

*THERMAL CONDUCTIVITY OF THE ONE-DIMENSIONAL CHAIN CONDUCTOR*



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We present measurements and analysis of the thermal conductivity of linear chain conductor  $(\text{NbSe}_4)_{10}\text{I}_3$ . We find that the thermal conductivity decreases from higher temperatures, showing a broad minimum below 280K down to 220K. Below, it increases monotonically with decreasing temperature. In addition, at 280K, an anomaly is found which we ascribe to the CDW transition.

1. INTRODUCTION

The chain conductor  $(\text{NbSe}_4)_{10}\text{I}_3$  shows a strong one-dimensionality, which favours the development of a charge-density-waves (CDW) transition as the consequence of the natural instability of a 1-D electron subsystem. Above the transition temperature  $T_p$ , metallic character is observed whereas below  $T_p$ , a temperature dependent gap opens at the Fermi level.  $(\text{NbSe}_4)_{10}\text{I}_3$  demonstrates some effects characteristic of collective CDW transport. At room temperature it is a semi-metal and below  $T_p \sim 280\text{K}$ , where the Peierls gap opens<sup>1,4</sup>, nonohmic conductivity, narrow band noise, switching and some metastabilities are observed<sup>2</sup>. One can expect a thermal conductivity of this crystals to display an anomaly at the CDW transition and here we report measurements in the range from 120K-320 K.

## 2. EXPERIMENTAL

Thermal conductivity was measured by a standard four-contact method, relative to a constantan foil. One end of a needle shaped single crystal elongated along the high conductivity axes, was thermally connected by indium soldering to a copper heat sink. The other end of the sample was glued by GE varnish to a constantan foil with the 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 reference<sup>(3)</sup>. The temperature gradient in the sample was always smaller than 1K. The typical sample dimensions were: 2.5 x 0.3 x 0.5 mm<sup>3</sup>. The relative accuracy was 1-2%; much better than the absolute one, which was 20%, mainly due to the uncertainty in defining the geometrical factor of thin samples.

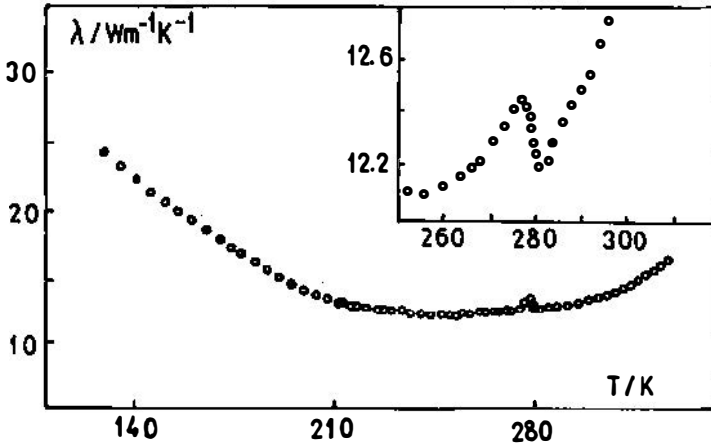


Fig.1 Thermal conductivity of  $(\text{NbSe}_x)_{1-x}\text{I}_x$ , as a function of temperature

In the insert is the anomaly at the Peierls transition.

The results obtained while cooling ( < 5K/h ) in the range from 120-320 K are shown in Fig.1. The temperature dependence of the thermal conductivity is similar to that of dielectric crystals; it decreases from higher temperatures, showing a broad minimum between 280K and 220K, and again increases monotonically with decreasing temperature. Especially interesting is the pronounced fine structure inside the minimum: an anomaly is present at  $T_p=280$  K. The height of the anomaly is between 3% and 5%, for different crystals and the width is approximately 20 K.

### 3. DISCUSSION

The thermal conductivity contains two contributions; one due to the lattice phonons  $k_{ph}$  and the other to electrons  $k_e$ .

$$k = k_{ph} + k_e, \quad \text{where} \quad k_e = L_0 \cdot T / \rho$$

$L_0$  is effective Lorentz number and  $\rho(T)$  - electrical resistivity obtained on crystals from the same batch. Although our sample is a semi-metal, or semiconductor below Peierls transition, in the first approximation we used free electron Lorentz number  $L_0=2.45 \cdot 10^{-9} \text{ W}\Omega\text{K}^{-2}$  getting at any temperature for the electron contribution almost two orders of magnitude lower thermal conductivity ( at room temperature  $k_e = 0.065 \text{ Wm}^{-1}\text{K}^{-1}$  ). We note that the calculated  $k_e$  is unable to reproduce the anomaly observed at Peierls transition. So, the thermal conductivity is mainly due to the lattice.  $(\text{NbSe}_4)_{10}\text{I}_3$  is the CDW system showing the highest ratio between the measured thermal conductivity and the calculated electron contribution ( 200:1 at room temperature ). The anomaly thus comes from  $k_{ph}$ . For temperatures above the Peierls transition it is not possible to find the explanation in the Debye theory.

The general behaviour of the thermal conductivity of several CDW

systems is the same - a more or less well defined minimum in the region of the Peierls transition and if the resolution allows, a small anomaly is observed at the transition temperature<sup>15,61</sup>. As far as we know there have been no attempts to explain what kind of phonon relaxation could cause such general behaviour except possibly the "pseudospin" concept, which appears to be valid for several order-disorder transitions, including ferroelectrics and dichalcogenides<sup>17)</sup>.

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