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Wolfgang Brütting, W. Rieß, P. H. Nguyen, G. Paasch

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Charge Density Wave Transport in Quasi-One-Dimensional Semiconductors

W. Brütting, W. Rieß[a], P.H. Nguyen
Experimentalphysik II and Bayreuther Institut für Makromolekülforschung (BIMF), Universität Bayreuth, D-95440 Bayreuth, Germany

G. Paasch
Institut für Festkörper- und Werkstofforschung, IFW Dresden eV., D-01171 Dresden, Germany

A model for the dc conductivity in quasi-one-dimensional charge density wave conductors is presented that allows for a determination of the magnitude and temperature dependence of both the Peierls gap below and the pseudogap above the phase transition. The application to different systems shows that there is a common dc conduction mechanism in organic and inorganic CDW materials. The theory enables us also to calculate related transport properties such as carrier concentration, mobility, scattering time, and mean free path directly from conductivity data.

1 Introduction

Due to their low-dimensional electronic structure in many quasi-one-dimensional (Q1D) conductors a metal-semiconductor transition (Peierls transition) to a charge density wave (CDW) ground state occurs at low temperatures [1,2]. A central feature of the Peierls transition is the occurence of fluctuations in a wide temperature range above the transition temperature. A direct consequence of these fluctuations is the formation of a pseudogap in the electronic density of states at the Fermi level. Though the theoretically determined density of states of the fluctuating gap has not been seen directly in experiments, there are various experiments like diffuse x-ray scattering, static magnetic susceptibility, and optical reflectivity that give evidence for the presence of CDW fluctuations in Q1D conductors [1]. Thus the independent determination of the temperature dependence of the gap below and above the transition temperature directly from dc conductivity data can provide additional information about fluctuation effects in Q1D CDW conductors.

2 DC Conductivity and Energy Gap

Fig. 1 shows the temperature dependence of the dc conductivity of the organic radical cation salt $(Fa)_2PF_6$ (Fa=fluoranthene=$C_{16}H_{10}$)[3], the molybde-

[a] now at: IBM Research Center, Zürich, Switzerland

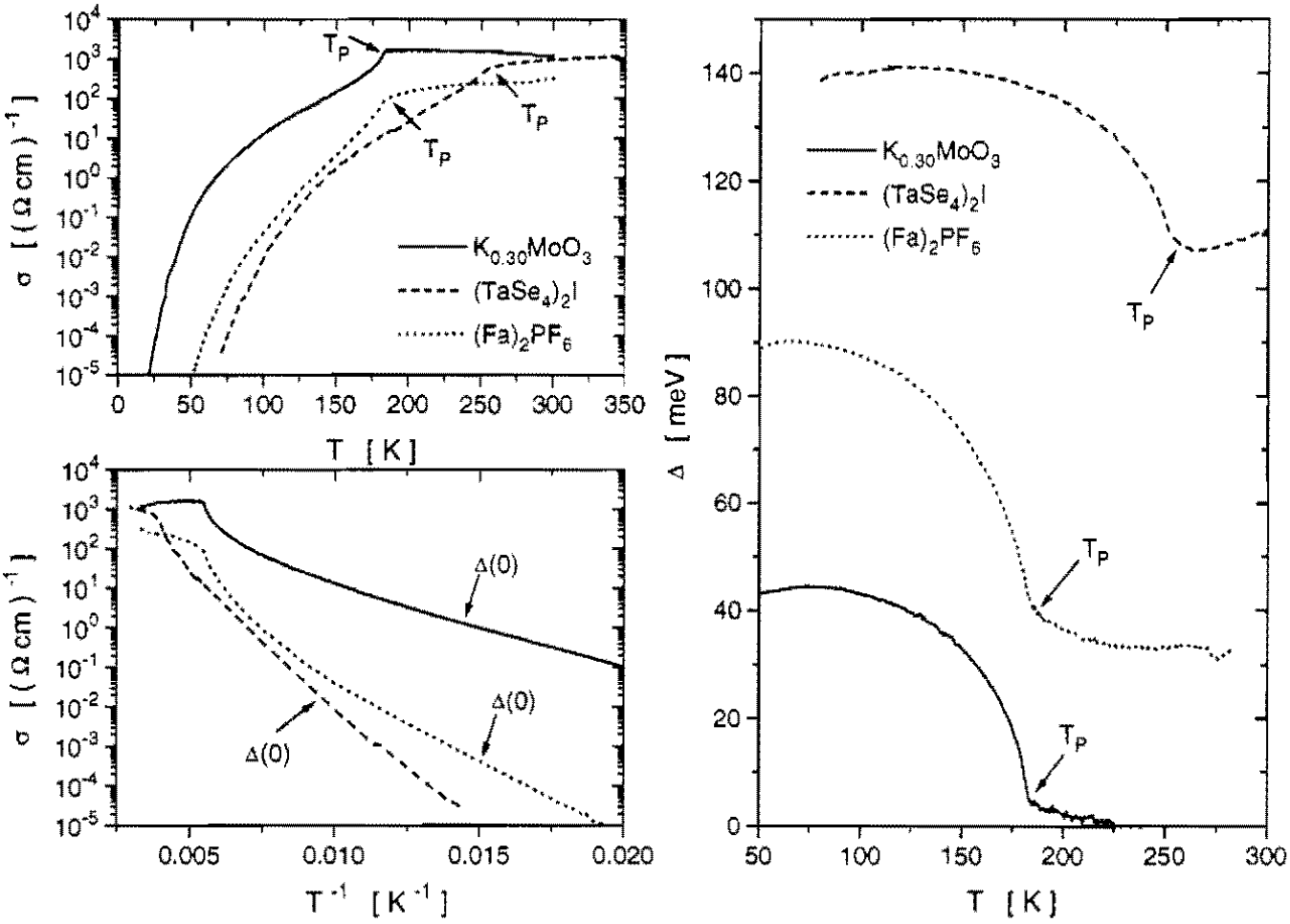

Figure 1: Temperature dependence of the dc conductivity in three different CDW materials (left) and temperature dependent energy gap calculated from the conductivity (right)

num oxide bronze $K_{0.30}MoO_3$ (blue bronze) [4] and the halogenated transition metal chalcogen $(TaSe_4)_2I$ [5] between room temperature and about 25K. All curves show qualitatively the same behaviour, however, there are characteristic differences in the Peierls transition temperature T_P, the room temperature conductivity and the ground state energy gap $2\Delta(0)$ (see Table 1).

At room temperature the systems show relatively high conductivities of typically $10^3(\Omega\text{cm})^{-1}$, however, apart from the blue bronze no increase of conductivity with decreasing temperature is observed, as should be expected for a Q1D metal. At the Peierls transition the slope of $\sigma(T)$ changes abruptly and, for temperatures below T_P, the conductivity rapidly decreases due to the opening of an energy gap at the Fermi level. At even lower temperatures the conductivity follows approximately a thermally activated law with $\sigma(T) \propto \exp[-\Delta(0)/k_BT]$. From the Arrhenius plot in Fig. 1 the characteristic energy gap $2\Delta(0)$ for each system can be determined.

Assuming that the transport is dominated by electrons and holes in bands, we have derived a model for the dc conductivity which is based on the Boltz-

	$(Fa)_2PF_6$	$(TaSe_4)_2I$	$K_{0.30}MoO_3$
T_P [K]	182	263	183
$\Delta(0)$ [meV]	$60-90$	$130-140$	$30-45$
$\sigma(300K)$ $[(\Omega cm)^{-1}]$	10^2-10^3	10^3	10^2-10^3
$\sigma_\parallel/\sigma_\perp(300K)$	10^4	10^3	100:10:1

Table 1: Parameters characterizing the three CDW systems. For the low temperature activation energy $\Delta(0)$ and the room temperature conductivity $\sigma(300K)$ the values can vary from crystal to crystal. In the table are given the typical values found in our experiments.

mann equation in the relaxation time approximation with a temperature and energy dependent relaxation time given by accoustical deformation potential scattering[6]. The conductivity due to both electrons and holes is then given by

$$\sigma(T) = \frac{C}{2k_BT}\int_0^\infty \frac{x^2+2xy}{(x+y)^2}\frac{e^{x+y}}{(e^{x+y}+1)^2}\,dx \tag{1}$$

with $x = \varepsilon/k_BT$, $y = \Delta(T)/k_BT$ and one constant C

$$C = \frac{2e^2\mathcal{N}Mc_s^2}{\pi\hbar a}\left(\frac{\hbar v_F}{E_a}\right)^2 \tag{2}$$

containing material parameters like the density of conducting chains $\mathcal{N}$, the molecular mass M, the sound velocity c_s, the lattice constant a and the acoustical deformation potential constant E_a. This equation includes on the one hand in the limit $\Delta \gg k_BT$ the well-known Arrhenius law $\sigma(T) \propto \exp(-\Delta(T)/k_BT)$ and on the other hand for $\Delta \equiv 0$ the metallic limit $\sigma(T) \propto T^{-1}$. Since equation (1) contains only the temperature dependent gap and one constant C, it is well suited to determine the temperature dependence of the gap from the measured conductivity data. The resultant energy gap for the three systems is shown in Fig. 1 in the righthand plot. Below the Peierls transition the temperature dependence follows a BCS-like behaviour, however, due to 1D fluctuations the BCS-relation $\Delta(0) = 1.76\,k_BT_P$ is not fulfilled. Also above T_P there remains a so-called pseudogap due to pretransitional fluctuations. The differences in the magnitude of this pseudogap are directly related to the degree of one-dimensionality in these systems (see Table 1).

With the knowledge of the temperature dependent energy gap $2\Delta(T)$ one can calculate several conductivity related quantities like the carrier concentration n, mobility μ, scattering time $\bar{\tau}$ and mean free path λ. The values are found to be in a reasonable range, e.g. $\mu = 10-1000$ cm^2/Vs, which again confirms the applicability of the Boltzmann equation in these materials[6].

Additionally to the low-field dc transport, which is based on single particle processes, we have also conducted electric field and frequency dependent measurements in a broad spectral range (10^{-4} - 10^{10} Hz) [7,8]. These experiments clearly show that below the Peierls transition there is a contribution of collective CDW excitations. We observe the response of the pinned CDW in the microwave range and a dielectric relaxation process in the radio frequency range due to internal deformations of the CDW. The static dielectric constant has large values of 10^3 - 10^6 in different materials and seems to diverge at low temperatures. This is interpreted as the transition of the CDW into a glass state at low temperatures.

3 Conclusion

We have developed a model for the dc conductivity in organic and inorganic CDW conductors, which allows for the determination of the temperature dependence of the energy gap in the entire temperature range below and above the Peierls transition directly from dc conductivity data. Our measurements confirm that one and the same conduction mechanism is responsible for the temperature dependence of the conductivity in the organic radical cation salt $(Fa)_2PF_6$, the blue bronze $K_{0.30}MoO_3$ and the transition metal compound $(TaSe_4)_2I$. In all three cases the calculated temperature dependence of the energy gap shows the typical behaviour of a Q1D conductor with a Peierls transition to a CDW ground state. Below T_P the Peierls gap follows a scaled mean field dependence, above the Peierls transition there remains a pseudogap due to CDW fluctuations.

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