Electronic state of $NbSe_2$ investigated by STM/STS

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Abstract

Scanning tunneling microscopy/spectroscopy (STM/STS) and resistivity(ρ) measurements were performed on $NbSe_2$ single crystals in which superconductivity and charge-density wave (CDW) coexist. We found a close correlation between residual resistivity ratio (RRR) and the resistive anomaly at the CDW transition, namely, RRR increases when the resistive anomaly becomes clearer. Topographic images at 4.4 K show 3×3 CDW superposed on atomic corrugations. Number of CDW domain boundary increases with decreasing RRR, while the CDW image and the tunneling spectrum within each domain are almost independent of RRR. Such a domain structure may reduce the anisotropy in the superconducting state.

Key words: STM/STS; charge-density wave; $NbSe_2$

1. Introduction

$NbSe_2$ has been regarded as one of the conventional s-wave superconductors. However, there are some peculiar features that can not be explained in terms of the simple s-wave superconductivity. One of them is a magnetic field H dependence of the electronic specific heat coefficient γ in the vortex state. In clean $NbSe_2$, γ is a sublinear function of H, which is in stark contrast with conventional $\gamma \propto H$ behavior [1]. Such γ anomaly has been observed in superconductors having anisotropic superconducting gap (SG) with nodes [1][2]. Recently, we performed systematic γ measurements on various $NbSe_2$ crystals with different RRR and suggested that anisotropy of SG and/or Fermi surface should be responsible for the γ anomaly although the SG of $NbSe_2$ is nodeless [3].

In s-wave superconductors, such as $NbSe_2$, anisotropy of SG is known to be smeared in a dirty sample where quasi-particle mean free path l is shorter than the coherence length ξ [4]. However, the γ anomaly in $NbSe_2$ begins to disappear even in the clean sample where l is 10 times longer than ξ [3]. This fact suggests that there is an additional mechanism that smears the anisotropy of SG and/or Fermi surface. Since CDW and superconductivity coexist in $NbSe_2$, it is interesting to examine the effects of CDW on the anisotropy. In this paper, we report the results of resistivity measurements and STM/STS on $NbSe_2$ with various RRR to examine this issue.

2. Experimental

Single crystals of $NbSe_2$ were grown by iodine vapor transport method. In-plane resistivity was measured by DC 4-probe method from 2 K to 300 K. RRR is defined as $\rho(300\ \mathrm{K})/\rho(T_c)$. The sample with RRR=10 was obtained by 5% Ta doping instead of Nb. STM measurements were performed on the samples with RRR=10, 30 and 100 using ultra-high vacuum STM. The observed surfaces were prepared by *in-situ* cleavages at room temperature. STM images were taken in the constant current mode at 4.4 K. Tunneling spectra were obtained by the numerical differentiation of the current-voltage characteristics.

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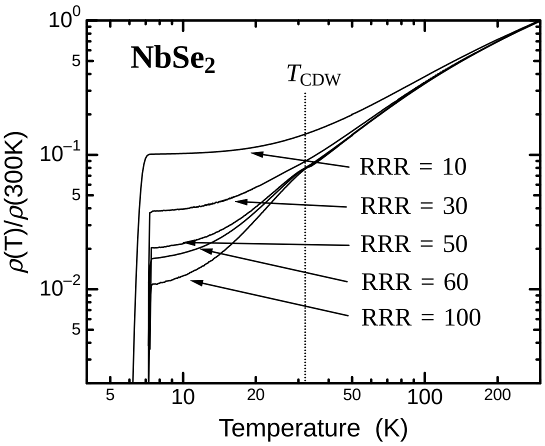

Fig. 1. Log-log plot of temperature dependence of ρ normalized by ρ(300K) for various RRR.

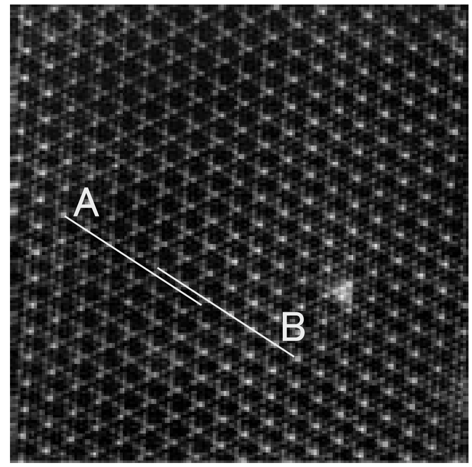

Fig. 2. Topographic image of $NbSe_2$(RRR=30) at 4.4 K. (I_t = 0.2nA, V_{sample}=10mV, 217Å scan range.)

3. Results and Discussion

Figure 1 shows the temperature dependence of in-plane ρ of various $NbSe_2$ crystals with different RRR. It is obvious that the resistive anomaly at the CDW transition temperature $T_{CDW} \sim 35$ K becomes clearer with increasing RRR. In analogy with the discussion on $2H$-$TaSe_2$ [5], which shows CDW similar to that of $NbSe_2$, this behavior can be explained as follows. Resistivity consists of three terms, namely $\rho = \rho_{phonon} + \rho_{imp} + \rho_{CDW}$. First two terms are contributions from phonon scattering and impurity scattering, respectively. Third term is a contribution from CDW phase fluctuations and is temperature independent above T_{CDW}. Below T_{CDW}, since phase fluctuations freeze up, ρ_{CDW} goes to zero at T=0. However, if the phase order of CDW is incompleted at T=0, ρ_{CDW} does not go to zero because carriers are scattered at the CDW domain boundaries. Such imperfections in the CDW phase order may be generated by small amount of impurities that hardly affect ρ_{imp}. If it is the case, CDW domain boundaries produce additional residual resisitivity with little effect on ρ above T_{CDW}. Thus RRR can be used as a measure of the completeness of the CDW phase order.

To confirm this model, we tried to image CDW directly using STM. The STM image of $NbSe_2$ with RRR=30 at 4.4 K is shown in Fig. 2. Both the atomic corrugation and 3×3 CDW modulation are clearly resolved. Line A and B, which connect the maxima of the CDW modulation from the left hand side and from the right hand side, respectively, are misaligned with just one atomic spacing. Namely, there exists a CDW domain boundary. In the sample with RRR=100, such a boundary was not observed. On the contrary, we found that the sample with RRR=10 consists of many CDW domains which may reflect the pinning by impurities. In fact, Fourier transformed STM image of the sample with RRR=10 shows that the spectral peaks which correspond to the CDW wave vectors are considerably broadened while the peaks which represent the atomic lattice still remain sharp. We found that CDW gap amplitude determined by STS is almost independent of RRR and the position where the spectrum was taken. These results support the model used to explain ρ, namely, the phase of CDW is distorted in the sample with lower RRR.

We consider that such a domain structure of CDW is responsible for the additional mechanism that smears the anisotropy of SG and/or the Fermi surface of $NbSe_2$. In the sample where CDW domain size is much longer than ξ, it may be possible that the CDW affects both the Fermi surface and the interaction which is responsible for the superconductivity in an anisotropic manner. However, if the CDW domain size becomes shorter than ξ, anisotropy of SG and/or Fermi surface which is brought by CDW should be averaged out. Actually, CDW domain size of the sample with RRR=10 is estimated to be 50∼60Å that is shorter than $\xi \sim$90Å. To study the relation between CDW and superconductivity more in detail, STM/STS at lower temperature is now in progress.

References

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