ISSN 0021-3640, JETP Letters, 2008, Vol. 87, No. 8, pp. 433–436. © Pleiades Publishing, Ltd., 2008.
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Energy Gap of a Charge Density Wave in $NbSe_3$ Induced by a High Magnetic Field above the Peierls Transition Temperature

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Received March 19, 2008

The effect of a magnetic field on the energy gap of the charge density wave (CDW) in $NbSe_3$ near the temperature T_{p2} of the lower Peierls transition has been investigated using interlayer tunneling spectroscopy. It has been shown that the magnetic field increases the energy gap and can even induce it at temperatures higher than T_{p2} by 15–20 K. As the field strength increases, the peak amplitude of the gap singularity of the tunneling spectrum first increases, reaches its maximum at 20–30 T, and then decreases. The increase in the gap peak amplitude is attributed to the field-induced improvement of the condition of the CDW nesting, while the decrease in the amplitude in high fields, to the breakdown of the ground state caused by its Zeeman splitting.

PACS numbers: 71.45.Lr, 71.70.Ej, 74.50.+r

DOI: 10.1134/S0021364008080092

The problem of the possible stimulation of the energy gap in $NbSe_3$ was raised more than 20 years ago [1] when an abnormally high magnetoresistance was revealed in this compound [2]. Balseiro and Falicov [3] assumed that an additional contribution to the magnetoresistance appears because a magnetic field suppresses the Fermi surface "pockets" with uncondensed carriers, thus increasing the number of carriers condensed in the charge density wave (CDW). The numerical results [3] indicated that the magnetic field can reduce the density of states to zero at the Fermi energy and increase the energy gap. Gor'kov and Lebed [4] considered the mechanism of the pocket suppression and attributed it to the improvement of the CDW nesting condition in the magnetic field. Until recently, no experiments on the energy gap in $NbSe_3$ in high magnetic fields have been performed.

In this study, we used the interlayer tunneling technique on the mesa-type layered nanostructures. This technique is based on the fact that the cross-layer transport is a result of the tunneling through the natural tunneling barriers separating the elementary conducting layers [5]. The mesa has the lateral dimensions 1 × 1 μm and contains 20–30 elementary conducting layers. Such structures prepared by double-sided etching in focused ion beams [6, 7] have been recently used in the spectroscopy of the CDW gap and intragap states in $NbSe_3$ [8–10].

The measurements were performed at Laboratoire National des Champs Magnetiques Pulse (LNCMP) in Toulouse, France, in the magnetic fields up to 55 T in a pulse with a duration of about 400 ms. The magnetic field pulse was produced by a high-voltage capacitor bank discharge through a liquid-nitrogen-cooled coil. The pulse shape is shown in Fig. 1a. The magnetic field reached its maximum in 60 ms and then relaxed in about 300 ms. A fast data acquisition system was developed for the measurements; it allowed one to record up to 2000 tunneling spectra for the pulse duration time, each of the spectra contained several thousand points. The measurement circuit is presented in Fig. 1b.

The current–voltage characteristics (CVCs) were measured as follows: the saw-tooth current with a period of 0.5 ms (2 kHz) (see Fig. 1a) was passed through the sample for the pulse duration time; the voltage and current measurements were synchronously performed at 0.5-μs (2 MHz) intervals. The high-speed CVC measurements were performed with an NI PCI-6110 digital card, which has a maximum speed of the analog-to-digital conversion (ADC) of 5 MHz with a 12-bit resolution, a digital-to-analog converter (DAC) with a speed of 4 MHz and a 16-bit resolution used for the formation of the saw-tooth current through the sample, and a trigger input for the start synchronized with the magnetic field pulse. Figure 1b demonstrates the sample-to-digital-card connection circuit. To match and disconnect the sample from the digital card, the differential preamplifiers ($K = 12$, $R_{in} > 100$ MΩ, and $\Delta F = 2$ MHz) and a unit of LC filters ($\Delta F = 0.03$ Hz–50 kHz) attenuating computer noise were produced. The pream-

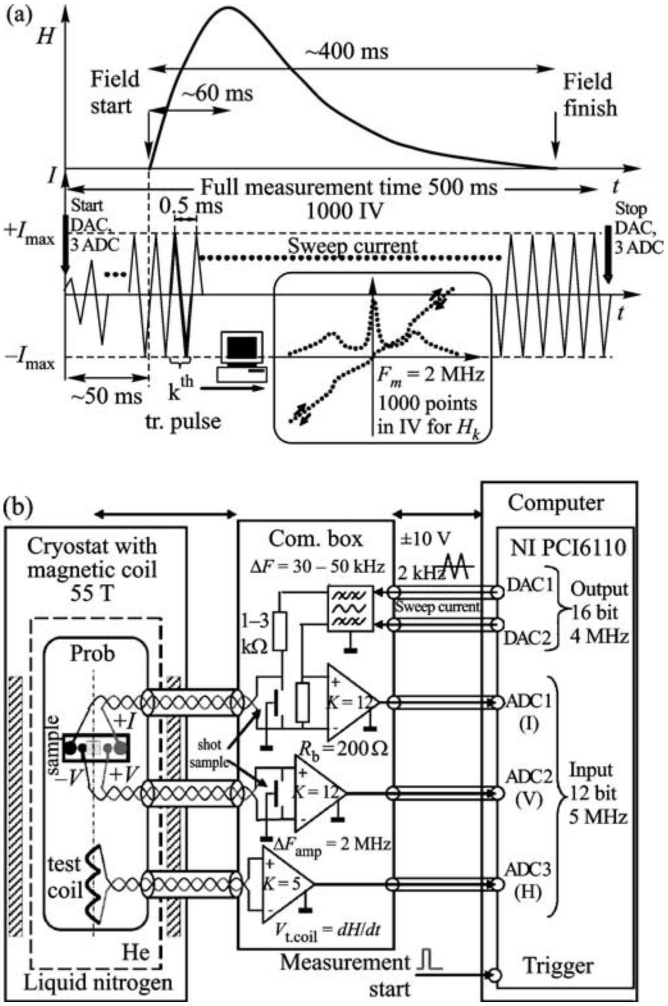

Fig. 1. (a) Time sweep of the magnetic field pulse combined with the sweep of the current through the sample; in the inset, the CVC of a single sweep period; (b) CVC measurement circuit in the pulsed magnetic field.

plifiers, filters, and the system of the sample stepwise short-circuiting to the ground were placed in a separate screened box (see Fig. 1b), which was connected via an insert to the sample by well-wounded screened wires no longer than 1 m to minimize the noise and to remove the magnetic field stray pickup. The system in the tuned state had a noise of 40 μV at the preamplifier input and a noise current of 200 nA at an effective measurement frequency of 2 MHz.

The assembled setup at a digitization rate of 4 MHz allowed 2000 points to be measured synchronously for current I, voltage V, and field variation rate dH/dt for one complete CVC (0.5 ms). On the whole, for one 500-ms magnetic field pulse, all data of the volume about 12 MB (3 × 2000 × 1000 × 16-bit reports) were stored in the computer. After filtration, averaging, and numerical differentiation of the stored data, we obtained the tunneling spectra $dI/dV(V)$ (comprised of 1000 points at a relative accuracy of no worse than 0.5%) of the $NbSe_3$ mesa measured in the magnetic field range of 0–55 T with a step of no more than 0.2 T. The method developed made it possible to obtain the complete 3D pattern of the $dI/dV(V, H)$ spectra for a single magnetic field pulse.

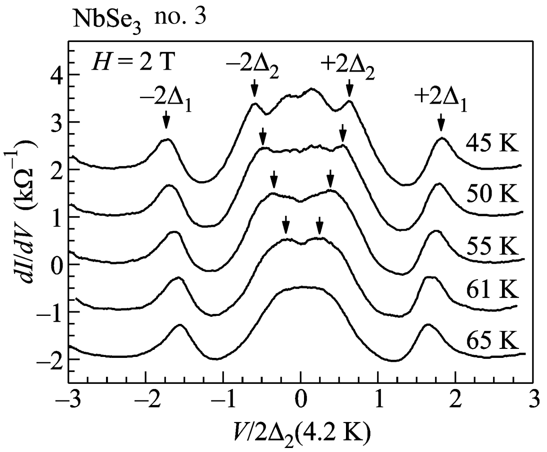

Fig. 2. Interlayer tunneling spectra in $NbSe_3$ as $T_p \approx 60$ K is approached. The spectra are equidistantly displaced along the vertical axis. The dI/dV scale corresponds to $T = 45$ K. The gap singularities of the low- ($V = \pm 2\Delta_2$) and high-temperature ($V = \pm 2\Delta_1$) CDWs are marked by the arrows; $2\Delta_2$(4.2 K) = 60 mV.

Figure 2 illustrates the evolution of the interlayer tunneling spectra of the layered $NbSe_3$ structure near the Peierls transition temperature in a certain comparatively low magnetic field. The energy gaps of the low- and high-temperature CDWs manifest themselves as the maxima on the $dI/dV(V)$ spectra marked by the arrows. It is seen in the figure that, as the lower Peierls transition temperature is approached (≈62 K), the gap peaks corresponding to the lower CDW merge into a wide maximum at zero bias; this maximum is attributed to the CDW fluctuations (the curve at 65 K in Fig. 2). In this case, the positions of the gap peaks of the upper CDW change slightly.

The effect of the magnetic field $H \parallel a^*$ on the tunneling spectra at 65 K is shown in Fig. 3. Clearly, the field restores the gap peaks of the low-temperature CDW.

The magnetic field $H \parallel a^*$ suppresses the density of states under zero bias, increasing the amplitude and voltage position of the gap singularity (Fig. 4). The gap induced by the magnetic field was observed up to the temperatures exceeding T_p by 20 K. These observations indicate that T_p increases under the action of the magnetic field since the gap singularity manifests itself at temperatures above T_p, at which it was absent in the absence of a magnetic field. Another feature is that the gap peak occurs only within a certain magnetic field range. For example, at 71 K, it appears at $H = 7$ T and almost disappears at $H = 52$ T (Fig. 4b).

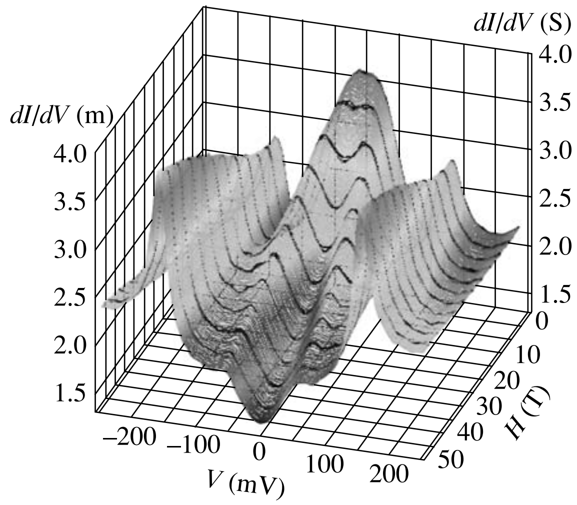

Fig. 3. Three-dimensional plot of the $dI/dV(V)$ spectra in the magnetic field range from 0 to 55 T at 65 K. NbSe$_3$ mesa no. 3. The dI/dV scale is in mS.

The amplitude Γ and position on the V axis of the gap peak as functions of the magnetic field at various temperatures are presented in Fig. 5. The features of the $\Delta_2(H)$ dependences at temperatures above T_{p2} are that the amplitude Γ of the gap peak vanishes, whereas the peak position in the V axis is nonzero (see Fig. 5). As follows from Figs. 4 and 5a, the Γ(H) dependence (Γ is defined in the inset of Fig. 5a) is nonmonotonic. As H increases, the value of Γ(H) first increases, has a maximum at about 25 T, and then decreases.

The magnetic field dependence of the CDW gap has not been theoretically studied. However, the authors of [11] considered the related problem of the magnetic field dependence of the Peierls transition temperature for systems of different nesting perfection degrees. In particular, for the system with imperfect nesting, a nonmonotonic $T_p(H)$ dependence was obtained similar to the experimentally observed Γ(H) dependence. It is qualitatively clear that the variation of T_p under the action of the magnetic field should correlate with the gap singularity amplitude at a given temperature. Therefore, we use the interpretation of [11] to explain the nonmonotonic dependence Γ(H).

Following [11], we attribute an initial growth of Γ(H) to the orbital effects of the magnetic field interaction with uncondensed carriers that increase their energy in the field and improve the nesting condition for the CDW formation. In high fields, the spin effects

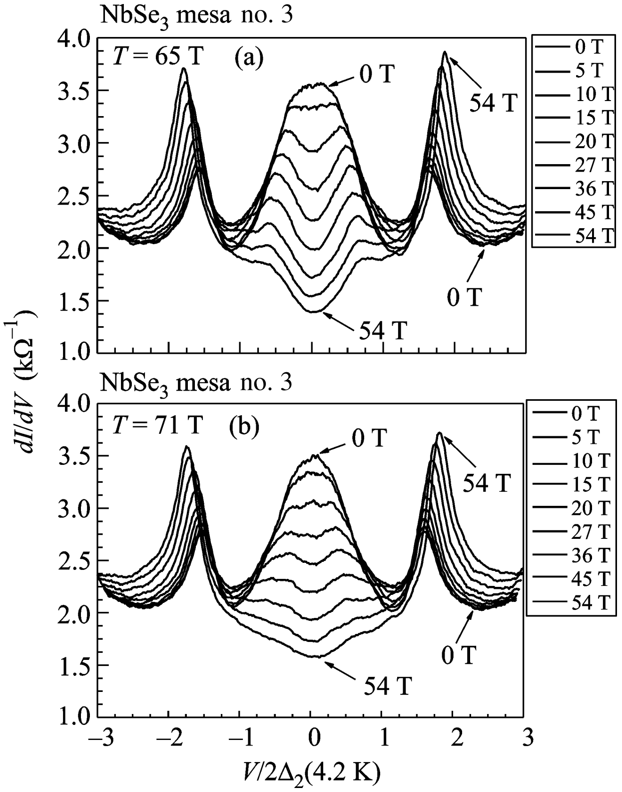

Fig. 4. Interlayer tunneling spectra in NbSe$_3$ at T = (a) 65 and (b) 71 K in various magnetic fields $H \parallel a^*$.

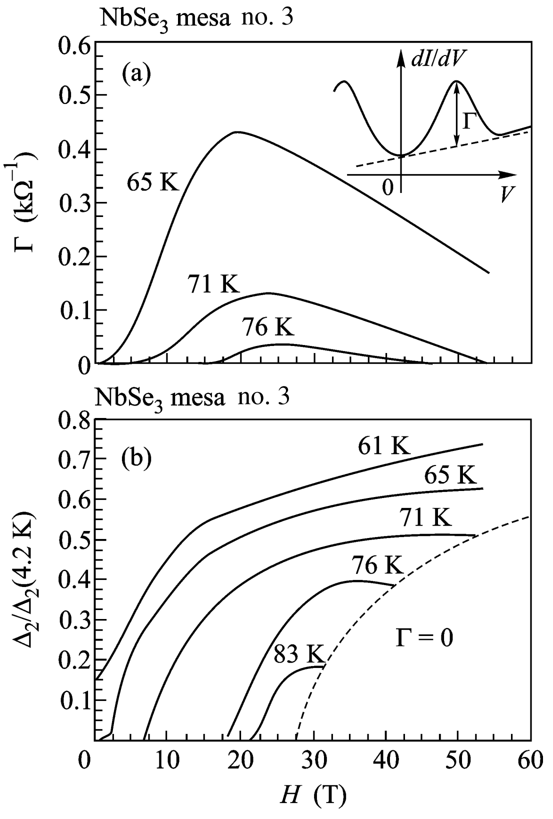

Fig. 5. Magnetic field dependences of the (a) amplitude Γ and (b) V position of the gap peak at the specified temperatures below and above T_p. The dashed line marks the region where the gap singularity amplitude Γ vanishes.

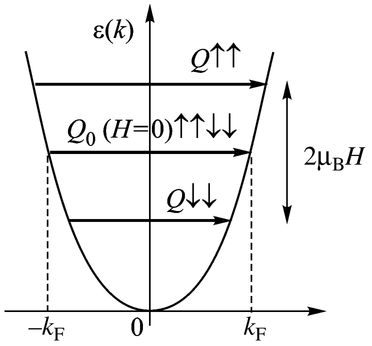

Fig. 6. Schematic diagram of the Zeeman splitting of the CDW ground state in the magnetic field.

become important. As is known (see, e.g., [4]), the electron–hole pairs forming the CDW have the parallel spins oriented conditionally upwards (↑↑) or downwards (↓↓). In the magnetic field, this degeneration is removed by the Zeeman splitting. The pairs with the upward spins increase their energy, while those with downward spins decrease it. The CDW wave vector for the ↑↑ pairs tends to increase, while that for the ↓↓ pairs, to decrease (Fig. 6). As a result, the initial CDW wave vector cannot be conserved, and the initial ground state breaks. This leads to the suppression of T_p in the field. The microscopic picture of the breakdown of field-induced CDW state has not yet been studied. For example, we can suppose the formation of the domains with the spins oriented upwards and downwards. We can also assume that the CDW transforms into a spin density wave, etc. We experimentally observe that the suppression of $\Gamma(H)$ starts in the fields higher than 25 T, which roughly meet the condition $2\mu_B H > kT_p$. Since the energy $\approx kT_p$ determines the energy of the transverse phase correlation, we can suppose that the transverse phase correlation of the CDW also begins to break in high fields. This condition means that the CDW phase dislocations can appear in the magnetic field by analogy with their appearance in the transverse electric field [10].

The numerically calculated nonmonotonic dependence $T_p(H)$ [11] also has a maximum at $2\mu_B H \approx kT_p$ close to the experimentally found condition of the maximum of $\Gamma(H)$.

The cause of vanishing the amplitude of the gap peak in high fields at a finite bias voltage still remains unclear and requires further investigations.

We are grateful to A.A. Sinchenko for assistance in carrying out the experiment and discussions of the results, to Th. Fournier for assistance in the preparation of the layered structures, and to S.A. Brazovskii and P.D. Grigor'ev for fruitful discussions of the results. This work was supported by the Russian Foundation for Basic Research (project nos. 08-02-01093-a and 06-02-72551-CNRSL-a), INTAS (project no. 05-100000-7972), and the Russian Academy of Sciences (programs "Quantum Nanostructures" and "Highly Correlated Electron Systems and Quantum Critical Phenomena").

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Translated by E. Perova