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STM spectroscopy of (TMTSF)₂PF₆

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Abstract

The SDW phase of $(TMTSF)_2PF_6$ was investigated by the electron tunneling spectroscopy using a low temperature STM. At room temperature and 86 K, the tunneling conductance is almost flat indicating metallic state. Below $T_{SDW}=11.5$ K, the spectrum shows the clear gap structure associated with the SDW state. The conductance curve is well explained by the mean field approximation for the quasi-one dimensional conductors. The SDW gap parameter Δ_{SDW} and ϵ_0 , which characterizes the transfer energy along the *b*-axis, are estimated as $\Delta_{SDW}=2.5-2.9$ meV and $\epsilon_0=2.0-2.6$ meV, respectively. The SDW-insulator-SDW tunneling spectrum was also observed.

Keywords: atomic force microscopy, scanning tunneling microscopy, metal-insulator phase transitions

1. Introduction

It is well known that a lot of quasi-one dimensional conductors undergo the density wave (DW) condensate, which is the charge density wave (CDW) or the spin density wave (SDW), as the ground state [1]. In such condensate phase of quasi-one dimensional conductors, many experiments have been developed. However, the exact shape of the electronic density of states for the DW state has been unclear, since there was less spectroscopic measurement to elucidate the electronic density of states.

The electron tunneling is the most useful spectroscopy in investigating such condensate state as DW and superconductivity [2] because of its high energy resolution. Additionally, it is easy to analyze the tunneling data: the tunneling differential conductance gives the electronic density of states directly. The electron tunneling study on the quasi-one dimensional conductor was energetically developed in the CDW state of NbSe, which is one of the most well-known inorganic quasi-one dimensional conductors. Fornel et al. [3] reported the tunneling differential resistance of NbSe₃insulator-lead junction under pressure. They claimed that the gap width decreases with increasing pressure while ratio of the gap to the transition temperature is constant. Ekino et al. [4] reported abut the both junctions of NbSe3-insulator-Au and NbSe3-insulator-NbSe₁. They explained their results by the mean field theory for quasi-one dimensional conductors [5]. In organic quasi-one dimensional conductors, the superconducting phase of $(TMTSF)_2ClO_4$ was studied by the junction method [6].

Among tunneling methods, STM spectroscopy has advantages due to its non-contacting tip configuration. There is less disturbance to the sample surface. The movable tip enables to probe the local electronic state with atomic spatial resolution.

In the present article, we report the electron tunneling study in the SDW state of $(TMTSF)_2PF_6$, which is one of the most famous quasi-one dimensional organic conductors, by using an low temperature STM.

2. Experimental

Single crystals of $(TMTSF)_2PF_6$, which are ribbon shape along the *a*-axis, were synthesized electro-chemically. The SDW transition temperature was determined as T_{SDW} =11.5 K from the resistive transition. As-grown surface of the *a-b* plane were investigated by low temperature STM.

3. Results and Discussion

Figure 1 shows the temperature dependence of the tunneling differential conductance obtained at the *a-b* surface of single crystals. As shown in the figure, there is some noise in spectra. The tunneling current in the present experiment was not stabilized well, partially due to less surface quality. It is difficult to prepare the fresh surface, since single crystals of $(TMTSF)_2PF_6$ are easily broken by a little stress. However, we could successfully obtain tunneling spectra both in the normal and SDW state. At room temperature and T=86 K, the tunneling differential conductance is almost flat, indicating the metallic state. At T=2.9 K, below $T_{SDW}=11.5$ K, the spectrum shows the clear gap structure associated with the SDW state. The conductance at zero bias voltage is well reduced to about 30 % of the normal conductance. The gap edge is observed near V=4.5 mV as the enhancement of the conductance.

At first, we tried to explain the obtained tunneling spectrum by the BCS density of states. Although the broadening of the oneelectron level is taking into account, the remained conductance inside the gap is not explained by the isotropic gap. The gap anisotropy is strongly suggested. However, the *d*-wave gap anisotropy, which is gapless, cannot explain the obtained spectrum.

In order to search for the origin of the gap anisotropy, we examine the mean field theory for quasi-one dimensional conductors [7]. The electronic band in TMTSF salts is almost one dimensional



Fig. 1. Temperature dependence of the tunneling differential conductance The zero conductance line of each curve is shifted by one division for clarity.



Fig. 2. Fitting of the calculation described in the text to the tunneling conductance at 2.9 K.

along *a* -axis. A band calculation predicted that the Fermi surface consists of a pair of slightly undulated sheet [8]. The transfer energy along the *b*-axis t_b is not negligible. Therefore, the two dimensionality in band structure must be considered. Consequently, the Fermi surface is additionally modulated and the nesting of the Fermi surface becomes imperfect. The two dimensionality of the

electronic band is represented by the parameter ϵ_0 , which is related with t_b and characterizes the imperfectness of the nesting. The conduction band is separated to two parts by the gap in the SDW state. In the case of imperfect nesting, the band dispersion of both split bands is undulated along k_b with the amplitude of ϵ_0 . Therefore, the electronic density of states is strongly modulated.

Huang et al. [5] proposed the calculation of the density of states in such an imperfect nesting DW state. The density of state spectrum in DW state has the finite gap of Δ_{SDW} - ϵ_0 , where Δ_{SDW} is the SDW gap parameter and enhancement at $\Delta_{SDW} + \epsilon_0$ instead of Δ_{snw} for the BCS prediction. We analyze the obtained tunneling spectrum according to the above calculation and the mean field theory developed by Yamaji [7]. As shown Fig. 2, in the obtained spectrum peak structure appears at 4.6 mV, corresponds to $\Delta_{spw} + \epsilon_0$. $\varDelta_{\rm SDW}$ is scaled to the transition temperature $T_{\rm e0}$ expected for the perfect nesting. The relation between $T_{\rm SDW}/T_{\rm c0}$ and $\epsilon_0/{\rm dSDW}$ is given [7]. Then we obtain parameters as Δ_{SDW} =2.5 meV and ϵ_0 =2.0 meV. The calculated density of states using above parameters is represented by the solid line in Fig. 2. Although the fitting is not always satisfactory, the qualitative behavior is explained by the model. From the fitting to the spectrum of different sample, we obtain as Δ_{spw} =2.8 meV and ϵ_0 =2.6 meV. The present estimated $\Delta_{\rm SDW}$ is consistent with the one obtained by the infrared absorption as 2.5-4.3 meV [9].

We observed another type of the tunneling spectrum, in which gap width is slightly larger and the conductance near zero bias is less than that described above. Since these spectra are often observed when we made tip contact to the sample, these spectrum is possibly due to the SDW-insulator-SDW tunneling. If small sample flakes are attached to the STM tip by contacting tip to the sample surface, the SDW-insulator-SDW tunneling would be possible. In the SDW-insulator-SDW tunneling spectrum, it is expected that the peak structure and an anomaly appear at $2\Delta_{\text{SDW}}$ and $2(\Delta_{\text{SDW}}+\epsilon_0)$, respectively [5]. The observed peak structure at V=5 mV, corresponds to $2\Delta_{\text{SDW}}$, is consistently explained with the above estimated Δ_{SDW} .

In summary, we succeeded to obtain the tunneling differential conductance in the SDW state of $(TMTSF)_2FP_6$ using low temperature STM. The tunneling spectrum is qualitatively explained by the mean field theory for quasi-one dimensional conductors. By the fitting, the gap and imperfectness parameters are estimated as Δ_{SDW} =2.5-2.9 meV and ϵ_0 =2.0-2.6 meV, respectively. We also obtained the SDW-insulator-SDW tunneling spectrum.

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