ANOMALOUS TRANSPORT PROPERTIES OF $ZrTe_5$

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Abstract

The measurements of thermal conductivity, thermal capacity and dc electrical conductivity as well as its anisotropy are presented. The anomalous character of these properties is discussed.

Special interest in the penetatellurides MTe_5 stems from the posibility of charge-density wave (CDW) instabilities in these "one-dimensonal" materials. The existence of these is suggested by giant resistivity anomalies found at 150 K for $HfTe_5$[1] and at 80 K for $HfTe_5$[2]. The resistivity peak in MTe_5 is even more marked than such resulting from CDW instabilities in $NbSe_3$ – a typical CDW conductor with a similar crystal structure. In MX_5 compounds triangular MTe_3 columns run parallel to the orthorhombic a – axis but are linked together along the c -axis. As a consequence, a two-dimensional character is expected in the properties of $ZrTe_5$. The presence of two polytypes: orthorhombic and monoclinic[4] has been confirmed.

Despite the accumulation of a large amount of experimental data[4] a unique explanation of the resistivity peak and other properties of $ZrTe_5$ has not been found. Band calculations[3] have shown a semi-metallic band overlap between valence and conduction bands arising from the coupling between adjacent $ZrTe_5$ layers. Therefore no CDW should be observed. The anomalies is transport properties might be related to temperature dependence of the carrier concentration and of the carrier mobility.

A new anomaly at 85 K[4] has been observed which is presumably associated with the existence of the monoclinic polytype.

In order to characterize our samples we have performed dc conductivity measurements in a, b and c directions. The electrical resitivity (Fig. 1) shows metal-like behaviour in the whole temperature region. The dc resistivity anisotropies in a-c and b-a layers at room temperature are 2—3 and 50 respectively and change slowly with temperature.

The measurements of thermal conductivity were done on cooling and heating above 60 K. At lower temperatures, because of the thermal link to the cold bath, we could measure only while heating. The thermal conductivity, shown in Fig. 2, continously increases as the temperature decreases from room temperature (10 W/mK) down to 15 K. There is a thermal hysteresis between 120 K and 220 K and a sharp anomaly around 40 K, presumably connected with a new phase transition.

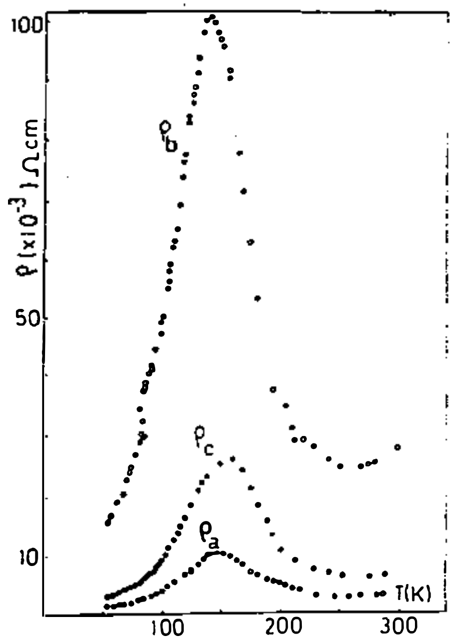

Figure 1.
DC resistivity in a, b and c directions

In the heat capacity of $ZrTe_5$ two peaks are observed: at 90 K and 135 K (Fig. 3). The first is ascribed to a phase transition in monoclinic inclusions, the second, at 135 K (the temperature of the peak in resistivity), to thermal excitations of electrons to a semimetallic energy band. In the same model the anomalies in transport properties (at this temperature) can be explained.

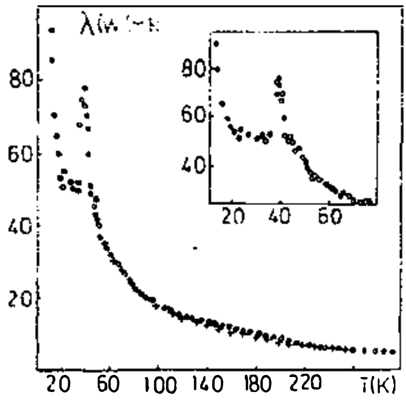

Figure 2.
Thermal conductivity of $ZrTe_5$ measured by cooling (+) by heating (o).

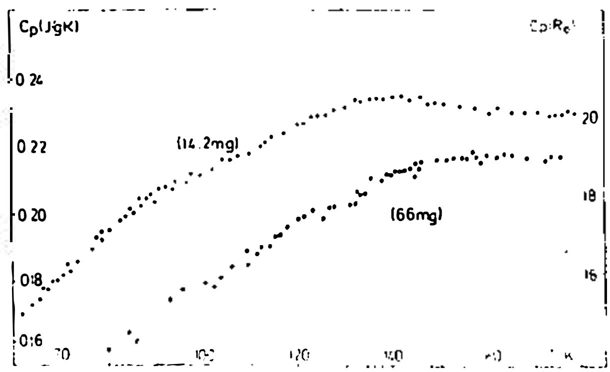

Figure 3
Specific heat of $ZrTe_5$ versus T measured during cooling in two separate runs on two different samples.

On the other hand susceptibility anisotropy measurements[5] have shown that the susceptibilities in all three directions are diamagnetic but only χ_b shows a strong and complex temperature dependence coresponding to anomalies in electrical resistivity as well as thermal conductity. Therefore we can also conclude that the transport properties are determined by the proposed open cylindrical Fermi surface (evidence for strong two dimensionality) along the b* direction, where cross section varies strongly and in a complicated way with temperature.

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