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TITLE: PRESSURE EFFECTS IN HAFNIUM PENTATELLURIDE AND ZIRCONIUM PENTATELLURIDE

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Pressure Effects in $HfTe_5$ and $ZrTe_5$

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Résumé - Nous avons mesuré l'effet de la pression sur la résistance électronique et le pouvoir thermoeléctrique de $HfTe_5$ et $ZrTe_5$ comme une fonction de la température. L'effet de la pression est différente pour les deux composés. La résistance montre un plus grande effet que le pouvoir thermoeléctrique. Aussi l'effet de la pression est plus grande pour le $HfTe_5$ que pour le $ZrTe_5$. Nous donnons deux expliquations: 1) l'instabilité de la surface Ferm. ou 2) c'est une semi-metal.

Abstract - We have measured the effect of pressure (0-17 kbar) on the resistivity and the thermopower of $HfTe_5$ and $ZrTe_5$ as a function of temperature. Pressure affects these two materials in different ways. The resistance shows a greater effect than the thermopower. There is a larger effect in $HfTe_5$ than in $ZrTe_5$. Possible explanations in terms of a Fermi surface instability and a semi-metal are given.

In the past several years there has been a growing interest in the compounds $HfTe_5$ and $ZrTe_5$./1-3/ These materials are reported to have a large resistive anomaly/1,3/ superimposed onto a metallic behavior. This anomaly is very reminiscent of those seen in $NbSe_3$, which have been identified as charge density wave (CDW) transitions. However, x-ray data/2,4/ has not shown the $2k_F$ scattering which would be associated with a CDW in these materials. The logarithmic derivative of the resistivity is a function of temperature shows no sharp behavior/2/ which would accompany a phase transition. The magnetic susceptibility as measured by the Bell group/2/ also shows no sign of a phase transition. However, the Hall coefficient/5/ and the thermoelectric power/6/ both show a sharp change of sign at a temperature corresponding to the peak in the resistance. This change of sign has been interpreted as arising from a change in carrier type./5,6/ The peak in the resistivity has been found to be unaffected by high electric fields (~ 50 V/cm for $ZrTe_5$ and ~ 20 V/cm for $HfTe_5$)./4/ The two materials do differ from each other when placed in a microwave field./4/ At 9.3 GHz Gruner (private communication) has found that the anomaly in $ZrTe_5$ is only partially suppressed while in $HfTe_5$ the anomaly is completely suppressed. Because of these puzzling results we undertook the measurement of the resistivity and thermoelectric power, S, of these materials as a function of pressure as well as temperature. In $NbSe_3$ it is well known that pressure suppresses the resistive anomalies./7/

The crystals of $HfTe_5$ and $ZrTe_5$ were grown as described in Ref. /4/. The measurements were made in a self-clamped beryllium copper pressure cell similar to that used by Harrison et al./8/ Four copper wires were attached to each crystal with indium solder to permit four probe resistivity measurements. A measuring current of ~ 500 μA was used. The pressure cell used permitted a series of pressure measurements (0-17 kbar) on each sample as well as a way to return to low pressures to check for destruction of the sample. No changes in the samples' characteristics were found upon return to low pressures. Four gold leads were attached with silver paint to evaporated gold contacts on $HfTe_5$ and $ZrTe_5$ for simultaneous thermopower and resistivity measurements. The temperature gradient, typically 0.25K, was measured with a chromel-constantan thermocouple placed next to the sample in the pressure cell. The pressure was determined from the superconducting transition of tin placed in the cell.

Figure 1 shows the results for $HfTe_5$ while Fig. 2 is for $ZrTe_5$. Only the extreme pressures are shown. In each case the resistance and thermopower are plotted as a function of temperature. As can be seen, pressure has a large effect on the size of the anomaly (as measured relative to the room temperature value) in $HfTe_5$, while hardly any difference in the size is seen in $ZrTe_5$. The temperature where the resistive anomaly peak occurs, T_p, decreases by about 10K at 17 kbar for the $HfTe_5$, while for the $ZrTe_5$ it increases by 20K. The temperature where S starts to drop from its high temperature behavior does follow T_p. At temperatures below the zero crossing the magnitude of the thermopower is larger when measured under pressure than at ambient pressure.

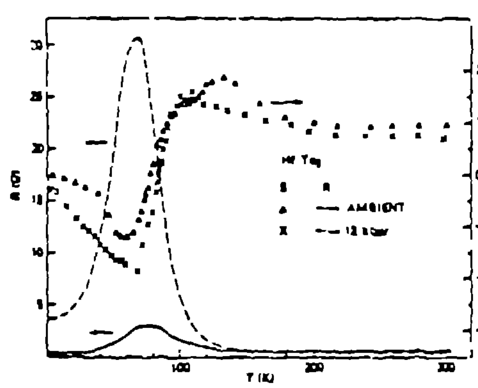

Fig. 1 The resistance and thermopower of $HfTe_5$ as a function of temperature for two extreme pressures. The two measurements at a given pressure were made simultaneously on one crystal. All the data is for this sample.

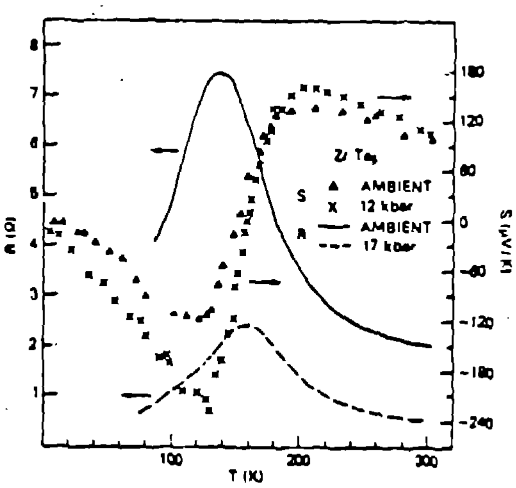

Fig. 2 The resistance and thermopower of $ZrTe_5$ as a function of temperature for two extreme pressures. The resistance data is on a different sample than the thermopower data.

A summary of the results for other pressures is presented in Table I. The features which should be noted are that T_p decreases by 12% in $HfTe_5$ while it increases by 15% in $ZrTe_5$ for 17 kbar. Thus, the relative change in the position of the peak is of similar magnitude but opposite direction for the two materials. The size of the anomaly, as measured by R_p/R_{300}, increases by a factor of 9 for $HfTe_5$ but it stays roughly constant for $ZrTe_5$ as the pressure increases. The room temperature resistance, R_{300}, of $HfTe_5$ stays roughly constant while it decreases by a factor of 8 for $ZrTe_5$. In $HfTe_5$ the resistance remained ohmic up to fields of 50 V/cm at 12 kbar.

The question of what the anomaly is due to remains opened. Two possible explanations are in terms of 1) a Fermi surface instability which is not accompanied by a structural transition or 2) a semi-metal, where due to band overlap the population of carriers changes. Both of these explanations rely on a two carrier model. This appears reasonable in light of the Hall effect and the thermopower data.

If the anomaly is due to a Fermi surface instability, then it appears that pressure causes a greater portion of the total Fermi surface to be affected by the instability in $HfTe_5$. Since the thermopower does not differ much with pressure, one would expect that pressure acts on the electron and hole surfaces in such a way that a compensation in the number of carriers occurs. In $ZrTe_5$ the amount of the Fermi surface affected by the instability does not appear to change with pressure. An instability is consistent with the Hall effect, thermopower and magnetoresistance

Table I

Pressure (kbar) ± 3 kbar	T_p(k) ZrTe$_5$ ±2K	T_p(k) HfTe$_5$ ±2K	R_p/R_{300} ZrTe$_5$ ±10%	R_p/R_{300} HfTe$_5$ ±10%
0	138	79	3.75	5
4.8		80		4.9
6	139		3.8	
7		79		8.3
9.5		80		18
10.5	147		4.0	
15.3		76		35
15.5	154		4.95	
17.7	158	73	4.6	45

Table I. A summary of the pressure effects on the resistivity of $HfTe_5$ and $ZrTe_5$.

data all of which appear to imply a phase transition. However, x-ray data suggest that if this is a phase transition it is not structural in origin. The difference in the behavior under pressure of the two materials could be explained by having the Fermi level on opposite sides of a peak in the density of states; thus pressure could increase T_p in one case and decrease it in the other.

A second interpretation would be in terms of a semi-metal where the band overlap is such that the population of the electron band changes with temperature. It is possible that at some point the number of carriers is increasing with increasing temperature faster than the electron-phonon scattering, this would lead to a negative temperature coefficient for the resistance. For this interpretation, one can explain the Hall effect and thermopower data by assuming the relative mobilities of the electrons and holes change with temperature. Pressure could change the band structure thereby affecting the population of the electron band. It would also affect the mobility of the carriers through the effective mass. However, it is difficult to explain the microwave results using a semi-metal model.

In conclusion pressure affects the resistive anomalies and the thermopower of $HfTe_5$ and $ZrTe_5$ in different ways. The effects in the resistivity is much more pronounced than those in the thermopower. The effect on the size of the resistive anomaly in $HfTe_5$ is more dramatic than in $ZrTe_5$. The effect of pressure on the position of the peak in the resistance is about the same, 12% in $HfTe_5$ and 15% in $ZrTe_5$. The data is inconclusive in terms of an interpretation of the anomaly. The data can be explained equally well by a fermi surface instability or by a semi-metal band structure.

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