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The effect of pressure on the charge-density wave and superconductivity in $ZrTe_3$

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Abstract
The charge-density-wave (CDW) transition temperature, T_{CDW}, of $ZrTe_3$ is found to increase for pressures up to 0.6 GPa, while the superconducting transition temperature, T_c, decreases with increasing pressure. According to a band calculation, it is found that the pressure-induced enhancement of the CDW and suppression of the superconductivity are not simply explained by the effect of nesting of the Fermi surface, suggesting the possibility of a new relation for the competition between the CDW and superconductivity.

1. Introduction

Over the past decade there has been considerable interest in charge-density-wave (CDW) transitions in transition metal trichalcogenides, MX_3 (M = transition metal, X = S, Se, Te). Among them, $ZrTe_3$ is unique, because an electron diffraction experiment [1] and a calculation of the Fermi surface [2, 3] show that the CDW nesting vector has no component in the chain-axis direction, only components perpendicular to the chain axis. In fact, a hump-like resistance anomaly is observed near 63 K when the current is supplied parallel to the *a*-axis, but no anomaly is observed in the resistance parallel to the *b*-axis [4]. Furthermore, $ZrTe_3$ enters a superconducting state at about 2 K [4]. However, the superconductivity is not of bulk nature but filamentary. The superconducting transition measured in the resistance parallel to the *a*-axis is wide and explained well by a one-dimensional fluctuation effect [4]. These features of the CDW and the superconductivity of $ZrTe_3$ lead us to be interested in whether the competition between the CDW and the superconductivity is explained by the usual effect of nesting of the Fermi surface.

In this paper, we report on experimental results on effects of pressure on the CDW and the superconductivity of $ZrTe_3$. We find pressure-induced enhancement of the CDW and suppression of the superconductivity, which is contrary to results observed for many quasi-one-dimensional metals. The possibility of a new relation for the competition between the CDW and superconductivity is discussed from the viewpoint of the filamentary nature of the superconductivity in $ZrTe_3$.

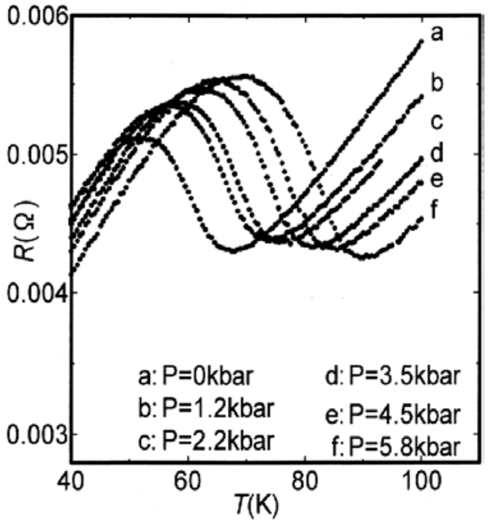

Figure 1. The temperature dependence of the resistance near T_{CDW} under various pressures.

2. Experiments

Single crystals are prepared by the chemical transport method using iodine as the transport agent. The pressure was generated by use of a piston and a clamp-type cylinder. The pressure-transmitting liquid was a 1:1 mixture of Fluorinert FC70 and FC77. Pressures were estimated from the pressure dependences of T_{CDW1} and T_{CDW2} in $\mathrm{NbSe_3}$ based on a previous result [5]. The resistance was measured by a usual four-probe dc method, where a current is supplied parallel to the a-axis. The samples were attached to four gold wires with Dupon silver paint (No 4929).

3. Results and discussion

Figure 1 shows the temperature dependence of the resistance between 40 and 100 K under various pressures. At ambient pressure a hump-like resistance anomaly associated with the CDW transition is observed around 60 K, which agrees with the previous result [4]. The temperature where the resistance anomaly appears rises with increasing pressure. Furthermore, the magnitude of the resistance anomaly is also enhanced by increased pressure. These results suggest a strongly pressure-induced enhancement of the CDW in $\mathrm{ZrTe_3}$.

Figure 2 shows the temperature dependence of the resistance near the superconducting transition temperature, T_c, under various pressures. The superconducting transition curves are shifted to lower temperatures with increasing pressure. In contrast to the pressure-induced enhancement of the CDW, the superconductivity is suppressed by increased pressure. Since the transition width is broad because of the filamentary nature of the superconductivity, we define three kinds of T_c as follows: the temperature corresponding to the onset of the transition, T_1, and the intercepts of the linear extrapolation of the transition curve to the normal value of resistance, T_2, and to zero resistance, T_3.

Figure 3 shows the pressure dependence of T_1, T_2, and T_3. All T_cs decrease almost linearly with increasing pressure in the pressure region of the measurements. The transition width defined as $T_1 - T_3$ decreases with increasing pressure. This means a good hydrostaticity under high pressures. However, the relative transition width, $(T_1 - T_3)/T_3$, increases under pressure, suggesting pressure-induced enhancement of the superconducting fluctuation.

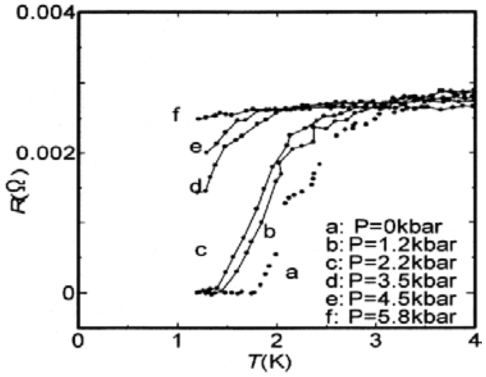

Figure 2. The temperature dependence of the resistance near T_c.

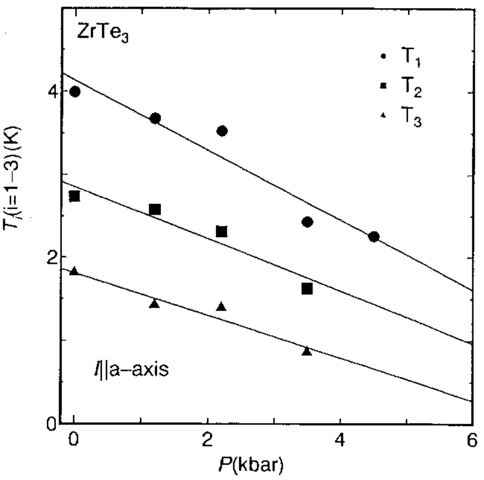

Figure 3. Pressure dependences of T_{c1}, T_{c2}, and T_{c3}.

According to the theory of Aslamazov and Larkin, the excess conductivity due to one-dimensional superconducting fluctuation, σ', is expressed by

$$\sigma' = (2\pi^2 e^2 \xi_0 / 16hS)[(T - T_c)/T_c]^{-3/2}.$$

Here, e is the electron charge, ξ_0 a coherence length at $T = 0$ K, S the cross-sectional area of a superconducting filament, h Planck's constant, and T_c a mean-field transition temperature. Figure 4 shows the relation of σ' versus $[(T - T_c)/T_c]^{-3/2}$ at pressures of $P = 0$ and 22 kbar, where σ' is calculated from data shown in figure 2 and T_3 is used as T_c. A good linear relation is observed at both pressures; the one-dimensional superconducting fluctuation effect appeared even under pressure. The value of S estimated is reduced from 2500 (±200) Å^2 at $P = 0$ kbar to 1700 (±200) Å^2 at $P = 2.2$ kbar. This suggests that the Josephson coupling between filaments is suppressed by increased pressure. It should be noted that the present result is in contrast with the normal behaviour in which pressure enhances the Josephson coupling between filaments.

Figure 5 shows T_{CDW} and T_3 plotted as a function of pressure. Here, T_{CDW} is defined as the temperature corresponding to the maximum value of $\mathrm{d}R/\mathrm{d}T$. Both T_{CDW} and T_3 varied linearly with increasing pressure. The pressure coefficient of T_{CDW} is $(\mathrm{d}T_{\mathrm{CDW}}/\mathrm{d}P)/T_{\mathrm{CDW}} \sim$ +0.07 kbar^{-1}, while that of T_3 is $(\mathrm{d}T_3/\mathrm{d}P)/T_3 \sim -0.14$ (±0.01) kbar^{-1}. Comparing the absolute value of the pressure coefficient for T_{CDW} and T_3, we find that the value for T_3 is about double that for T_{CDW}. The large difference in magnitude of the pressure coefficient between T_{CDW} and T_3 suggests that competition between the CDW and the superconductivity is not occurring on the same Fermi surface. This is consistent with the result of the band calculation where the CDW is formed on a Fermi surface with the character of 3p electrons of the Te atom, while the superconductivity is formed on a Fermi surface with the character of 3d electrons of the Zr atom [2, 3]. Furthermore, the band calculation predicts that the CDW would be suppressed by increased pressure, because the Te–Te chain interactions parallel to the a-axis increase with increasing pressure. These experimental and theoretical results suggest strongly that the competition between the CDW and the superconductivity is not simply explained by the effect of nesting of the Fermi surface.

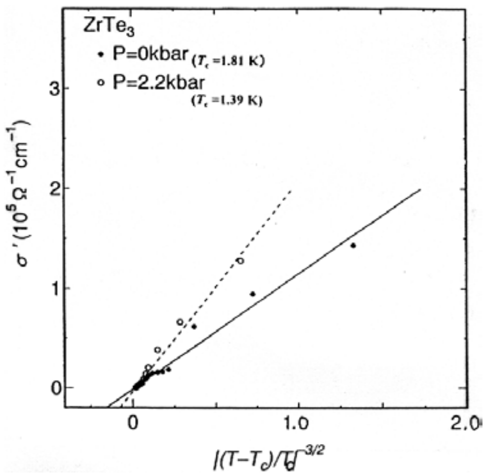

Figure 4. Excess conductivity due to one-dimensional superconducting fluctuation as a function of temperature.

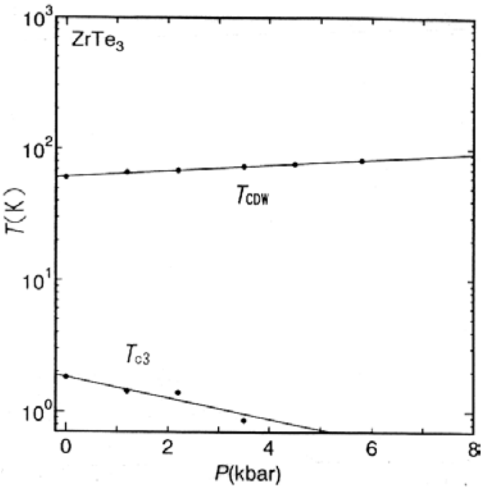

Figure 5. Pressure dependences of T_{c3} and $T_{\rm CDW}$.

When we consider possible explanations other than the effect of nesting of the Fermi surface, it is important to pay attention to the correlation between the enhancement of the CDW and the suppression of the Josephson coupling under pressure. Since the CDW nesting vector is $\boldsymbol{q} \sim (1/14, 0, 1/3)$ [1], the CDW in real space can be represented as a wave with wavelength components of (∼80 Å, 0, ∼30 Å). The large component is in the direction parallel to the a-axis—that is, parallel to the superconducting filaments. Thus, the Josephson coupling between the superconducting filaments is coupled through the CDW region; the strength of the Josephson coupling depends on the amplitude of the CDW. This suggests that competition between the CDW and the filamentary superconductivity occurs in real space. To make the competition in real space clearer, we need to measure the superconducting transition in the direction of the Josephson coupling, parallel to the b-axis. Such measurements are in progress.

In the present situation, the origin of the pressure-induced enhancement of the CDW in ZrTe$_3$ is an open question. Further studies, such as diffraction experiments under pressure, are required.

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