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HOPPING CONDUCTIVITY IN THE PEIERLS GAP IN HYDRAZINE INTERCALATED TaS_2

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Abstract The hydrazine intercalation complexes formed with the layered compound 1T-TaS_2 exhibit very strong Fermi surface driven structural distortions. They are non-metallic below room temperature due to Anderson localization of states near the Fermi level which lies in the Peierls pseudo-gap. Resistivity, ρ, and thermopower, S, measurements indicate that transport is by variable range hopping, and a proportionality is demonstrated between $\ln\rho$ and $\sqrt{(S/T)}$ over a wide temperature range. The conduction mechanism in this intercalation complex may be compared with that in lightly-doped polyacetylene, in which the Fermi level also falls in the Peierls gap.

1T-TaS_2 belongs to a class of "two-dimensional" metals which have a layered structure and exhibit Fermi surface related structural phase transitions[1,2]. Hydrazine may be intercalated reversibly between the layers[3,4] and two complexes are produced, $3R_I$ with $0 < x < 2/3$ and $3R_{I.I}$ with $2/3 < x < 4/3$. Each shows a well-defined layer separation indicating one and two layers of hydrazine respectively between adjacent layers of the host material[5].

The intercalated materials are non-metallic as shown in figure 1 where the resistivities of the $x = 2/3$ and $x = 4/3$ complexes are compared with that of the pure material which has an incommensurate to commensurate Peierls transition at $\sim$ 200K and shows weakly non-metallic behaviour below 50K. In a previous paper[4] we present evidence for an intercalate induced enhancement of the Peierls pseudo-gap to $\sim$ 1eV in the $3R_{I.I}$ complex and for Anderson

localization of the electronic states near the Fermi level, E_F, which lies in this gap. We discuss here the mechanism of conduction in the light of recent transport measurements.

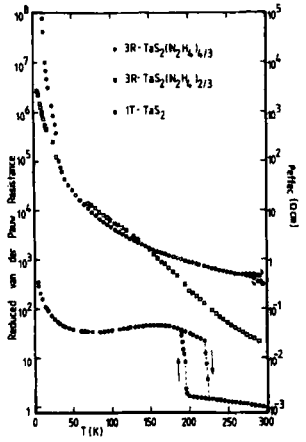

FIGURE 1 Resistivity of 1T-TaS_2 and the two hydrazine intercalation complexes

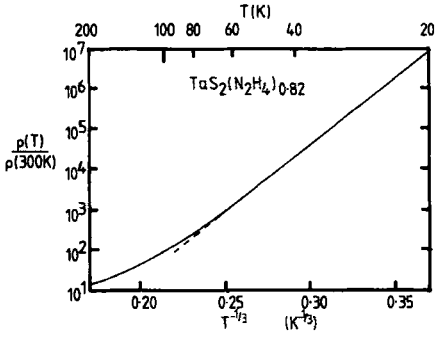

FIGURE 2 Logarithm of resistivity of $TaS_2(N_2H_4)_{0.82}$ plotted against $T^{-1/3}$

The temperature dependences of the resistivity for both complexes do not show simple activated behaviour but for the $3R_{I.I}$ material, the plot in figure 2 shows that the two dimensional variable range hopping (VRH) relation $\rho = \rho_o \exp[T_o/T]^{1/3}$ is approximately obeyed with $T_o = 4.6 \times 10^5$K (fitting below 100K). If we assume a localization length, α^{-1}, of 10Å, this value of T_o corresponds to a density of states, $N(E_F) \sim 1.3 \times 10^{20} eV^{-1} cm^{-3}$ [4,7]. Such a value is a factor of 100 below the typical metallic value for a d-band and is an acceptable value for E_F located in the Peierls pseudo-gap.

The thermopower, S, for the $3R_{I.I}$ complex is plotted in figure 3 and has a large negative value which shows little variation with temperature. For activation to a mobility edge at E_C, $S \propto (E_C - E_F)/k_B T$ and a strong temperature dependence is expected[7]. On the other hand, for VRH, $S = A(k_B/e)^2 . \gamma . (W^2/k_B T)$ where W is the most probable hopping energy at a given temperature, $\gamma = (1/N)(dN/dE)|_{E_F}$ and A is a constant with a model dependent value[7,8,9] between 0.5 and 0.05. For VRH in a constant density of states $W \propto T^{3/4}$ in 3D and $W \propto T^{2/3}$ in 2D. Clearly the density of states is not constant (otherwise $\gamma = 0$) but a similar type of relation between W and T is expected which would lead only to a weak dependence of S on T (S is constant if $W \propto T^{1/2}$). We conclude that conduction in the $3R_{I.I}$ material is by VRH and not by activation to a mobility edge.

It is interesting to note that the resistivity in the VRH regime may be expressed as $\rho = \rho_o \exp[(1+m)W/k_B T]$ where m is related to the effective dimensionality for hopping by $W \propto R^{-m}$ and R is the most probable hopping range at a given temperature. We may relate this with the expression for thermopower discussed above to obtain the relation $\ln \rho = \ln \rho_o + (1+m) B \sqrt{(S/\gamma T)}$. Thus, for γ constant, $\ln \rho \propto \sqrt{(S/T)}$ for any dimensionality. This is the behaviour observed in figure 4 over a much wider range of temperature than the range over which $\ln \rho$ is proportional to $T^{-1/3}$ in figure 2.

From this plot we estimate a value $4 < \gamma < 40 eV^{-1}$ (the range reflects the different values calculated for A). For an incommensurate PLD we expect E_F to lie in the middle of the Peierls pseudo-gap and hence a small value for γ. However, if the PLD is commensurate E_F will be displaced from the centre of the Peierls gap and γ may be quite large. We consider the value estimated for γ to be acceptable in the present case where the PLD is commensurate[6].

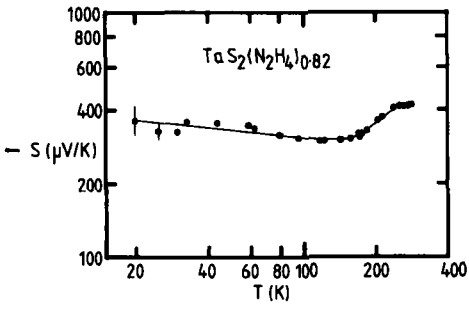

FIGURE 3 Thermopower vs. T in $TaS_2(N_2H_4)_{0.82}$

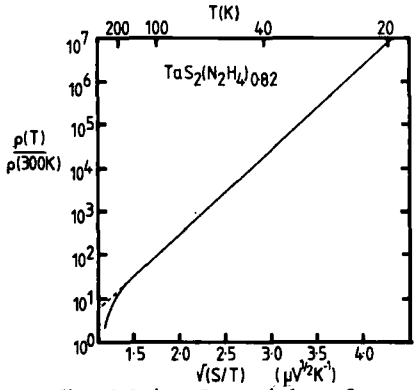

FIGURE 4 Logarithm of resistivity vs. square root of thermopower divided by temperature in $TaS_2(N_2H_4)_{0.82}$

Finally, we point out that a close relationship may exist between the conduction mechanism in the present intercalation complexes and that in lightly-doped samples of polyacetylene which exhibit non-metallic properties. In those samples the Fermi level should also lie in the Peierls gap, the gap between the soliton and conduction bands[10].

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