Charge-Density-Wave Mechanism in 2H-NbSe$_2$: Photoemission Results

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The quasi-two-dimensional transition metal dichalcogenide (TMDC) NbSe$_2$ is well known to undergo a phase transition at $T_{CDW} \approx 33$ K from normal metallic into an incommensurate charge-density-wave (CDW) state [1]. The threefold degenerate CDW vectors are oriented parallel to the ΓM directions of the hexagonal Brillouin zone (BZ) and have a magnitude of $|\mathbf{q}_{CDW}| = 2/3 \, |\Gamma\mathrm{M}| (1 - \delta)$ with $\delta = \delta(T) \approx 0.02$ determining the incommensurability. As the resistivity of 2H-NbSe$_2$ exhibits metallic behavior below T_{CDW} and shows only a small anomaly at the transition, only a small modificaton of the Fermi surface can be involved by the CDW [2].

The origin of the CDW instability in 2H-NbSe$_2$ and similar 2H-polytypes has been a matter of debate for years. Mainly two alternative explanations are discussed. The first one is based on FS nesting similar to the Peierls instability in one-dimensional metals, except that only fractions of the FS satisfy the required nesting condition [3]. The remaining parts of the FS are responsible for the metallic resistivity below T_{CDW}. The CDW vector is then given by the distance $\mathbf{q}_N$ of the nesting FS.

Rice and Scott have proposed a completely different mechanism [4]. They have shown that a two-dimensional conduction band with saddle points close to the Fermi level is unstable against CDW formation. The CDW vector is determined by the **k**-space separation $\mathbf{q}_S$ between two saddle points.

Both suggestions were exclusively based on band structure calculations [5, 6] due to a lack of experimental information on the conduction bands. The relevant FS sheets have never been observed in de Haas–van Alphen (dHvA) experiments [7–10]. A recent high-resolution photoemission study on the related compound 2H-TaSe$_2$ confirmed saddle points near the Fermi energy and seems to favor the Rice-Scott mechanism for this material.

To elucidate the origin of the CDW instability in 2H-NbSe$_2$ we determined its band dispersion $E(\mathbf{k}_{\|})$ in the **k**-region of the expected saddle point by means of angle resolved photoemission. Since this compound exhibits three conduction bands that are separated only by some ten meV one needs a spectrometer with very high energy resolution. To avoid a modulation of the spectra by a broad room temperature Fermi edge the sample must be cooled down to some degrees above the phase transition. A further specification for the experiment is a reasonable angular resolution to identify the **k**-position of the saddle points with sufficient accuracy. These prerequisites are all excellently met by the high energy resolution spectrometer (HERS) at beamline 10.0.1.1 in connection with the small spot monochromator and the high precision manipulator with its many degrees of freedom. Thus we used the very sophisticated experimental parameters $\Delta E = 11$ meV, $\Delta\vartheta < 0.5°$, $T = 40$ K, $h\nu = 34.9$ eV.

We took spectra on a grid of emission angles that have been separated by 0.3° in one direction and 1° perpendicular to it. The band energies have been extracted from the spectra by fitting the sum of two Lorentzians and a multiplied by the Fermi function to each spectrum as shown in Fig. 1. This was only possible since the two peaks are well separated due to high energy and angular resolution.

The experimental band structure is shown in Fig. 2. As is clearly seen there exists a saddle point with binding energy of 45 meV at 1/2 ΓK.

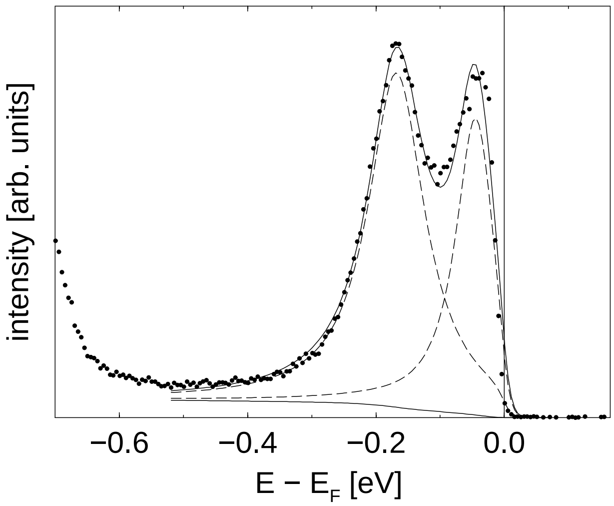

Figure 1: Particular angle resolved spectrum with two fitted Lorentzians and an inelastic background.

But the only vector that connects to another saddle point and is parallel to ΓM has the magnitude $|\mathbf{q}_S|$ = 1.05 Å^{-1}. This value does not agree with the magnitude of the CDW vector $|\mathbf{q}_{CDW}|$ = 0.688 Å^{-1} as mentioned above. For this reason *the existence of saddle points in the conduction band cannot be the origin for the CDW instability in 2H-NbSe$_2$*.

With the high energy and angular resolution data presented here it was possible to show that although saddle points obviously exist in the conduction band they cannot account for the observed CDW periodicity due to their **k**-space locations. This confirms previous results which were restricted to higher temperatures and lower E- and k-resolution [11].

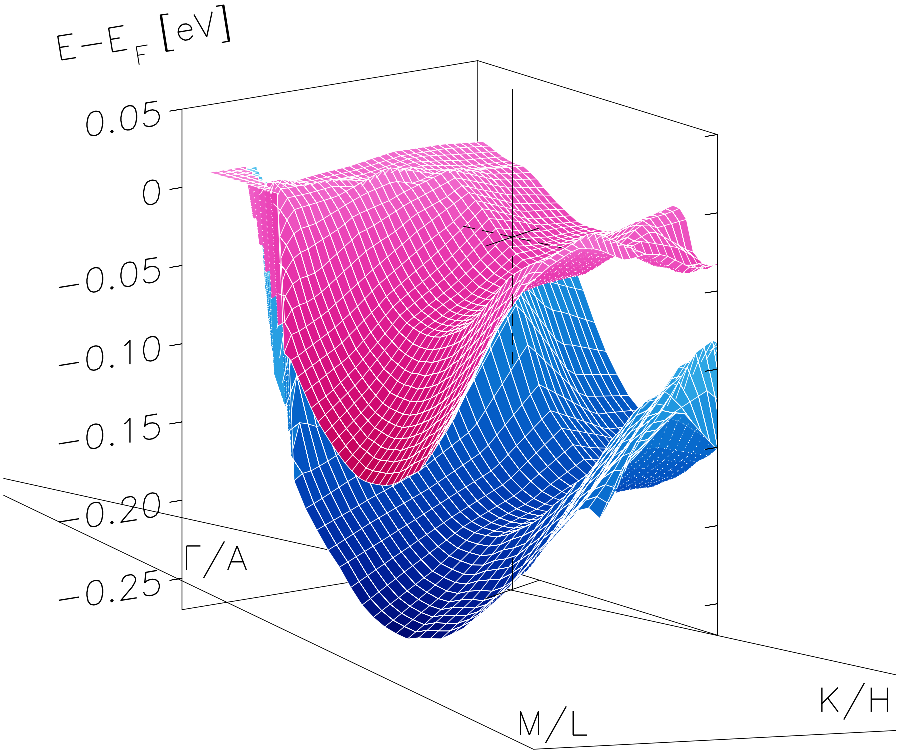

Figure 2: Experimental band structure of 2H-NbSe$_2$ in the vicinity of the saddle point which is located at 1/2 ΓK.

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This work was supported by Deutsche Forschungsgemeinschaft and Bundesministerium für Bildung und Forschung.

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