

Anderson Localization of 1T-TaS₂

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1T-TaS₂ with a layered structure has been recently investigated by many researchers because it has a strong charge density wave (CDW) fully to destroy the original Fermi surface and shows Anderson localization at low temperatures. The main origin of this localization is crystalline defects. 1T-phase of TaS₂ is stable above 750°C and is retained at room temperature by quenching, which introduces the vacancies in the crystal. Furthermore, the constitutional tantalum is self-intercalated in the Van der Waals gap site during the crystal growth. The present paper reports the electrical and magnetic properties of 1T-TaS₂ with different intra- and inter-layer crystalline defects.¹⁻³⁾

(1) Electrical resistivity

Figure 1 shows the temperature dependence of electrical resistivity for two typical samples.

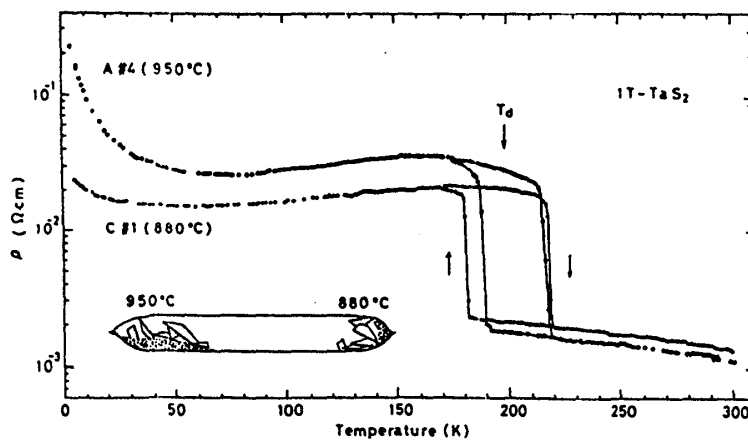
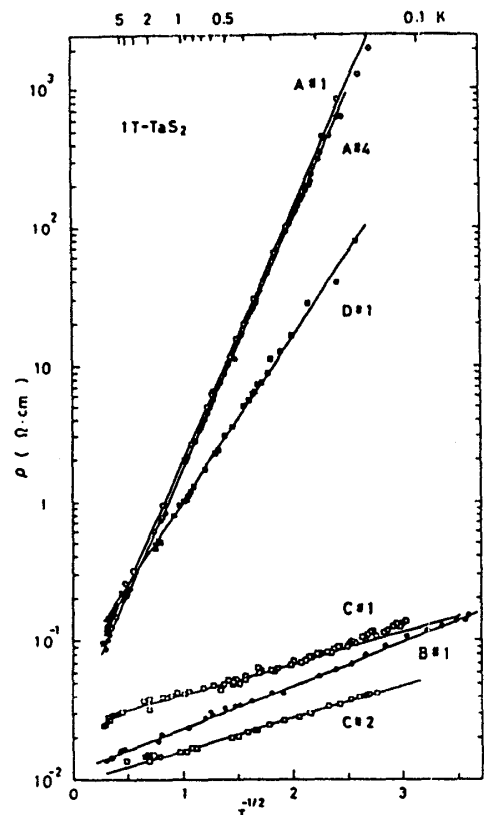


Fig. 1 Temperature dependence of 1T-TaS₂ (A & C-samples).

Fig. 2 Electrical resistivity of 1T-TaS₂ in the temperature region of 10K to 0.1K, where the abscissa is taken as $T^{-1/2}$.



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Growth temperatures are 950°C (A-sample) and 880°C (C-sample), respectively, as shown in the insert of Fig.1. The A-single crystal was grown in the hotter part of the quartz tube where the powder materials were put out. On the other hand, the C-single crystal was grown at the lower temperature part where the excess sulphur vapor is high in the density. Therefore, the A-sample should have much crystalline(inter-layer) defect compared with the C-sample. The resistivity increase at low temperatures is due to the variable range hopping conduction of Anderson localization, which is enhanced for the A-sample with a much defect.

Futhermore, Fig.2 shows the electrical resistivity of 1T-TaS₂ at lower temperatures, ca. 10-0.1K, where the temperature axis of abscissa is taken as $T^{-1/2}$. The logarithmic resistivity data for 1T-TaS₂ with different crystalline defects fit with a $T^{-1/2}$ dependence, which is the same result for the previous data by Kobayashi and Muto⁴⁾ and the present authors⁵⁾. On the other hand, it is not in agreement with the $T^{-1/3}$ one by DiSalvo and Graebner⁶⁾, which is simply expected in the possible quasi-two dimensional nature of the layered material.

(2) Hall coefficient

Figure 3 shows the temperature dependence of Hall coefficient of 1T-TaS₂. At a nearly commensurate - commensurate CDW transition of $T_d =$ ca. 200K, the electrical resistivity increases from $2 \times 10^{-3} \Omega \cdot \text{cm}$ to $3 \times 10^{-2} \Omega \cdot \text{cm}$ when the temperature is lowered and the corresponding carrier concentration decreases from $4 \times 10^{21} \text{ cm}^{-3}$ (a negative Hall coefficient) to $4 \times 10^{19} \text{ cm}^{-3}$

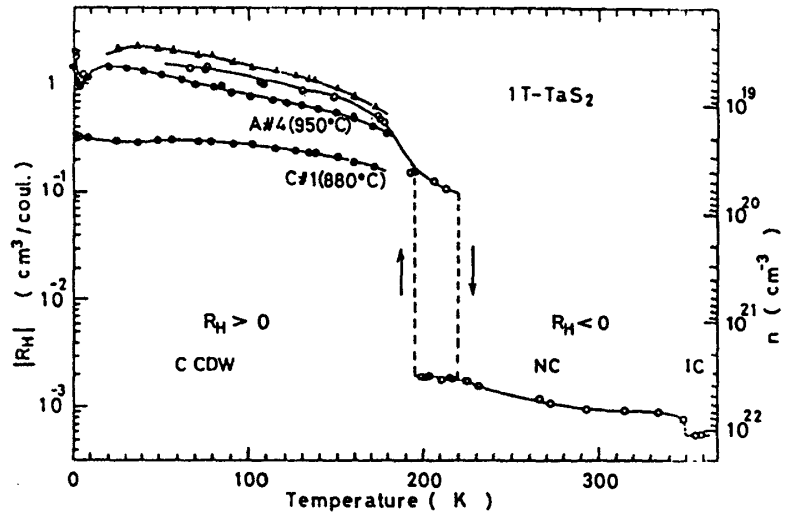


Fig.3 Temperature dependence of Hall coefficient of 1T-TaS₂.

(a positive one) under a single carrier model.^{1,7)} The Hall coefficient for the A-sample with a much defect has a peak around 20-40K, while constant for the C-sample with less defects.

(3) Magnetoresistivity

Large positive and negative magnetoresistances associated with the Anderson localization in 1T-TaS₂ was reported by Kobayashi and Muto⁴⁾ and the present authors^{2, 5)}. The negative magnetoresistance was explained by Fukuyama and Yosida⁸⁾ in such a way that

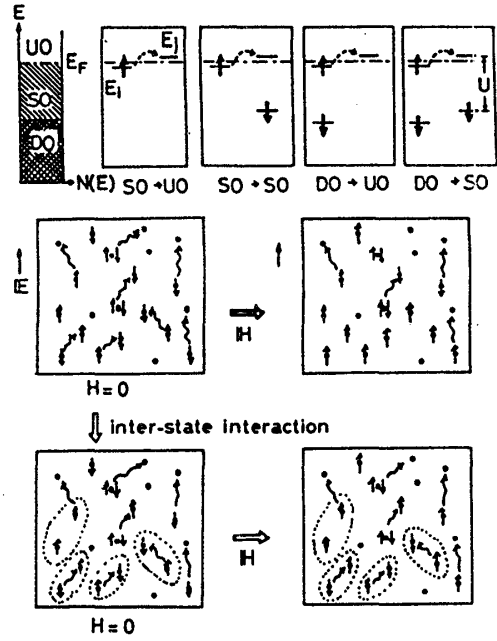
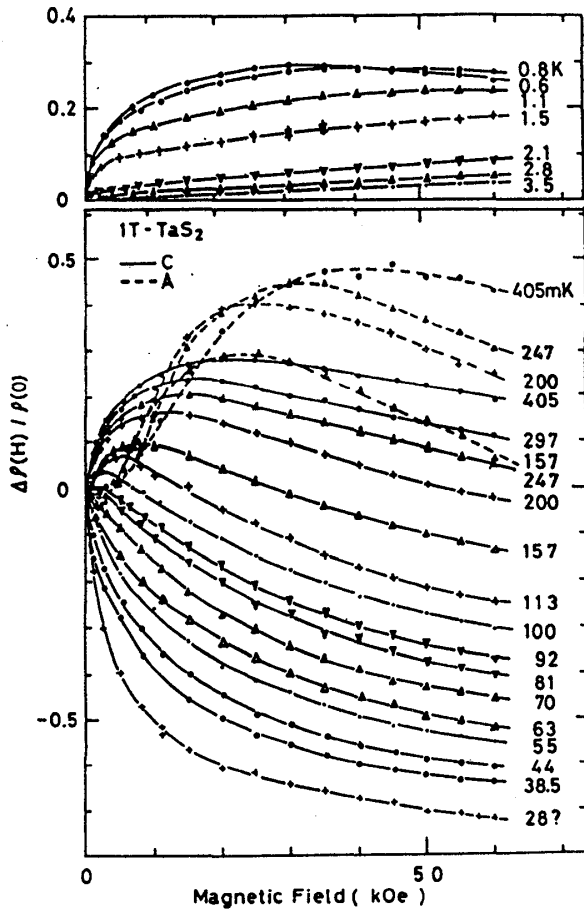


Fig.5 Hopping processes in the presence of intra- and inter state correlations.

Fig.4 Magnetoresistance of 1T-TaS₂ (A & C-samples).

the highest occupied state has an upward linear Zeeman shift to make the energy difference between the mobility edge E_c and the Fermi energy E_F smaller under magnetic fields and to make the hopping conduction larger. Figure 4 shows an overall trend of magnetoresistances from negative to positive with the increase of temperature, which has been explained in the following way by Kamimura, Takemori and Kurobe.⁹⁾ For the localized electrons which make hopping conduction, the intra-site and inter-site correlations should be taken into account. For the former correlation, four kinds of hopping processes exist as shown in Fig.5, where SO, UO and DO mean singly occupied, unoccupied and doubly occupied states, respectively, and U the correlation energy. All of these four processes contribute to the conductivity in the absence of magnetic field. The processes SO+SO and DO+UO trend to be suppressed under the applied field. Therefore, the positive magnetoresistance increases with the increase of magnetic field and saturates above a certain field, while the Zeeman effect dealt by Fukuyama and Yosida decreases the magnetoresistance. The magnetoresistance is then expected to have a maximum at a certain field, as shown in Fig.4. At low enough temperature, the inter-site correlation plays such a role that an antiferromagnetic coupling between two SO-states stops the spin flip under the field and the suppression of SO +SO and DO+UO transitions are released. Thus the negative magnetoresis-

tance takes place due to the Zeeman effect again.

(4) Magnetic susceptibility

Figure 6 shows the temperature dependence of magnetic susceptibilities of $1T-TaS_2$ and $1T-TaS_{1.7}Se_{0.3}$. The susceptibility consists of a diamagnetic part and a paramagnetic one. The paramagnetic contribution appears below ca. 100K and shows a

Curie like temperature dependence, which is not due to the magnetic impurities but due to the correlation effect of

Anderson localized electrons.¹⁰⁾ Replacing sulphur by selenium makes a intra-layer random potential, which scarcely changes the carrier concentration and enhances the localization.⁵⁾ Namely, a density of the paramagnetic moments of about one in 10^3 Ta atoms is twice larger than the one of $1T-TaS_2$.

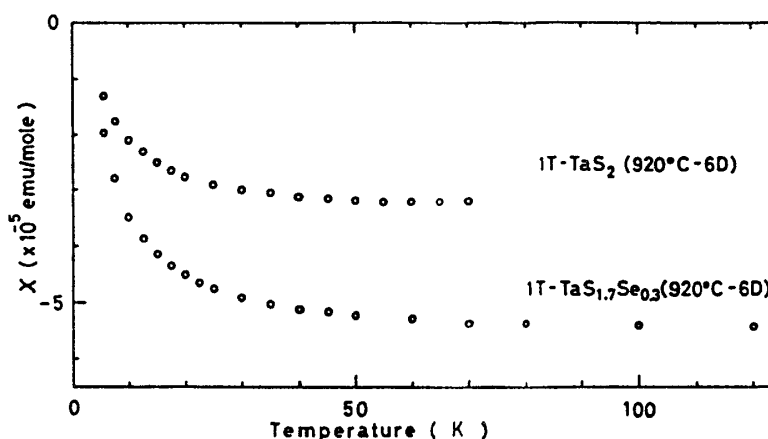


Fig.6 Temperature dependence of magnetic susceptibilities of $1T-TaS_2$ ($\chi = (11.5/(T-2.5) - 3.42) \times 10^{-5}$ emu/mole) and $1T-TaS_{1.7}Se_{0.3}$ ($\chi = (22.7/(T-0.08) - 5.64) \times 10^{-5}$ emu/mole).

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