THERMAL CONDUCTIVITY OF SOME CDW COMPOUNDS IN THE REGION OF THE PEIERLS TRANSITION

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ABSTRACT

We report thermal conductivity data for several 1-D inorganic CDW compounds, the members of the $(MX_4)I_nI$ family as well as blue bronze ($K_{0.3}MoO_3$) in the temperature range between 80K and 320K. The thermal conductivity decreases from higher temperatures showing a broad minimum in the vicinity of the Peierls transition and the small anomaly just below this transition.

INTRODUCTION

All compounds in our investigation undergo a Peierls transition: $(TaSe_4)_2I$ at T_p=265K, $(NbSe_4)_{10}I_3$ at T_p=280K and blue bronze ($K_{0.3}MoO_3$) at T_p=180K. Below this temperature they exhibit nonlinear transport properties due to CDW current-carrying state[1]. We will compare them to $(NbSe_4)_3I$[2] which does not show same properties but is structurally very similar.

Thermal conductivity was measured by the standard four-contact method, relative to a constantan foil. One end of a needle shaped single crystal (along the high conductivity axis) was thermally connected with indium solder to a copper heat sink. The other end of the sample was glued with GE varnish to a constantan foil which had a small heater at the other end. Both thermal gradients, on the sample and on the constantan reference, were measured using constantan-chromel thermocouples. The unknown thermal conductivity is determined by the ratio of the gradients, a geometrical factor and the thermal conductivity of the constantan as reference[3]. The thermal gradient in the sample was always smaller than 1K except in the transition region where it was 0.2K. The typical sample dimensions were 2.5*0.3*0.5 mm^3. The relative accuracy (1-2%) was much better than the absolute one (20%), mainly due to the uncertainty in defining the geometrical factor of thin samples.

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RESULTS AND DISCUSSION

The results obtained on cooling (slower than 5K/h in the whole temperature region except around the transition where the rate was smaller than 1K/h) in the temperature range from 80 to 320K are shown in Fig.1.

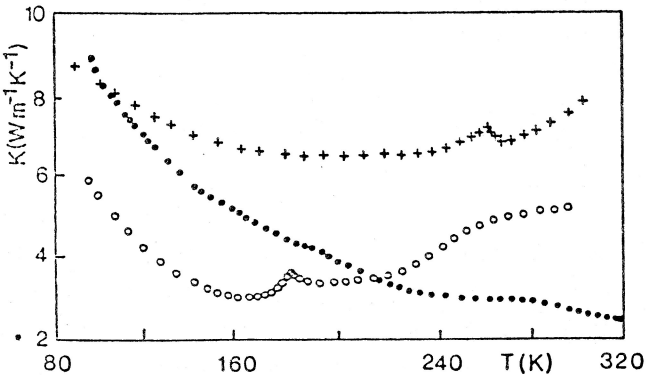

Fig.1. Thermal conductivity of $(NbSe_4)_3I$[2] (•), $(TaSe_4)_2I$[4] (+) and $(K_{0.3}MoO_3)$ (o)

In comparison to $(NbSe_4)_3I$[2], which does not undergo a Peierls distorsion and where the thermal conductivity increases almost monotonically with decreasing temperature, the thermal conductivities of other compounds which are CDW systems [4,5,7] show a common general behaviour: a more or less well defined minimum in the region of the Peierls transition and a small anomaly of a few percent of total conductivity at the transition temperature. The same general feature has the thermal conductivity of TaS_3[7] as well as blue bronze for which we obtained similar results as Lopes at al.[8].

We note that electronic contribution calculated from the Wiedemann-Franz law, as shown in Table 1., is less than six percent for the tetracalcogenides and does not explain the decrease of thermal conductivity from the higher temperatures down to the Peierls transition temperature as well as the anomalous behaviour at the Peierls transition. Therefore it seems that thermal conductivity is mainly due to the lattice. However for temperatures above the Peierls transition it is not possible to find an explanation for the thermal conductivity within the Debye theory. Similar behaviour of the thermal conductivity has been observed in dichalcogenides which are 2D CDW systems where an order-disorder picture has been used for the explanation of the lattice conductivity. Nunez-Requeiro at al[9] introduced a "pseudospin" concept for analysing the thermal conductivity of

that CDW compound but they already noticed that its extension to some other CDW compounds (as $NbSe_3$) could be difficult because their transition entropy is much smaller. It is suggestive to look for a possible mechanism for the additional contribution to the thermal conductivity above the Peierls transition in the existence of a wide regime of 1-D fluctuations which is characteristic for materials we have investigated (the large ratio $2\Delta/kT_p$ - see Table 1/. We will discuss it in more detail elswhere[5].

	T_p (K)	$2\Delta/kT_p$	$\varrho_{R.T.}$ ($\mu\Omega$m)	$(k_e/k)_{R.T.}$	Δk_{Tp}(%)
$(NbSe_4)_3I$	274		10 000	1/3000	
$(NbSe_4)_{10}I_3$	280	13.7	150	1/200	5
$(TaSe_4)_2I$	263	11.4	15	1/20	6
$(K_{0.3}MoO_3)$	180	12.2	6.7	1/4	8

Table 1. Data pertaining to Peierls or structural transitions in tetrachalcogenides and blue bronze at room temperature. Listed are: the phase transition temperature, the ratio of the amplitude of the Peierls gap and the Peierls temperature, resistivity at room temperature, electronic thermal conductivity over the total thermal conductivity at room temperature, the hight of the anomaly in the thermal conductivity below the Peierls transition.

As for the explanation for the anomaly in the thermal conductivity just below the Peierls transition some arguments could be possibly used as in high Tc- superconductors[10]: the phonon mean free path below Tp is enchanced because the phonons cease to dissipate their momentum in collisions with CDW condensate and it increases as more and more carriers are condensed but finally other scattering mechanisms come into play at a few degrees lower temperatures[5].

The other explanation for the occurrence of the anomaly at Peierls transition was given by Kwok at al[11]. They claim that the anomalies they observed in blue bronze and $(TaSe_4)_2I$ are related to the heat carried by soft phonons with wave vector close to $2k_F$. However, the interpretation of the anomaly at the Peierls transition as the contribution of soft phonons is questionable because the softening was not seen in $(TaSe_4)_2I$[12]. In blue bronze[13] the softening exists but accompanied by the significant increase of the damping[14].

It seems to us that the nature of the observed anomalies in all these CDW systems should be the same as well as their driving mechanism[5].

CONCLUSION

We point out two general characteristics of the thermal conductivity of quasi 1D CDW systems. First is the minimum in the region of the Peierls transition and the second is a small anomaly just below the transition temperature. We hope that the results will stimulate further theoretical efforts towards final explanation of the measured thermal conductivity of CDW materials.

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REFERENCES

1 P.Monceau in: Electronic Properties of Inorganic Quasi One Dimensional Materials II, ed.P.Monceau (Riedel, Dordrecht), The Netherlands)p.139

2 A.Smontara, K.Biljaković and L.Forró, Synthetic metals, 19 (1987) 859

3 R.W.Powers, J.B.Ziegler and H.L.Johnston, USAF, TR.(1951) 264

4 A.Smontara, K.Biljaković and L.Forró, Second European Workshop on Charge Density Waves, Aussois, France, 21-25 September, 1987.

5 A.Smontara and K.Biljaković, to be published

6 A.Smontara, K.Biljaković, T.Futivić and T.Idžotić, Proceedings of the XI Yugoslav Symposium of the Physics of Condensed Matter, Donji Milanovac, 3-7 October, 1988,Fizika,21,Suppl 1 (1989)84

7 A.V.Inyushkin, A.N.Taldenkov and V.V.Florentiev, Synthetic metals, 19(1987)843

8 E.B.Lopes, M.Almeida, J.Dumas and J.Marcus, Phys.Lett.A, 130 (1988) 98

9 M.O.Nunez-Requeiro, J.M.Lopez-Castilla and C.Ayache, Phys.Rev.Lett.55(1987)1931

10 C.Uher and A.B.Kaiser, Phys.Rev.B, 36(1987) 5680
D.T.Morelli, J.Heremans and D.E.Swets, Phys.Rev.36(1987)3917

11 R.S.Kwok and S.E.Brown, Phys.Rev.Lett.,63(1989) 895

12 P.Monceau, L.Bernard, R.Currat, F.Levy and J.Rouxel, Physica, 136B (1986) 352, Synthetic Metals,19(1987)819 and private communication.

13 J.P.Pouget and R.Comes, 1989 in: Charge Density waves in Solids, ed.by L.P.Gor´kov and G.Grüner (Elsevier Science Publishers B.V.)p.85

14 The possible explanation for this damping follows from the result of numerical simulations of 1-D systems, E.Tutiš and S.Barišić, this Conference.