

## Effect of elastic tension on the electrical resistance of HfTe<sub>5</sub> and ZrTe<sub>5</sub>

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We have measured the effect of elastic, uniaxial stress  $\sigma$  in the  $a$  direction on the resistance  $R$  of ZrTe<sub>5</sub> and HfTe<sub>5</sub> for  $\sigma$  up to more than 1.0 GPa and for temperatures  $T$  from 2 to 300 K. We find little change with stress of the magnitude of the resistance peak for either material. The change of the temperature of the resistance peak with stress is not simple for HfTe<sub>5</sub>, but for ZrTe<sub>5</sub> there is a linear increase. For sufficiently low temperatures ( $<20$  K for HfTe<sub>5</sub> and  $<15$  K for ZrTe<sub>5</sub>) the resistance rises sharply with stress to a saturation level. We discuss two possible Fermi-surface changes as explanations for the sharp rise of resistance to saturation under tension: first, a change in the energy of the conduction bands relative to each other, and second, effects due to band bending. The first appears adequate to explain the size and the saturation of the resistance changes measured, whereas the latter can play only a secondary roll.

### I. INTRODUCTION

The electrical resistivities of the quasi-one-dimensional compounds HfTe<sub>5</sub> and ZrTe<sub>5</sub> show large, broad peaks as a function of temperature<sup>1</sup> (Fig. 1). The temperatures  $T_p$  at which the peaks occur are sample dependent, but are  $\approx 70$  and  $\approx 150$  K, respectively.<sup>2</sup> Two somewhat similar resistance peaks which occur in NbSe<sub>3</sub> at  $\approx 60$  and  $\approx 140$  K are due to the formation of two independent charge-density waves (CDW),<sup>3-5</sup> i.e., spacially periodic modulations of the lattice and the charge density. Because of this similarity and the similar quasi-one-dimensional structures of these materials, considerable effort has gone toward a search for a CDW or other type of phase transformation in these pentatellurides. Jackson<sup>6</sup> *et al.* found large reductions in the resistance peaks at high frequencies; a result similar to those for NbSe<sub>3</sub>. They interpreted these results as being due to the response of a collective mode to the high-frequency field. Other efforts, however, including the Hall effect and magnetoresistance,<sup>7</sup> the effect of pressure on the electrical resistance and thermoelectric power,<sup>8</sup> specific heat,<sup>9</sup> elasticity,<sup>10</sup> and x-ray diffraction studies,<sup>11</sup> have resulted in no clear evidence

for such a transition. The Fermi-surface studies of Kamm<sup>12,13</sup> *et al.* show that these pentatellurides remain electronically compensated at low temperatures. It seems highly unlikely that a CDW transition would preserve compensation, and so we may view their results as evidence against such a transition. The nature of the resistance peaks and associated phenomena remains poorly understood.

HfTe<sub>5</sub> and ZrTe<sub>5</sub> have the same crystal structure:<sup>14</sup> orthorhombic with the  $Cmcm$  space group. The lattice constants for HfTe<sub>5</sub> (ZrTe<sub>5</sub>) in angstroms are  $a = 3.974$  (3.9876),  $b = 14.492$  (14.502), and  $c = 13.730$  (13.727). Each has 24 atoms (four formula units) per unit cell (the primitive cell has half the volume of this cell). The metal atoms lie at the centers of right trigonal prisms of Te atoms stacked along the  $a$  direction, which is the direction of minimum electrical resistivity,  $\rho$ . Parallel chains of trigonal prisms are coupled in the  $c$  direction by intermediate Te atoms to form sheets in the  $ac$  plane. These sheets are loosely bound by van der Waals forces in the  $b$  direction, which is the direction of maximum  $\rho$ .

### II. EXPERIMENTAL PROCEDURE AND ANALYSIS

The crystals used in this investigation were grown by Levy by the iodine vapor-transport method, described by Levy and Berger,<sup>15</sup> from elemental powders having purities 99.99% for the metals and 99.999% for the Te. As grown they are needle shaped with the long axis parallel to  $a$ . Usually these crystals are larger in cross section than desired for our tension experiments; in addition, their surfaces were somewhat irregular. They are, however, easily cleaved along planes parallel to the  $a$  direction. Samples which appeared to have no surface imperfection when viewed in an optical microscope were cleaved from the as-grown crystals. Typical samples had lengths of 2 mm and transverse dimensions 2–10  $\mu\text{m}$ .

All resistance measurements were made using the four-probe dc technique. Electrical contacts were made to the samples by sputter-coating two small regions near each end of each sample with Au-Pd. These coated re-

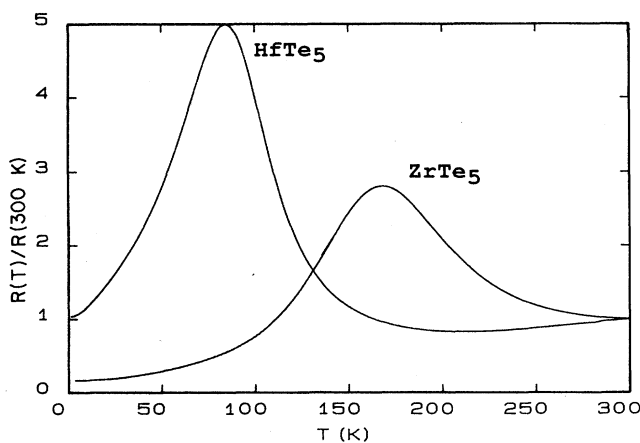


FIG. 1. Resistance vs temperature for HfTe<sub>5</sub> and ZrTe<sub>5</sub>.

gions were then placed over four No. 36 copper wires attached to the stressing device. Silver paste was used to cement the samples to the wires.

The stressing device has been described elsewhere.<sup>16</sup> With this device, the extension  $\Delta L$  (where  $L$  is the length of the sample subjected to stress) of the sample in the  $a$  direction is measured, not the uniaxial stress. The stress must be calculated using the appropriate elastic modulus. The stressing device was placed in a variable-temperature, gas-cooled cryostat the temperature of which was controlled to within 1% over the range 2–300 K.

Plots of resistance versus extension were made on an X-Y recorder at several fixed temperatures down to 2 K. Data from these plots were subsequently digitized at approximately 30 equal intervals of extension and stored for further analysis. In some cases the data were taken originally with digital equipment under computer control. Plots of  $R$  versus  $T$  at constant  $\epsilon$  ( $\epsilon = \Delta L/L$  is the axial component of the strain tensor) were constructed from these data.

### III. EXPERIMENTAL RESULTS

Samples of  $\text{HfTe}_5$  ( $\text{ZrTe}_5$ ) sustained maximum elastic extensions of  $\approx 1\%$  (1.5%) of their lengths. Table I gives data pertinent to the samples used in this study. These samples have smaller transverse dimensions and lower values for  $T_p$  than those of other investigators. Figures 2 and 3 show plots of  $R$  versus  $\epsilon$  at several representative temperatures for  $\text{HfTe}_5$  (sample 2) and  $\text{ZrTe}_5$  (sample 4). The temperatures are (a) room temperature, (b) the temperature of the resistance minimum,  $T_m$ , (c) a temperature between  $T_m$  and  $T_p$  at approximately the half maximum of the peak of the unstrained sample, (d)  $T \approx T_p$ , (e) a temperature less than  $T_p$  at approximately the half maximum, and (f) a temperature below which no further qualitative change in the  $R$  versus  $\epsilon$  curves takes place. Similar data were taken at many other temperatures. Other samples give substantially the same results.

The resistance changes with stress are very large compared to those typical of metals such as copper and they are highly nonlinear. Similar large changes are found in the semimetal Bi (Ref. 17) and in other low-dimensional materials.<sup>18</sup> Some of the nonlinearity near  $T = T_p$  is asso-

TABLE I. Data for samples used in these experiments.  $L$  is the length of the sample which was subjected to stress. It is also the distance between electrical potential leads.  $A$  is the sample cross-sectional area determined from the resistivities  $\rho(300 \text{ K}) = 380(700) \times 10^{-6} \Omega \text{ cm}$  for  $\text{HfTe}_5$  ( $\text{ZrTe}_5$ ), resistances  $R(300 \text{ K})$ , and  $L$ .  $T_p$  is the temperature at which the resistance peak occurs.

Sample	$L$ (mm)	$A$ ( $\mu\text{m}^2$ )	$T_p$ (K)	$R(300 \text{ K})$ ( $\Omega$ )
$\text{HfTe}_5$ 1	2.18	5.5	37.5	1501
	2	1.45	28.5	193
$\text{ZrTe}_5$	1.88	42.8	144	308
	2	2.22	135	1088
	3	1.32	23.5	392
	4	2.45	3.24	5290

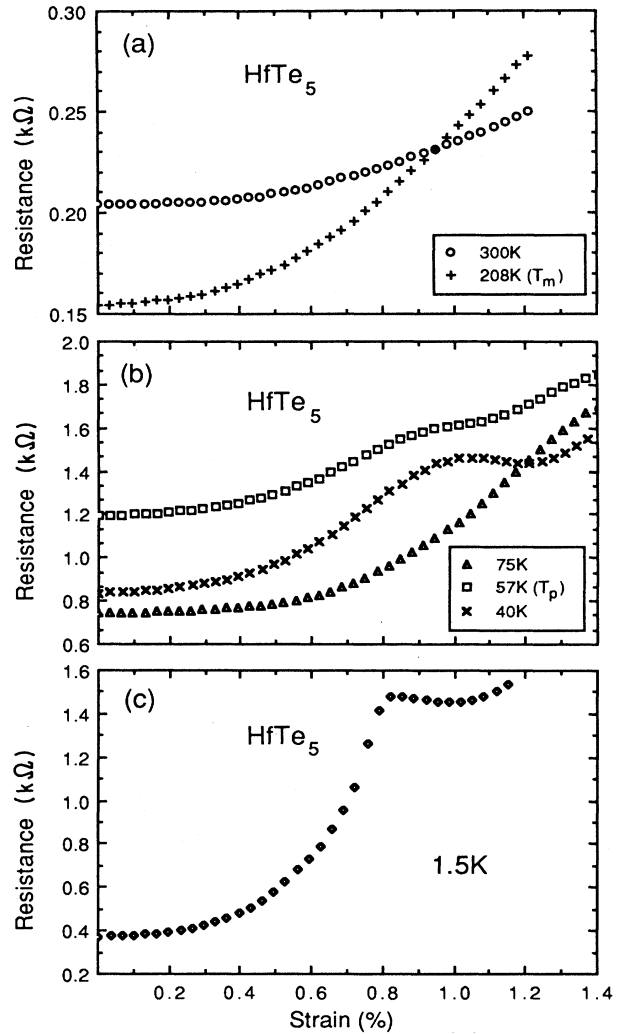


FIG. 2. Resistance vs axial strain at several temperatures for  $\text{HfTe}_5$ . (a) Room temperature and  $T_m$ , (b)  $T_p < T < T_m$  at approximately the temperature of the half maximum of the peak for the unstrained sample,  $T = T_p$ , and  $T < T_p$  again at the half maximum, and (c)  $T = 1.5 \text{ K}$ .  $T_m$  and  $T_p$  are the temperatures of the resistance minimum and the resistance peak, respectively.

ciated with a shift with strain of  $T_p$  and with a change in the width of the resistance maximum. At the lowest temperatures each material shows a very large initial increase in resistance with stress followed by saturation.

Figure 4 shows  $R$  versus  $T$  at several values of  $\epsilon$ . These plots were made from many  $R$  versus  $\epsilon$  plots at constant  $T$ . For  $\text{HfTe}_5$ ,  $T_p$  decreases at low  $\epsilon$  followed, at larger  $\epsilon$ , by an increase. The two samples of  $\text{HfTe}_5$ , even though cleaved from the same larger crystal, had quite different values of  $T_p$  and showed some differences in their  $T_p$  versus  $\epsilon$  curves. For  $\text{ZrTe}_5$ ,  $T_p$  increases and the width of the peak increases with  $\epsilon$ . There is little change in the ratio of  $R(T_p)/R(300 \text{ K})$ . These changes are shown in detail in Fig. 5. The change of  $T_p$  with  $\epsilon$  is linear for  $\text{ZrTe}_5$  with slope  $\partial T_p / \partial \epsilon$  that is dependent on the sample. For the two samples which were completely analyzed (samples 3 and 4) the slope was 2200 and 2700 K.

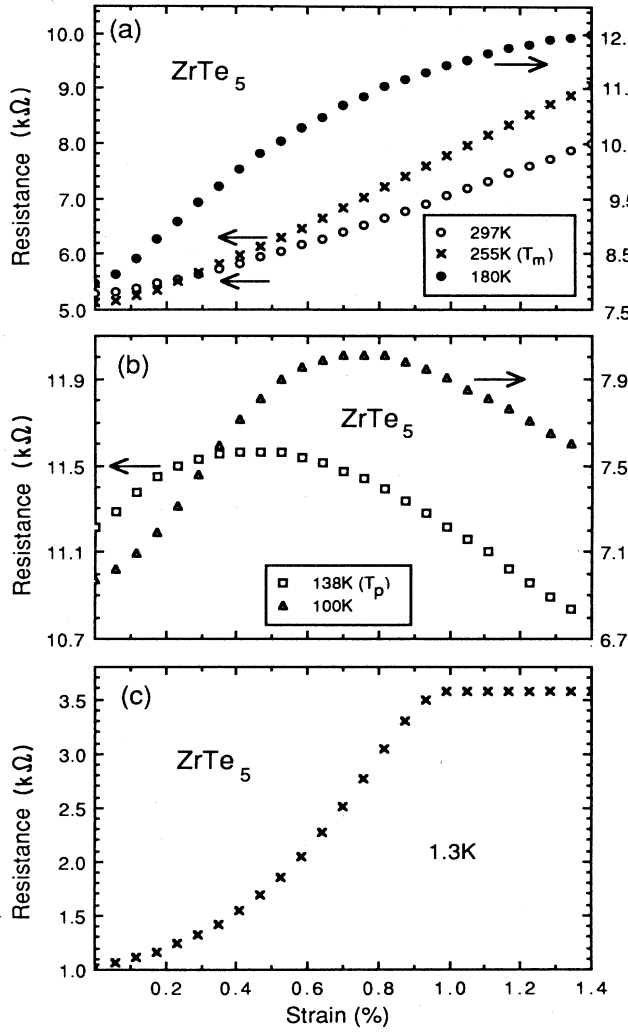


FIG. 3. Resistance vs axial strain at several temperatures for  $\text{ZrTe}_5$ . (a) Room temperature,  $T = T_m$ , and  $T_p < T < T_m$  at approximately the temperature of the half maximum of the resistance peak for the unstrained sample, (b)  $T \approx T_p$  and  $T < T_p$  again at approximately the temperature of the half maximum and, (c)  $T = 1.3$  K.  $T_m$  and  $T_p$  are the temperatures of the resistance minimum and peak, respectively.

#### IV. DISCUSSION

##### A. Comparison of the results of tension and pressure

The effect of hydrostatic pressure  $P$  on the resistance of  $\text{HfTe}_5$  and  $\text{ZrTe}_5$  has been measured as a function of temperature.<sup>8</sup> Using the measured elastic constant for  $\text{ZrTe}_5$  (Ref. 10) we may compare pressure and stress results. The elastic constant  $C_{aa}$  for  $\text{ZrTe}_5$  is  $(1.1 \pm 0.3) \times 10^2$  GPa. No other elastic constants have been measured for either material. In the absence of a value of  $C_{aa}$  for  $\text{HfTe}_5$  we use the value for  $\text{ZrTe}_5$ . The correct value is not likely to be much different given the strong similarity of the two compounds. In the absence of elastic con-

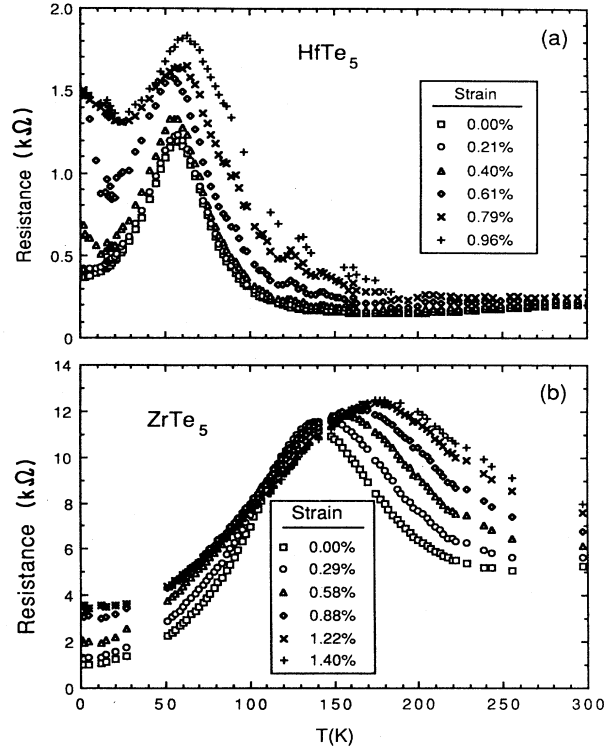


FIG. 4. Resistance vs temperature at several axial strains  $\epsilon$  for (a)  $\text{HfTe}_5$  and (b)  $\text{ZrTe}_5$ .

stants  $S_{ab}$  and  $S_{ac}$  the effect of tension on the transverse dimensions of the samples cannot be determined. In most orthorhombic materials both transverse dimensions contract under tension, though it is not impossible for one or both to expand. Thus, it is likely that the dimensional changes due to pressure and tension are of the same sign for the transverse directions, but of opposite sign for the longitudinal direction. We assume this to be true for these two materials.

Notable effects of pressure on  $R$  of  $\text{HfTe}_5$  are<sup>8</sup> (a) a large enhancement of the magnitude  $M = R(T_p)/R(300\text{ K})$  of the resistance peak, (b) a decrease of  $T_p$  which, if fit to a parabola,  $T_p = T_p(0) + BP^2$ , gives  $B = -2.0$  K/GPa<sup>2</sup>, and (c) for  $T < 20$  K a pressure of 1.2 GPa increases the resistance by a factor of more than 3. In tension, (a) there is only a small enhancement of the magnitude of the peak, and (b) for  $\sigma < 0.7$  GPa  $T_p$  decreases with  $\sigma$ , according to the expression  $T_p = T_p(0) + B_1\sigma + B_2\sigma^2$  with  $B_1 = -(0.7 \pm 0.4)$  K/GPa and  $B_2 = -(6.9 \pm 0.7)$  K/GPa<sup>2</sup> (sample 2) in which the errors reflect only the scatter in the data, not sample-to-sample variations. For  $\sigma > 0.7$  GPa  $T_p$  increases. (For sample 1, there was a small initial increase in  $T_p$  to  $\sigma = 0.1$  GPa followed by a decrease to  $\sigma = 0.4$  GPa, then an increase for larger  $\sigma$ .) (c) for all  $T < \approx 15$  K the resistance increases rapidly with stress to a saturation level of  $R(\sigma_s)/R(0) = 4$  (2) at  $\sigma_s = 0.75$  (0.77) GPa for sample 2 (1).

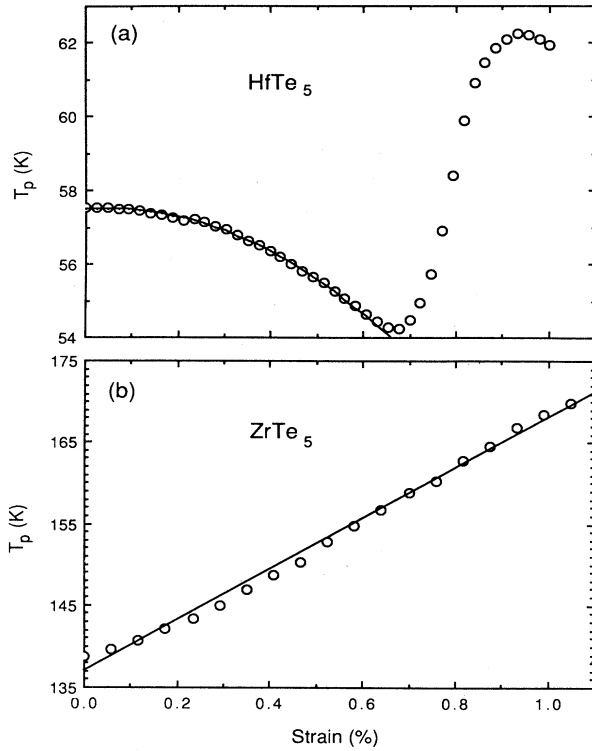


FIG. 5. Temperature of the resistance peak vs axial strain for (a) HfTe<sub>5</sub> and (b) ZrTe<sub>5</sub>.

The results above suggest that for HfTe<sub>5</sub>, (a) the magnitude of the resistance peak is more strongly associated with the change of  $b$  and/or  $c$  than with  $a$ , (b) the change of  $T_p$  is more strongly associated with the change of  $b$  and/or  $c$  than with  $a$ , and (c) the resistance change due to  $P$  or  $\sigma$  at low  $T$  is more strongly associated with the change of  $b$  and/or  $c$  than with  $a$ . (Whether the resistance change with  $P$  saturates is, unfortunately, not known.) Further,  $R(\sigma_s)/R(0)$  is sample dependent while  $\sigma_s$  is not.

For ZrTe<sub>5</sub> notable effects of pressure  $P$  are<sup>8</sup> (a) almost no change of the magnitude  $M$  of the peak, (b) a linear increase in  $T_p$  with  $P$  with slope of 1.2 K/GPa, and (c) an increase in  $R$  at each temperature at which measurements were made (the range was 80 to 300 K), with  $R(1.7 \text{ GPa})/R(0)$  changing with  $T$  from  $\approx 4$  at 80 K to  $\approx 2.5$  at 300 K. For stress  $\sigma$  there is (a) almost no change of  $M$ , (b) a linear increase of  $T_p$  with  $\sigma$  with slope of 2–2.5 K/GPa depending on the sample, and (c) an increase of  $R$  with  $\sigma$  at all temperatures for low stress. At intermediate  $T$  large  $\sigma$  reduces  $R$  because of the shift with stress of  $T_p$ . For  $T < 15$  K the resistance saturates with  $R(\sigma_s)/R(0) = 2.5$  (3.5) for sample 4 (3). The saturation stress  $\sigma_s = 0.8$  GPa for both samples.

The above results for ZrTe<sub>5</sub> suggest that (a) the magnitude of the peak is insensitive to small changes of  $a$ ,  $b$ , or  $c$ , (b) the increase of  $T_p$  is more strongly associated with changes of  $b$  and/or  $c$  than with  $a$ , and (c) the increase of

$R$  with  $P$  or  $\sigma$  is associated more strongly with changes of  $b$  and/or  $c$  than with  $a$  for  $T$  above 80 K. For  $T < 80$  K we have no data for the effect of  $P$ . Further,  $R(\sigma_s)/R(0)$  is sample dependent but  $\sigma_s$  is not.

### B. Origins of the transport properties

McMillan<sup>19</sup> has shown that in a one-dimensional system CDW transitions from the normal state are first (second) order if the CDW is commensurate (incommensurate). If there is a transition in these pentatellurides there is no evidence to suggest that it is of first order. At a second-order transition<sup>20</sup>

$$\Delta E/E = -(E\Delta C_p/T_c)(\partial T_c/\partial \sigma)^2 \quad (1)$$

in which  $\Delta C_p$  is the change of the specific heat due to the transition, and  $T_c$  is the transition temperature. Brill and Sambongi<sup>10</sup> have shown that there is no abrupt change in the elastic modulus ( $\Delta E/E < 3 \times 10^{-4}$ ) in ZrTe<sub>5</sub> in the temperature range of a possible transition. Sambongi *et al.*<sup>9</sup> have found  $\Delta C_p$  (obtained from a transition over a rather broad temperature interval) to be  $3.5 \times 10^4 \text{ J/(m}^3 \text{ K)}$ . Assuming that Eq. (1) applies and taking  $T_c \approx T_p$  then the right-hand side of Eq. (1) is about  $10^{-2}$ , which seems to rule out a second-order transition. Similar data are not available for HfTe<sub>5</sub>. Brill and Sambongi did find a sharp increase with  $T$  in modulus  $\Delta E/E \approx 4 \times 10^{-3}$  at 84 K in ZrTe<sub>5</sub>. A shift in  $C_p$  was found near 84 K in Ref. 9 but was attributed by those authors to a transition in an inclusion of a monoclinic polytype phase of ZrTe<sub>5</sub>. We found no unusual behavior at or near this temperature.

A most interesting result of this investigation is the rapid rise to saturation of the resistance with stress at low temperature. This result is similar to that of Tritt<sup>21</sup> *et al.* for the linear-chain compound TaSe<sub>3</sub>. This saturation appears to be unassociated with the resistance peak that occurs at higher temperatures in ZrTe<sub>5</sub>. However, for HfTe<sub>5</sub>, saturation occurs at approximately the same  $\sigma$  as does the minimum of the  $T_p$  versus  $\sigma$  curve, and  $T_p$  is lower than for ZrTe<sub>5</sub>. Thus, the negative dependence of  $T_p$  on  $\epsilon$  appears to be associated with the rapid rise of resistance and saturation that occurs at low temperatures.

A possible explanation for the rapid resistance increase to saturation may be that a Fermi-surface (FS) topology change occurs as a function of stress. This change is completed at a critical stress  $\sigma_c$  which is the saturation stress  $\sigma_s$ . Lifshitz<sup>22</sup> has developed a theory of such transitions, called “electron transitions” or “2.5-order transitions,” and there is convincing experimental evidence for their existence.<sup>23</sup> They are manifested in highly nonlinear electronic properties such as those observed in these experiments.

Kamm *et al.*<sup>12,13</sup> have reported detailed determinations of the FS of HfTe<sub>5</sub> and ZrTe<sub>5</sub>. The surfaces are very similar to each other, each consisting of three nested ellipsoidal surfaces centered at the center of the zone. The two inner surfaces are electron surfaces; the outer is a hole surface (Fig. 6). The two electron surfaces enclose

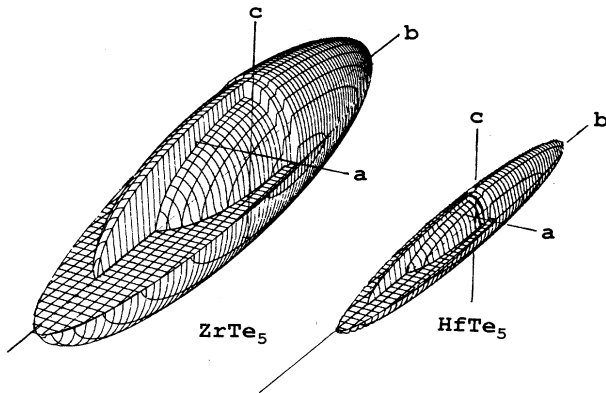


FIG. 6. Fermi surfaces of  $\text{HfTe}_5$  and  $\text{ZrTe}_5$ , as determined by Kamm *et al.* (Refs. 12 and 13).

total volume equal to that of the outer hole surface. These surfaces are very small and the two electron surfaces were shown to be very near one another in the  $ac$  plane. The topology of these surfaces might easily change under tension, and such a change could easily increase  $\rho$  by the factors found in these experiments.

In particular, measured from the edge of each band, the Fermi energy for all the surfaces is approximately 15 meV. It would not be difficult to imagine that the bands could be displaced in energy relative to each other enough to reduce the number of electrons and holes very significantly. Calculations for Si and Ge on the one hand,<sup>24</sup> and for Ca on the other,<sup>25</sup> have shown that effects of a 1% change in lattice parameter could move different bands relative to each other at least this much. Thus, for example, one of the electron bands, say the larger, could move up sufficiently in energy relative to the hole band to become empty. This would produce the correct order-of-magnitude change in electrical resistivity. In addition it provides a mechanism for the saturation of resistivity that is observed in these materials, for once the band is emptied further increasing the gap has no effect at very low temperatures.

Another possible origin of the rapid rise of resistance with strain at low temperature is band shape changes. The crystal structure of these materials can be expected to lead to a very soft material in the transverse directions. Furthermore, the energy dispersion curves are much flatter in the transverse directions than in the longitudinal directions (higher transverse effective masses). Thus, a reduction in the transverse lattice parameters caused by either isotropic pressure or longitudinal strain can be expected to result in a reduction in the relatively large transverse effective masses of both the electrons and holes. This implies a reduction in both the number of holes and electrons even in the absence of energy shifts of the bands relative to each other and thus an increase of resistivity.

A more subtle question is the effect of such a change in band shape on the impurity scattering relaxation time  $\tau$ . In order to evaluate this we have carried out a calculation of the electrical resistivity,  $\rho$ , of a one-dimensional conductor under the influence of elastic (impurity) scattering in the semiclassical Boltzmann equation approximation.

The calculation closely parallels the well-known treatment found in many standard texts for spherical-band materials. In our case the Fermi volume can be thought of as having a very flat ellipsoidal shape; i.e., we assume quadratic dispersion relationships between the energy  $E$  and wave vectors  $k_i$  in the three principal directions with the effective masses in the two transverse directions much larger than in the current-carrying direction. The scattering potential is the usual screened-Coulomb potential  $V_s$  and the electron wave functions are approximated by plane waves. Then, if  $z$  is the longitudinal (current-carrying) direction, the relevant equations are

$$\frac{1}{\rho} = \frac{ne^2\tau}{m_z}, \quad (2)$$

$$\frac{1}{\tau} = N_i v_z \int \sigma(\theta, \phi) (1 - \cos\theta) d\omega, \quad (3)$$

$$\sigma(\theta, \phi) = \left[ \frac{2m_z}{2\pi\hbar^2} \right]^2 |\langle i | V_s | f \rangle|^2, \quad (4)$$

$$V_s = \frac{Ze^2}{r} e^{-qr}, \quad (5)$$

$$q^2 = 4\pi e^2 \eta(E), \quad (6)$$

where  $1/\rho$  is the conductivity of a single band with  $n$  carriers and  $z$  component of the effective mass  $m_z$ ,  $N_i$  is the number of scattering centers,  $v_z$  is the  $z$  component of the carrier Fermi velocity,  $\sigma(\theta, \phi)$  is the differential scattering cross section into solid angle  $d\omega$ ,  $\langle i | V_s | f \rangle$  is the matrix element between initial and final plane-wave states,  $Z$  is the difference in atomic number between the impurity and the atom usually found at the site,  $q$  is the scattering length, and  $\eta(E)$  is the density of states at the Fermi surface.

The evaluation of the matrix element in Eq. (4) is identical to the spherical band case.  $\sigma(\theta, \phi)$  can then be inserted under the integral in Eq. (3), but here a problem arises. The integral cannot be evaluated over the non-spherical (pancake shaped) Fermi surface that we are assuming. Instead, and only for the purpose of evaluating this integral, we approximate the true Fermi-surface shape by a disc; i.e., a thin right circular cylinder. This implies that the electrons have velocities only in the plus and minus  $z$  direction. The factor  $(1 - \cos\theta)$  is then either 0 or 2 depending on whether the scattering takes place between states on the same side or opposite sides of the disk respectively. Using cylindrical coordinates  $1/\tau$  can be calculated exactly for the initial state at the center of a surface of the disk and to a good approximation elsewhere. For what we wish to learn, i.e., the fractional change in resistivity that accompanies a change in the Fermi-disk diameter, the results should be quite good. We obtain for  $1/\tau$

$$\frac{1}{\tau} = \frac{\pi}{2} N_i \left[ \frac{2m_z Z e^2}{\hbar^2} \right]^2 \frac{\hbar k_z^2}{m_z q^5} G(q/k_z), \quad (7)$$

where

$$G(q/k_z) = \frac{2}{\left[1 + \frac{k_z}{q}\right]^2 \left[\frac{k_z}{q}\right]} + \frac{3}{\left[\frac{q}{k_z} + \frac{k_z}{q}\right]} + 3 \left[ \tan^{-1} \frac{k_z}{q} - \tan^{-1} \frac{k_r}{q} \right]. \quad (8)$$

This is remarkably similar to the spherical-band case except for the somewhat different nature of  $G(q/k_z)$ . When  $k_z/q$  is small, which is the case for the two pentatellurides we are discussing, we can replace  $G(q/k_z)$  in  $1/\tau$  by the first (linear) term in its expansion in powers of  $k_z/q$ . Using this and the usual expression for  $n$  in Eq. (2), we obtain

$$\rho = \frac{c}{\alpha_x^3 \alpha_y^3 k_z^4}, \quad (9)$$

where  $c$  is a numerical factor and  $\alpha_i = k_i/k_z = (m_i/m_z)^{1/2}$  and  $i = x, y$ . This differs from the spherical case only by a numerical factor and the fact that the  $\alpha_i$  are not unity.

In order to determine the change in resistivity from band bending under the influence of tension or pressure it remains to estimate the change in  $m_i$  accompanying a change in lattice parameter resulting from tension or pressure. For this we employ the tight-binding approximation in the transverse directions and assume a free-electron dispersion relation in the  $z$  direction. Then if  $k_i a_i$  is small, as is expected in a semimetal,

$$E(k) = A + \frac{\hbar^2 k_z^2}{2m_z} + \gamma_x a_x^2 k_x^2 + \gamma_y a_y^2 k_y^2, \quad (10)$$

where  $A$  is a constant, the  $a_i$  are the interatomic spacing (the lattice parameters in a simple-cubic structure), and the  $\gamma_i$  are matrix elements between the atomic orbitals centered on neighboring sites.<sup>26</sup> It follows that  $m_i = \hbar^2/2\gamma_i a_i^2$ . Further, in the tight-binding formalism

there is a scaling law connecting  $\gamma_i$ , and therefore  $m_i$ , with the interatomic spacing  $a_i$  and the angular momentum quantum numbers of the atomic orbitals on the neighboring sites,<sup>27</sup> to wit:

$$\gamma_i \propto a_i^{-(l+l'+1)} \propto 1/m_i, \quad (11)$$

where  $l$  and  $l'$  are the angular momentum quantum numbers on the (weakly) overlapping orbitals.

The right-hand side of Eq. (9) varies basically as  $(1/m)^3$ . Whangbo *et al.* and Bullet<sup>28</sup> have calculated the states at the Fermi surface of ZrTe<sub>5</sub> as primarily  $p$  states but with some admixture of  $d$  states. Thus  $(l+l'+1)$  is between 3 and 5 and from Eq. (11) there will be a 3–5% change in  $m_i$  for each 1% change in the transverse lattice parameters. This predicts a roughly 10–15% change in  $\rho$ . Thus, in order to account for even half the factor of 4 increase we see in electrical resistivity with 1% longitudinal strain, this mechanism requires a 3–4% decrease in the relevant transverse interatomic distances. Although a particular transverse interatomic distance could possibly undergo a percentage change twice as much as the lattice parameter change in the complex unit cell found in these pentatellurides, even a 2% change in the former would be unprecedented, to our knowledge. We conclude, therefore, that although band bending may be making a significant contribution to the change in the electrical resistivity it is unlikely that it is contributing half or more of the change we observe.

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