fermi surfaces, but it is different in 2H-$TaSe_2$, exhibiting a different topology [9,10]. As seen in Fig. 1, a continuous expansion of the outer Fermi surfaces of 2H-$NbSe_2$ would lead to their merging along the Γ–K line and thus to a set of electron-like "dogbone" Fermi surfaces centered around M-points. This is indeed observed in 2H-$TaSe_2$.

This difference in topologies of the outer Fermi surfaces is interesting since the mentioned point of junction on the Γ–K line is a saddle point and it is this Van Hove singularity that is located

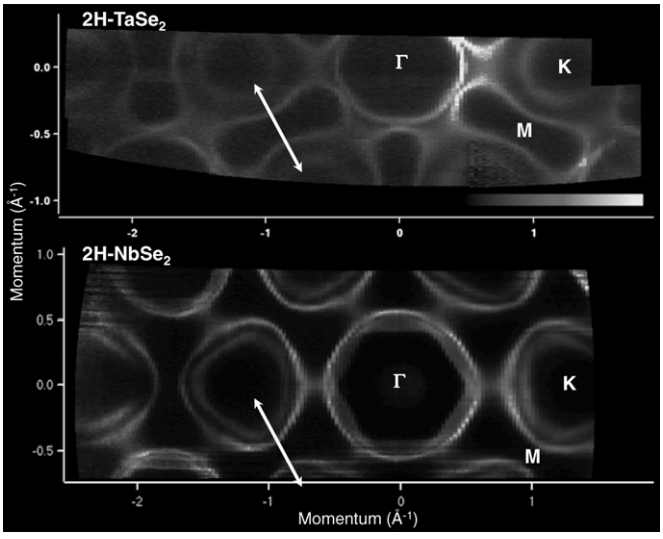

Fig. 1. Fermi surface maps as seen by ARPES in 2H-$TaSe_2$ (top panel) and 2H-$NbSe_2$ (bottom panel). The white double-headed arrows show cuts in momentum space where the photoemission intensity has been recorded also as a function of energy.

* Corresponding author.
E-mail address: S.Borisenko@ifw-dresden.de (S.V. Borisenko).

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doi:10.1016/j.jpcs.2010.10.063

below the Fermi level in 2H-$NbSe_2$ and above in 2H-$TaSe_2$. We note that such a relatively negligible distinction between the positions of the saddle points (~60 meV) may appear to be responsible for a rather crucial change in the physical properties of these two materials. Transition temperature to the charge-density wave state in the Ta compound (122 K) is nearly four times higher than that for the Nb compound (33 K) and the latter becomes a superconductor at 7.2 K whereas the former remains resistive down to 300 mK.

Even smaller differences between the electronic structures follow from the results of the band-structure calculations presented in Fig. 2.

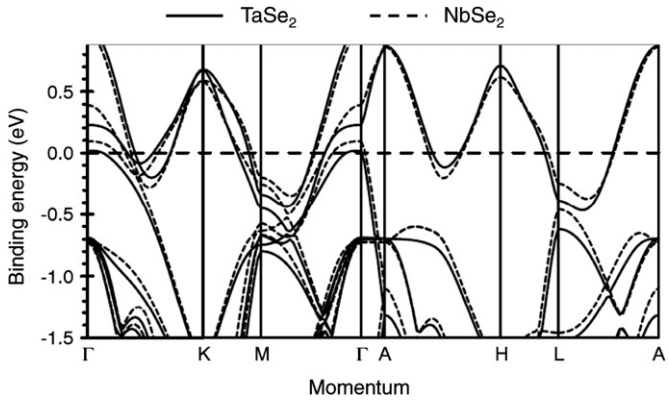

Fig. 2. Band structure of 2H-$TaSe_2$ (solid) and 2H-$NbSe_2$ (dashed) along the high symmetry directions in the Brillouin zone.

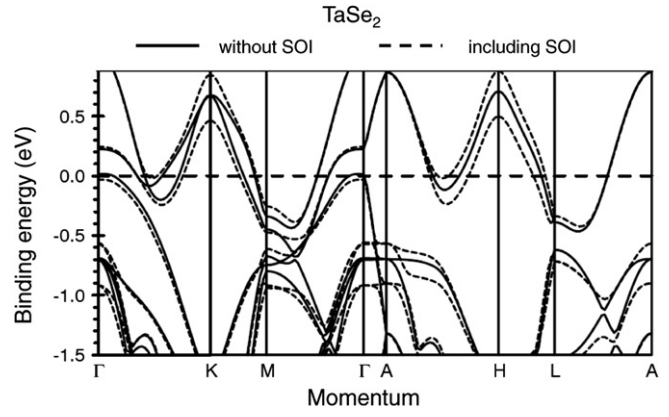

Fig. 3. Band structure of 2H-$TaSe_2$ calculated: solid, without SOI and dashed, with SOI.

The saddle points are seen here as local minima of the bands near the Fermi level along the Γ–K line. As seen in Fig. 2 the saddle points of both bands in 2H-$TaSe_2$ remain occupied similar to the Nb compound, which is at variance with the experimental data in Fig. 1. Another disagreement with the experiment is the presence of a small Fermi surface around Γ with pronounced 3D character (as follows from the strong k_z dispersion along the Γ–A line). However, both discrepancies are effectively removed by inclusion of the spin–orbit interaction (SOI) into the computational scheme (Fig. 3). Since Ta is a rather heavy element, the relativistic treatment is justified. Thus, considering the experimental Fermi surfaces and calculated bands one may arrive at the conclusion that the low-energy electronic structures are fairly similar.

In Fig. 4 we present the central result of this work. The ARPES data are recorded along the cuts through the M-points in order to determine the energy positions of the local minima of both main bands. The striking disparity is obvious. The minimum of the dispersive feature, which forms the outer Γ- and K-Fermi surfaces in 2H-$NbSe_2$, is at ~100 meV whereas the minimum of the "dogbone" pocket of 2H-$TaSe_2$ is at ~320 meV. Comparing these numbers with the results of the calculations (200 and 340 meV, respectively), one obtains a factor of two renormalization in 2H-$NbSe_2$ and nearly no renormalization in the case of the Ta material.

What is the reason for such different renormalizations in two seemingly similar dichalcogenides? One should point out that from Nb (4d) to Ta (5d) the localization of the valence d-shell is not changed significantly (less than 4% in atoms) and the considerable renormalization cannot be attributed to the larger U. For comparison, the valence d-shell radius of V (3d) is nearly twice shorter than that of Ta (5d). As pointed out earlier, the only principal difference between the electronic structures of these compounds is the energy location of the saddle point, which lies on the Γ–K line. The presence of additional states near the Fermi level increases the probability for other electrons to scatter and thus decreases their lifetime. In terms of electronic self-energy, their imaginary part will be higher for the Nb compound and thus the real part of the self-energy will renormalize the bare dispersion stronger. The effect of life-time broadening can indeed be seen in Fig. 4, comparing the widths of the momentum distributions at the same energy.

Projecting this situation to the pnictides, one can also relate the presence of the Van Hove singularity with strong bandwidth renormalization, though the energy scales are different. In 2H-NbSe2 the saddle point has a binding energy of 30 meV and the occupied bandwidth is less than 200 meV, whereas in e.g. LiFeAs the flat top of the band near the Γ-point is closer than 10 meV to the Fermi level and the lowest binding energy of the

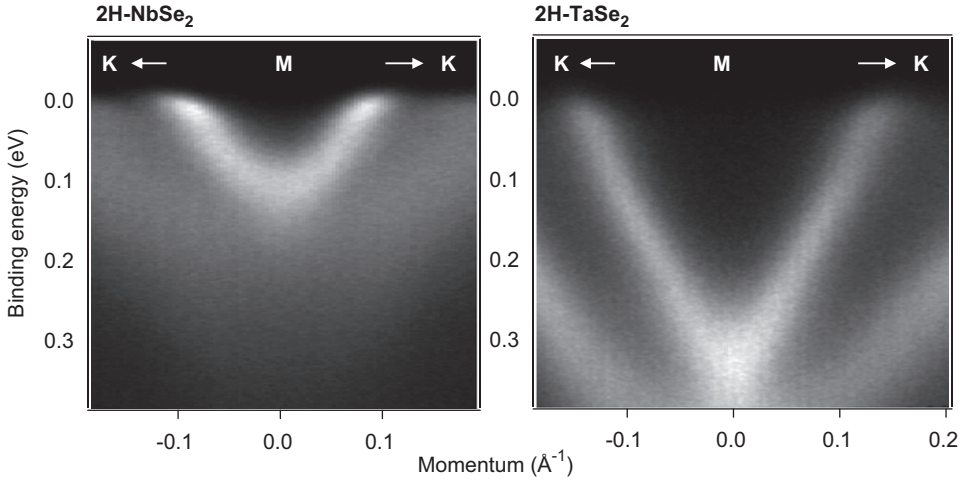

Fig. 4. ARPES spectra taken at 50 eV excitation energy along the KMK high symmetry directions in 2H-$NbSe_2$ (left) and 2H-$TaSe_2$ (right).

bands supporting the Fermi surface is $\sim$700 meV. It is therefore probably hard to expect global renormalization of the whole bandwidth by a factor of three, but in the light of the presented data one should certainly take the discussed effect into account.

Acknowledgements

This project was supported, in part, by the DFG under Grant nos. KN393/4 and BO 1912/2-1 as well as priority program SPP1458.

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