In-Chain Tunneling Through Charge-Density Wave Nanoconstrictions and Break-Junctions

K. O’Neill, E. Slot, and H. S. J. van der Zant
Kavli Institute of Nanoscience Delft, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands
R. E. Thorne
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853
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We have fabricated longitudinal nanoconstrictions in the charge-density wave conductor (CDW) NbSe$_3$ using a focused ion beam and using a mechanically controlled break-junction technique. Conductance peaks are observed below the $T_{P1} = 145$ K and $T_{P2} = 59$ K CDW transitions, which correspond closely with previous values of the full CDW gaps $2\Delta_1$ and $2\Delta_2$ obtained from photo-emission. These results can be explained by assuming CDW-CDW tunneling in the presence of an energy gap corrugation $\epsilon_2$ comparable to $\Delta_2$, which eliminates expected peak at $\Delta_1 + \Delta_2$. The nanometer length-scales our experiments imply indicate that an alternative explanation based on tunneling through back-to-back CDW-normal junctions is unlikely.

Charge-density wave (CDW) conduction remains of major interest despite its experimental discovery nearly 30 years ago. Much of the existing work has focused on transport properties of as-grown single crystals. More recently, micro/nanofabrication methods for CDW materials has allowed the study of mesoscopic CDW physics. Structures for tunneling spectroscopy are of particular interest because of the unusual gap structure with large one-dimensional fluctuation effects expected in these highly anisotropic materials, and because of predictions of unusual mid-gap excitations of the collective mode. Tunneling studies in fully gapped CDW conductors like the "blue bronze" K$_{0.3}$MoO$_3$ suffer from band-bending effects at the interface akin to semiconductor-insulator-metal junctions. These effects are absent in the partially gapped CDW conductor NbSe$_3$, which remains metallic down to 4.2 K.

Tunneling perpendicular to the direction $b$ of quasi-one-dimensional chains, along which the CDW wavevector lies, has been studied in ribbon-like whiskers of NbSe$_3$ by Scanning Tunneling Microscopy (STM). by lead contacts evaporated over the native oxide on the $b-c$ plane, and by tunneling through a gold wire or a NbSe$_3$ crystal that is laid across another NbSe$_3$ crystal, forming junctions in the $a-b$ or $b-c$ planes. Peaks in the T=4.2 K differential conductance at 35 and 101 mV, 35 mV, 36 mV and 90 mV, and 37 mV and 100 mV from metal-NbSe$_3$ junctions correspond well with the CDW gaps $\Delta_1 = 110$ mV and $\Delta_2 = 45$ mV for NbSe$_3$’s $T_{P1} = 145$ K and $T_{P2} = 59$ K CDWs as determined by angle-resolved photo-emission (ARPES). Crossed NbSe$_3$-NbSe$_3$ crystals yielded peak voltages of 60 mV and 142 mV, and interlayer tunneling in micro-fabricated NbSe$_3$ mesas yielded peaks at 50 mV and 120 mV. A single in-chain tunneling study using a gold ribbon mechanically positioned near the end of a NbSe$_3$ crystal gave a peak at 100 mV for the $T_{P1}$ CDW.

Here we demonstrate that a small constriction in a

![Image](cond-mat/0509171v3)
where $a_{k\sigma}$ ($a_{k\sigma}^\dagger$) is the electron creation (annihilation) operator for the states with wavevector $k$ and spin $\sigma$. Like conventional superconductors, the CDW condensate produces peaks in the density-of-states (DOS) at $\pm \Delta$ relative to the Fermi energy. Applying the semiconductor model for electron tunneling in superconductor junctions \[13\] to CDW systems, tunneling between occupied and unoccupied states in a CDW-insulating-CDW junction should produce peaks in the conductance at voltages equal to $\pm \Delta$. In a CDW-normal junction, peaks should be observed at voltages equal to $\pm \Delta$. To fabricate nanoscale constrictions using the FIB, a single-crystal whisker of NbSe$_3$ with a typical width of 20 $\mu$m was placed on a silicon dioxide/silicon substrate having 2 $\mu$m wide Au electrical contacts that were pre-patterned by photo-lithographic techniques. The NbSe$_3$ crystal was then carved using an FEI/Philips FIB-200 focused ion beam. At low magnification (10,000×), two large transverse cuts were made from either side to create a constriction in the b$^\ast$/b direction. At high magnification (50,000×), further line cuts were made at low currents of 350 pA until the constriction had a width of around 100 nm and its resistance (which dominated the overall sample resistance) exceeded 150 $\Omega$ at room temperature. Images of both cuts, taken in the FIB, are shown in Figure 1(b). To find the cross-sectional dimension of the junction we can make a simple estimate using the classical (diffusive) resistance formula, the contact’s room temperature resistance of 165 $\Omega$, NbSe$_3$’s bulk resistivity (1.86 $\Omega\mu$m), and a contact length of around 100 nm (estimated from the device image in Figure 1(b)), which gives a conducting area of roughly 20 nm$^2$.

Differential conductance versus voltage data was measured between $T_{P1} = 145$ K and 4.2 K using a conventional four-probe technique \[14\]. Figure 2(a) shows that the constriction’s zero-bias resistance increases monotonically with decreasing temperature, and at 4.2 K has a value close to 2 k$\Omega$. This contrasts with the bulk behavior of NbSe$_3$, which shows large resistance increases just below the two Peierls transitions and then a strong metallic (roughly linear) decrease down to 4.2 K (inset).

To fabricate constrictions by the mechanically-controlled break-junction technique, a single crystal whisker of NbSe$_3$ was placed on a Kapton-tape capped piece of flexible phosphor-bronze. The crystal was held to the Kapton, which had pre-patterned gold electrical contacts, using cellulose. The crystal was controllably broken at 4.2 K in a custom-built cryostat \[15\], which allowed the sample to be broken and re-contacted several times in the course of an experiment. Transport measurements at $T = 4.2$ K were performed in two-probe configuration, with a contact resistance of $\sim 10 \Omega$ estimated from the total sample plus contact resistance before breaking. Because of the quasi-one-dimensional bonding and very strong bonds along the chains, the NbSe$_3$ crystal’s response to stress likely involved successive breaking of fibers within its cross-section, as in the

![Graph](image-url)
The analysis of Fig. 2(b) shows the absence of any feature at $\Delta_1 + \Delta_2 \approx 145$ meV, which might be expected for tunneling between the $T_{P1}$ CDW on one side of the constriction and the $T_{P2}$ CDW on the other.

The conductance peak widths do not significantly vary below $\frac{4T}{P}$ for either transition, implying a temperature-independent intrinsic broadening of the CDW DOS. Down to the lowest temperatures, the conductance also shows a substantial tail as the voltage decreases below the gap, indicating that the DOS does not cut off sharply at the nominal gap energy. This is consistent with optical absorption measurements [17], and calculations of the zero-temperature CDW DOS with one-dimensional fluctuations [18]. Suppression of conductance peaks at $> \frac{2T}{P}$ for each CDW is likely due to the strong effect of thermal fluctuations on the DOS in a quasi-one-dimensional system [19].

Our results may be explained in terms of CDW-CDW tunneling in the presence of a transverse corrugation of the $T_{P2}$ CDW's energy gap, as shown in Figure 3. Inter-chain coupling results in band structure dispersion in momentum perpendicular to the chains ($b$-direction), which should produce transverse corrugations in the CDW gap and imperfect nesting [20]. In NbSe$_3$, the measured electrical anisotropy implies a bandwidth in the $c$-direction a factor of 10 larger than in the $a$-direction, qualitatively consistent with band structure calculations [21], so that the former should dominate in tunneling involving the $T_{P2}$ gap. Analysis of measurements on metal-NbSe$_3$ tunnel junctions at low biases [8] and of bulk low-temperature thermal and electrical conduction [22] have both suggested a transverse bandwidth comparable to the $T_{P2}$ gap itself.

We consider a semiconductor tunneling model [18] including finite transverse dispersion in the $c$-direction. This dispersion is characterized by a single parameter $\epsilon_0 = \frac{r_t^2}{2\hbar^2} \cos(bk_F)$, $t_{\perp}$ and $t_b$ being the bandwidths of the dispersion perpendicular and parallel to the chains, and $b$ the inter-chain separation. Figure 3(a) illustrates this dispersion, showing by brightness the density of states $N(E, k_{\perp})$ as a function of energy and perpendicular wave vector within one half Brillouin zone (left), and the den-
osity of states at a $N(E)$ at a fixed wavevector (right). The conductance is then calculated by integrating the product $N(E,k_f)N(E-eV,k_f)$ over all energies $E$ and wavevectors $k_f$, assuming a BCS $T = 0$ DOS broadened by a Gaussian distribution of width $\sigma = 24$ meV to mimic the experimental peak broadening. The computed $\frac{dI}{dT}(V)$ curves for $\varepsilon_2 = 0$ (no corrugation) and $\varepsilon_2 = 50$ meV are shown in Figure 2(b). As expected, with no corrugation $\frac{dI}{dT}(V)$ exhibits a strong peak at $(\Delta_1 + \Delta_2)/e$. As $\varepsilon_2$ is increased, this peak splits in energy and shrinks in height. While all conductance peaks remain visible with a divergent DOS, with a broadened DOS the peaks at $\Delta_1 + \Delta_2 - \varepsilon_2$ and $2\Delta_2$ merge at around 100 meV, resulting in a conductance curve that closely resembles the present data. The transverse gap corrugation we assume to obtain the best fit to our data is in agreement with the conclusion of Sorbier et al. \[2\] that the corrugation for the $T_p \nu$ CDW $\varepsilon_2$ is slightly larger than the CDW gap $\Delta_2$.

An alternative explanation is that the peak structure results from back-to-back N-CDW junctions. Provided that the relaxation length of the non-equilibrium distributions is long compared with the characteristic length that the relaxation length of the non-equilibrium distribution results from back-to-back N-CDW junctions. Provided an intermediate peak. We can estimate the dimensions of the constricted region assuming that the narrow region consists of NbSe$_3$ chains. The length of the constriction can be determined by comparing the low-field residual resistance ratio $\frac{R(T=293\,K)}{R(T=4.2\,K)}$ with NbSe$_3$ nanowires of different cross-sectional dimensions \[22\]. We find that our FIB junction most closely resembles a wire with resistance per unit length $R/L \sim 10^6 \, \Omega/\mu$m at 4.2 K, corresponding to a cross-section of 600 nm$^2$. From the measured junction resistance $R(T = 4.2 \, K) = 1798 \, \Omega$ we obtain a junction length $\sim 1.8$ nm. This is comparable to the known CDW amplitude coherence length in NbSe$_3$, and is too short to allow the full loss of CDW order required to achieve the tunneling characteristics of back-to-back CDW-normal junctions. Furthermore, despite the strong zero-bias low-temperature resistance increase, the FIB constriction shows no hints of anomalies at the two Peierls transitions. These are clearly seen even in the smallest cross-section nanowires (500 nm$^2$) studied to date.

The back-to-back junction interpretation might be viable if the FIB somehow disorders the constricted region in a way that eliminates the Peierls transitions and causes the resistance to increase strongly with temperature, while producing a resistivity whose magnitude is smaller than in nanowires having similar temperature dependence. But even in this case the observed zero-bias junction resistance cannot easily be accounted for \[24\]. In addition, the relevance of the back-to-back junction explanation to MCBJ samples, where the sample has simply been broken and brought back close together is unclear due to the absence of an intermediate conducting structure. We therefore attribute the conductance peaks in our devices to CDW-CDW tunneling.

In conclusion, we have fabricated in-chain nanoconstrictions in a CDW material. These constrictions behave like a tunnel junctions, and conductance peaks are observed at biases that correspond well with the full CDW gaps $2\Delta_1$ and $2\Delta_2$ determined from independent measurements. The peaks disappear at around two-thirds the respective Peierls transition temperature, in agreement with calculations of the effects of fluctuations on the DOS for one-dimensional compounds.

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