Electrical conductivity of the uniaxially strained quasi-one-dimensional Peierls insulator TaS_3

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A strong, nonmonotonic dependence of the conductivity of TaS_3 on the uniaxial strain of the sample has been observed over a wide range of temperatures near and below the Peierls transition temperature. Possible mechanisms explaining the observed phenomena are discussed.

Because of its clearly defined, low-dimensional properties, tantalum trisulfide is the most suitable material for studying experimentally the properties of a quasi-one-dimensional electron gas. At $T_p = 215$ K TaS_3 transforms from the high-temperature metallic phase to the Peierls insulator state with an "almost commensurate" ($\lambda = 4$ cm) charge density wave (CDW).[1,2] In this state it exhibits several unusual properties related to the existence and motion of the CDW: strong nonlinear conductivity, anomalously high dielectric constant ($\epsilon \approx 10^7$), and generation of high-frequency electric oscillations accompanying the passage of a CDW.[1,3]

The least studied aspects of quasi-one-dimensional conductivity are those associated with commensurate-incommensurate transitions in systems with CDW and with the effect of the interaction between conducting chains on the mobility of charge carriers and the stability of single-particle excitations in quasi-one-dimensional conductors.[4] The solution of these problems requires a systematic study of the properties of quasi-one-dimensional compounds under conditions when the lattice parameters change.

We have studied the effect of uniaxial tensile strain S in the direction of the conducting chains (c axis) on the electrical conductivity $\sigma^{\parallel}$ of orthorhombic TaS_3 in the temperature range 65–315 K, which includes the region of existence of CDW, where the conductivity in weak fields is attributable to the thermal excitation of carriers through the Peierls gap, and the region of metallic conductivity.

Samples of orthorhombic TaS_3 comprised of whiskers 3–5 mm long with characteristic diameters of several microns were obtained by using the procedure we described previously.[3] The uniaxial extension of the samples was realized with the help of a strain converter proposed in Ref. 5. The samples were attached to an extension device with silver paste, which simultaneously served as a conducting electrode, or by means of gold clamping contacts. Both methods give identical results. In order to avoid the nonlinear contribution to the conductivity, the measurements were performed in weak fields ($E < 100$ mV/cm) with a dc current or 66-Hz ac current.

For all samples investigated, the following characteristic features are observed (Fig. 1). The changes in the conductivity with $S < 2\%$ are completely reversible. For small extensions and temperatures above 80 K the conductivity increases linearly with the strain. The strain-sensitivity coefficient

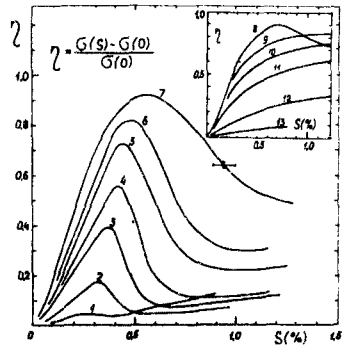

FIG. 1. Strain dependence of the relative change in the electrical conductivity of TaS_3 at different temperatures. 1) 65 K; 2) 95 K; 3) 125 K; 4) 145 K; 5) 165 K; 6) 175 K; and, 7) 185 K. The inset: Evolution of strain curves near the Peierls transition [199 K (8); 206 K (9); 211 K (10); 217 K (11); 232 K (12); 264 K (13)].

$$\beta(T) = \frac{1}{\sigma(0, T)} \frac{\partial\sigma(S, T)}{\partial S}$$

(Fig. 2) varies slightly from sample to sample; moreover, after repeated (> 50) cycles of extension of the sample, β increases (by $\sim 20\%$), whereas $\sigma(0,T)$ remains unchanged, at least to within 3% (Fig. 2). For large extensions the conductivity drops sharply. The magnitude of the strain S^* corresponding to the sharpest drop in the conductivity depends strongly on the temperature (the inset in Fig. 3).

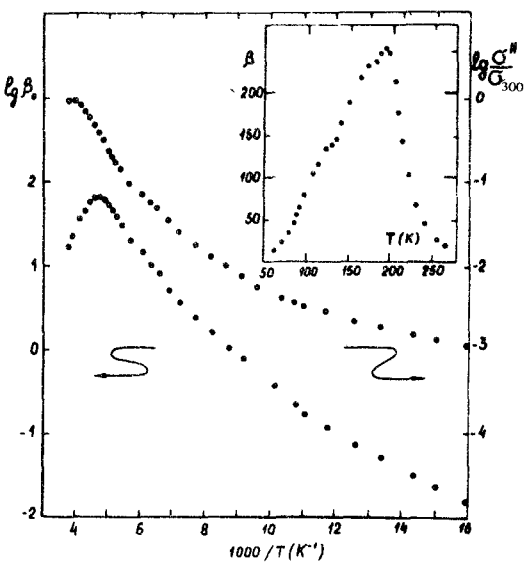

FIG. 2. Temperature dependence of the coefficient $\beta_0 = (1/\sigma(0, 300))(\partial\sigma(S,T)/\partial S)$ and of the normalized electrical conductivity $\sigma^{\parallel}/\sigma_{300}$. The inset: Temperature dependence of the strain-sensitivity coefficient $\beta = (1/\sigma(0, T))(\partial\sigma(S,T)/\partial S)$

The strain-induced change in the conductivity of TaS_3, we might note, is unexpectedly large, exceeding by almost an order of magnitude the effects observed in ordinary metals and semiconductors in the absence of structural and electronic phase transitions. Similar studies have not been performed for other quasi-one-dimensional materials.

The dependence of the conductivity of TaS_3 on the strain could be due to both a change in the carrier mobility and a change in the size of the Peierls gap Δ, which is associated with the change in the width of the conduction band and of the phonon spectrum. A decrease in the width of the conduction band (and, correspondingly, the Fermi energy ϵ_F) would be expected to be the dominant factor in this case. From

$$\Delta \sim \epsilon_F \exp\left(-\frac{1}{\lambda}\right), \tag{1}$$

where $\tilde{\lambda} = g^2/\omega_Q \epsilon_F$ (g is the electron-phonon coupling constant, and ω_Q is the frequency of the phonon mode, $Q = 2k_F$), it follows that the derivative

$$\frac{1}{\Delta}\frac{d\Delta}{d\epsilon_F} = -\frac{1}{\epsilon_F}\left(\frac{1-\lambda}{\lambda}\right)$$

is always negative. Consequently, the conductivity should decrease when the sample is extended. Thus the change in the width of the gap cannot explain the behavior of $\sigma(S)$, at least for small strains. Furthermore, if it is assumed that the strain-induced increase in the conductivity is a consequence of the change in the gap width, then the experimentally observed increase in the conductivity by a factor of nearly two should correspond to a decrease of Δ by approximately 15%. As is evident from Fig. 3, however, the gap width in TaS_3 (and T_p associated with it) remains virtually unchanged under the strain.

Thus the strain dependence of the conductivity which we observed is primarily related to changes in the mobility, rather than to the change in the gap width.

The strain dependence of the relative change in the conductivity η can be represented in the form

$$\eta(S) = \alpha_1 S_\parallel + \alpha_2 S_\parallel^2 + \alpha_3 S_\perp + \alpha_4 S_\perp^2 \alpha_5 S_\perp S_\parallel + \ldots, \tag{2}$$

where $S_\parallel$ and $S_\perp$ are related by Poisson's relation. An approximately twofold increase in the conductivity of TaS_3 is observed under hydrostatic compression up to 13 kbar.[6] Since in our experiments the change in the conductivity due to small extensions depends linearly on the strain, and since it has the same sign as under hydrostatic compression of the samples in Ref. 6, we can assume that it is associated primarily with the third term, rather than with the first and second terms in (2), which takes into account the transverse compression of the sample that accompanies the convergence of the conducting filaments.

The coefficient $\beta_0 = (1/\sigma(0, 300))(\partial\sigma(S,T)/\partial S)$ varies with temperature according to an activation law with $E_\beta \simeq 800$ K. Here E_β, like $E_\sigma^\perp$ (the activation energy of conductivity in a direction perpendicular to the chains), is approximately constant over the entire temperature range studied, whereas $E_\sigma^\parallel$ decreases by a factor of ap-

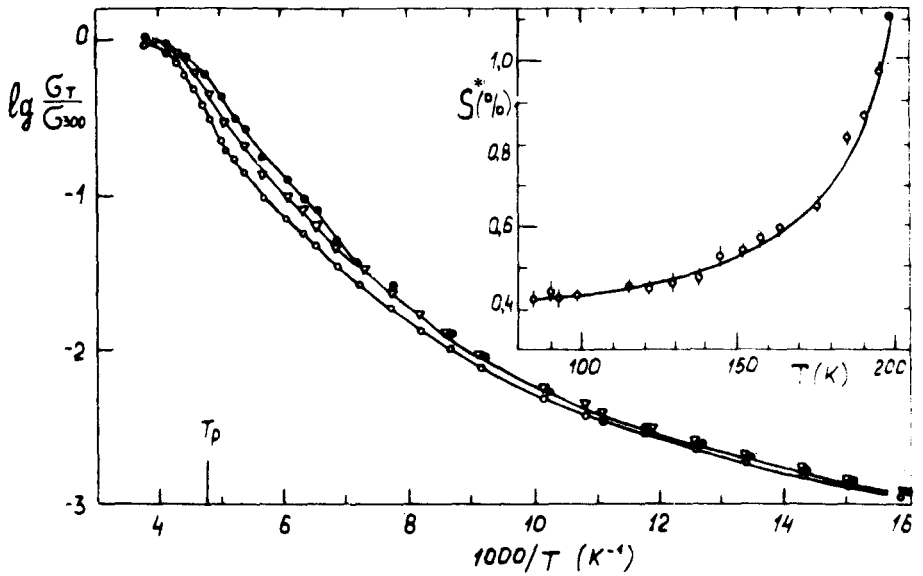

FIG. 3. Dependence of the normalized electrical conductivity on $1/T$ for three fixed values of the strain on the sample. 1) $S=0$; 3)$S=0.25\%$; 2) $S=0.45\%$; $(\sigma_{300}\approx 2\times 10^3\ (\Omega\ \text{cm})^{-1}$. The inset: The temperature dependence of S^*. The solid curve corresponds to the equation $S^*=(A/(T_p-T)^{1.04})+C$.

proximately three at $T<100$ K (Fig. 2). This also confirms the assumption that the strain-induced increase in conductivity is caused by the enhanced interaction between chains.

We shall examine some of the possible mechanisms which account for a strong dependence of the longitudinal conductivity on the transverse compression of the sample. If structural defects, inhibiting the motion of charge carriers along a chain, are present in a quasi-one-dimensional material, then the longitudinal conductivity will depend on the transfer of electrons from chain to chain, bypassing the "nonconducting" section. In this case, the longitudinal conductivity will increase as the distance between chains decreases. In addition to the breaks in the filaments, such defects in TaS_3 can also be the "nonconducting" sections of the chains with a different charge state of the sulfur atoms, as in the case of $NbSe_3$.

Free charge carriers, as we know, cannot exist in a weakly coupled one-dimensional system, since they are transformed in a time on the order of I/ω_{ph} into less mobile solitons or polarons due to a strong polarization of the CDW.[4] The interchain coupling suppresses this instability, i.e., it increases the lifetime of the carriers. The transverse compression of the sample in this case will also increase the conductivity.

Thus, although the reason for the strong changes that we observed in the conductivity remains unclear, our data, taken collectively, show that these changes seem to be related to the dependence—peculiar to quasi-one-dimensional system—of the mobility of charge carriers on the interaction between chains.

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