THERMAL CONDUCTIVITY OF QUASI-ONE DIMENSIONAL CONDUCTORS

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ABSTRACT

The thermal conductivity of $K_0.3MoO_3$, $(TaSe_4)_2I$ and $TaS_3$ have been measured by two different methods and are found to be independent, within experimental uncertainties, of applied electric field. The enhanced zero-field thermal conductivity observed at the Peierls transition is possibly from extra heat carried by the soft mode associated with the structural distortion.

Since the discovery of quasi-one dimensional materials[1] in the early 1970's and the observation of non-ohmic electrical conductivity[2] in $NbSe_3$, the charge transport properties of the incommensurate charge-density-wave (CDW) systems in $NbSe_3$ and related materials have been studied extensively[3]. It is also well known that interesting field-dependent behavior is observed for the thermopower and related Peltier heat coefficient[4]. These two observations have prompted experimental efforts to measure all the Onsager transport coefficients related to CDW motion. However, for various reasons, the change in the thermal conductivity from a sliding CDW remains unknown. The following is a brief report on the thermal conductivity of the CDW systems $K_0.3MoO_3$, $(TaSe_4)_2I$ and $TaS_3$, measured by two different methods with and without an applied electric field.

The zero-field thermal conductivity of $K_0.3MoO_3$ and $(TaSe_4)_2I$ have been measured using a steady-state linear heat-flow method described in detail elsewhere[5], and the results are shown in Figs.1(a) and (b), respectively. The overall temperature dependence of $\kappa_T$ is similar for both materials, with the slightly stronger temperature dependence above $T_p$ for $(TaSe_4)_2I$ probably related to the stronger fluctuations in this material[6]. A sharp peak is observed at $T_p$ in all of the

FIG.1 – Thermal conductivity of (a) $K_0.3MoO_3$ and (b) $(TaSe_4)_2I$ measured by a linear heat-flow method.

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blue bronze and (TaSe₄)₂I samples that were measured, even though the details of the peak depend on the quality of the samples. We also observed that samples with a higher κₜ maximum at low temperature have a sharper and narrower anomaly at T_p. Since all samples measured have similar geometrical dimensions, it is likely that the correlation is from lattice defects.

In general, κₜ is modelled as a sum of the lattice κₚ and electronic κₑ contributions. For normal metals, κₑ can be estimated from the Wiedemann-Franz law. The situation here is complicated by the presence of a pseudo-gap and Peierls gap in the electronic spectrum above and below T_p, respectively. This will in general enhance the total thermal conductivity due to an extra contribution from recombination of electrons and holes[7]. As in the case of the new high-temperature superconductors[8], the opening of the energy gap at T_p decreases the phonon-electron scattering and therefore enhances the lattice contribution κₚ. On the other hand, enhanced fluctuations near the phase transition shorten the mean-free-path of the heat carrying phonons. As a consequence, a 'dip' is expected in the measured κₜ, as in the case of the antiferromagnets[9]. Such analyses have been carried out but could not explain the sharp peak observed in κₜ[10,11].

Recently, Deland et al.[12] also observed an extra 'bump' in the lattice thermal conductivity of blue bronze around T_p, although the anomaly is somewhat smeared out compare to what we report here. The authors suggested that the excess contribution was related to the fluctuation effects.

The thermal conductivity can also be measured by a steady-state self-heating technique[13] in which the specimen is heated directly by passage of an electric current. Such a method has been employed by Brill et al.[14] for measurement on NbSe₃. Using this technique, we have measured κₜ of orthorhombic TaS₃. Results for the zero-field limit are shown in Fig.2. The overall magnitude of κₜ is the same as previously reported[15]. However, the peak at T_p was not observed using the indirect method of Ref.[15]. The κₜ feature of TaS₃ around T_p is similar to, but significantly larger than that of blue bronze and (TaSe₄)₂I, indicating that the anomaly observed at T_p is an intrinsic property of CDW systems.

The specific heat of blue bronze has been measured by a relaxation method[5]. A non-mean-field type of anomaly observed at T_p [10,16] indicated that the lattice contributed significantly to the specific heat anomaly[17]. Since the softening of phonons near q=2k_F results in a non-zero group velocity dω/dk, it is possible that the increase in κₜ is a result of extra heat carried by the soft phonons.

To study the electric field dependence of κₜ of blue bronze, the linear heat-flow method
was modified slightly[18]. The result is that, within the 2% uncertainty of our apparatus, $\kappa_T$ of blue bronze is field independent up to 6 times the threshold field.

We were motivated to study the field dependence of the thermal conductivity of TaS$_3$ because the field dependence of the thermopower of that material is stronger than that of the blue bronze[4]. Due to the fragility of TaS$_3$, the linear heat-flow method is replaced by the self-heating technique described in Ref.[13]. By thermally anchoring the ends of the specimen to a base temperature $T_0$ and measuring the mid-point temperature $T_{\text{max}}$, one can calculate $\kappa_T$ (assuming $\kappa_T$ and the electrical resistance $R$ are weak functions of temperature) using:

$$\kappa_T = \frac{PL}{8A\Delta T}$$

where $\Delta T = T_{\text{max}} - T_0$, $P = I^2R$ is the joule heat applied to the sample of cross-sectional area $A$ and length $L$. Also, the resistance of the sample is given by:

$$R = \frac{1}{A} \int_{-qz}^{qz} \rho(x)dx = R_0 \left(1 + \frac{I^2L}{12\kappa A} \frac{dR}{dT}\right)$$

where $\rho$ is the resistivity and $R_0$ is the zero-field resistance of the sample.

Four representative curves of $P$ vs. $\Delta T$ are shown in Fig.3 for four distinctive temperature ranges. For $T>230K$, $\kappa_T$ and $R$ are weak functions of temperature and Eq.(5) predicts $\Delta T$ to be linear with $P$. Around the Peierls transition at about 220K, the curvature of $\Delta T(P)$ is dominated by the temperature dependence of $\kappa_T$. The measurement at $T_0=205K$ shown in Fig.3 follows the prediction of $\kappa_T(T)$ from Fig.2 as $\Delta T$ rises. For $150K<T<210K$, $\kappa_T$ is weakly temperature dependent as is the case for $T>230K$. However, $R$ is a stronger function of temperature and consequently, $T_{\text{max}}$ is much smaller than that predicted by Eq.(1) because the mid-point resistivity is much lower than the average $\rho$. This is revealed in the slightly concave down $\Delta T(P)$ of the $T_0=160K$ curve in Fig.3. A calculation of $\kappa(I_{\text{max}})$ at $T_0=160K$ from Eq.(2), using the measured $I$-$V$ curve and the appropriate $dR/dT$, gives the result that $\kappa(I_{\text{max}})=\kappa(0)$ to within 5%. Finally, for $T<150K$, the upturn of $\Delta T(P)$, due to the rapid decrease of $\kappa_T$ as $T_{\text{max}}$ increases, is partly compensated by the concave down effect due to the fast dropping mid-point

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**FIG.3** – Four typical $\Delta T$ vs. $P$ curves for TaS$_3$ as discussed in text. Arrows show where the threshold field ($rV_T$) is from resistivity measurements.
resistivity. The net effect is a slight upward concavity of $\Delta T(P)$ as shown in the $T_0=120K$ curve in Fig.3.

We have checked the previous result for $K_{0.3}MoO_3$ using the same method over the temperature range of 100-160K. $\Delta T$ is found to be linear with $P$, to within 1%, up to about 25mW or equivalently $\Delta T=6K$. This corresponds to applied fields of about 8 times the threshold field. Combined with the earlier experiments, we conclude that $\kappa_T$ is field independent for $TaS_3$ as well as for blue bronze to within 5 and 1%, respectively.

In summary, we observed a peak in $\kappa_T$ of the CDW systems $K_{0.3}MoO_3$, (TaSe$_4$I$_2$ and $TaS_3$. Together with the specific heat measurements on blue bronze, we suggested that the anomaly is related to the heat carried by phonons with $q$ near $2k_F$. Furthermore, $\kappa_T$ of blue bronze and $TaS_3$ are found to be field independent within the uncertainty of our apparatus, which is about 1 and 5%, respectively.

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