factorily. Moreover, using this model and the hydrogenic wave functions for the ground and the excited states of a donor, we have calculated the effective donor-acceptor pair separation corresponding to the observed peak in the emission band; the calculated number is consistent with the impurity content of the sample deduced from electrical measurements.

In conclusion, we may mention that the shallow donor states in GaAs may be masked by band-tail effects in more impure materials. This may explain why the excited donor states have not been observed previously in GaAs.

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Band Inversion and the Electrical Properties of $Pb_xSn_{1-x}Te$†

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The electrical resistivity and Hall coefficient of $Pb_xSn_{1-x}Te$ alloys were determined as a function of temperature from 4 to 300°K. The measurements were intended as a test of Dimmock, Melngailis, and Strauss's band-inversion model in the immediate region of band crossing. The resistivity is characterized by a predominantly linear dependence upon T, and by the distinct breaks which occur in this dependence. The linearity is attributed to degenerate lattice scattering. The temperatures at which the breaks occur depend upon alloy composition, and are relatively independent of carrier concentration and carrier mobility. These break temperatures are in excellent agreement with band-crossing temperatures predicted on the basis of the band-inversion model. This fact, along with several other features of the results, strongly supports the band-inversion model.

I. INTRODUCTION

PROPERTIES of the $Pb_xSn_{1-x}Te$ alloy system have been studied in several laboratories over the past few years.[1] It has been shown that these solids are semiconductors having the rocksalt crystal structure throughout the range $0 \leq x \leq 1$. Considerable interest has centered around the unusual dependence of the valence-conduction band gap E_g upon alloy composition and temperature. This dependence is illustrated in Fig. 1, using a type of plot first presented by Dimmock, Melngailis, and Strauss[2] (DMS). The data represent experimental determinations of the magnitudes of E_g by various optical[2–11] and electrical[9,11–13] methods. The assignment of negative values to the band gaps of SnTe is based upon the proposal by DMS that E_g becomes zero at some intermediate alloy composition and that this is followed by an inversion of the states forming the valence- and conduction-band extrema. Their proposal was based upon a band model in which E_g varies with alloying because of differences in the relativistic band effects associated with Pb and Sn. Such a model explains the observed variation of E_g with x and the change in sign of the temperature coefficient of E_g in going from PbTe to SnTe.[2] Unfortunately, no experimental determinations of E_g have been carried out near the proposed band-crossing points, and only two values are reported on the Sn-rich side of the alloy system. Efforts

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† This work constitutes part of a thesis to be submitted to the University of Maryland by R. F. Bis in partial fulfillment of the requirements for the Ph.D. degree in physics.

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TABLE I. Properties of $Pb_xSn_{1-x}Te$ samples.

Sample	Type	Lattice constant (Å)	x	Carrier concentration (cm^{-3})	Slope (ρ versus T) (10^{-7} ohm cm/°K)	
					Below T_B	Above T_B
A	Bulk	6.349	0.25	5.3×10^{20}	...	...
B	Bulk	6.380	0.45	2.5×10^{20}	5.9	7.5
C	Bulk	6.386	0.50	2.9×10^{20}	6.4	7.0
D	Film	6.395	0.52	4.3×10^{19}	23	30
E	Bulk	6.392	0.54	2.4×10^{20}	6.5	7.7
F	Film	6.398	0.55	2.6×10^{19}	7.7	11
G	Bulk	6.403	0.61	1.4×10^{20}	7.6	9.2
H	Bulk	6.426	0.77	1.1×10^{20}	...	...
A (A&H)[a]	Bulk		0.00	1.40×10^{20}	...	...
7 (A&H)[a]	Bulk		1.00	1.45×10^{20}	...	...

[a] Samples and data of Allgaier and Houston (Ref. 24).

to obtain additional values in these regions by optical methods have been unsuccessful because of the large free-carrier concentrations that characterize the materials. Furthermore, no other properties have been measured through regions in which band crossing is expected to take place. In contrast to this incompleteness, a relatively thorough and impressive confirmation of the DMS model as applied to the $Pb_xSn_{1-x}Se$ alloys has been carrier out by Strauss.[14]

The obvious desirability of obtaining experimental information on the behavior of the $Pb_xSn_{1-x}Te$ alloys in the immediate region of proposed band crossing was the motivation for the work reported here. It was hoped that such information would serve as a useful test of the band-inversion model. For this purpose, we chose to make precision measurements of the resistivity of selected alloys as a function of temperature. The alloy compositions were selected so that the proposed band crossing would take place somewhere within the temperature range of measurement. For example, the alloy range involved for measurements from 12 to 300°K is indicated in Fig. 1 by the width of the shaded region. Our hypothesis, based upon the validity of the band-inversion model, was that the change in sign of the temperature coefficient of E_g occurring at the point of band crossing would be manifested as a change in the temperature dependence of the resistivity. We could not anticipate the exact nature of the expected variation because details of carrier scattering mechanisms and band structure for these materials are not known. The results show that, in fact, distinct breaks do occur in the temperature dependence of the resistivity. These results are described and related to the band-inversion model in Secs. III A and III B. An unexpected and simplifying feature of our observations was the linear dependence of resistivity upon temperature over wide temperature ranges. This feature and its implications as to carrier scattering mechanisms and band structure are discussed in Secs. III C and III D.

II. EXPERIMENTAL

The alloys that have been studied are listed in Table I along with their properties. Some were in the form of single-crystal epitaxial films, while others were bulk single crystals.

The two films were prepared by vacuum evaporation onto a cleaved (100) surface of an NaCl substrate, using the double-source method described previously.[15] Lattice constants a_0, listed in the table, were determined from a standard analysis of Bragg x-ray spectra obtained using the $K\alpha$ line of Cu. Alloy fractions x were estimated from these values of a_0. This was done by applying Vegard's law, using as endpoints the lattice constants 6.461 and 6.327 Å for PbTe[16] and SnTe,[17] respectively. The lattice constant for SnTe has been

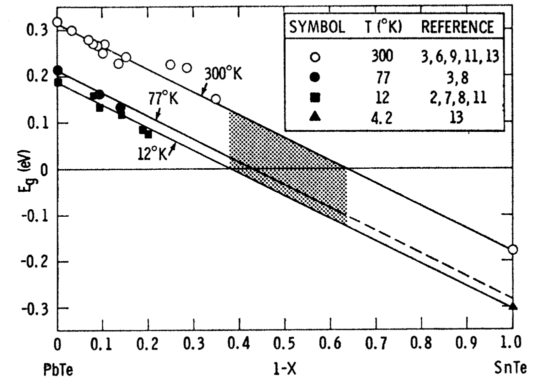

FIG. 1. Valence-conduction band gap of $Pb_xSn_{1-x}Te$ as a function of alloy composition and temperature. The assignment of negative gaps for SnTe is based upon the band-inversion model of Dimmock, Melngailis, and Strauss.

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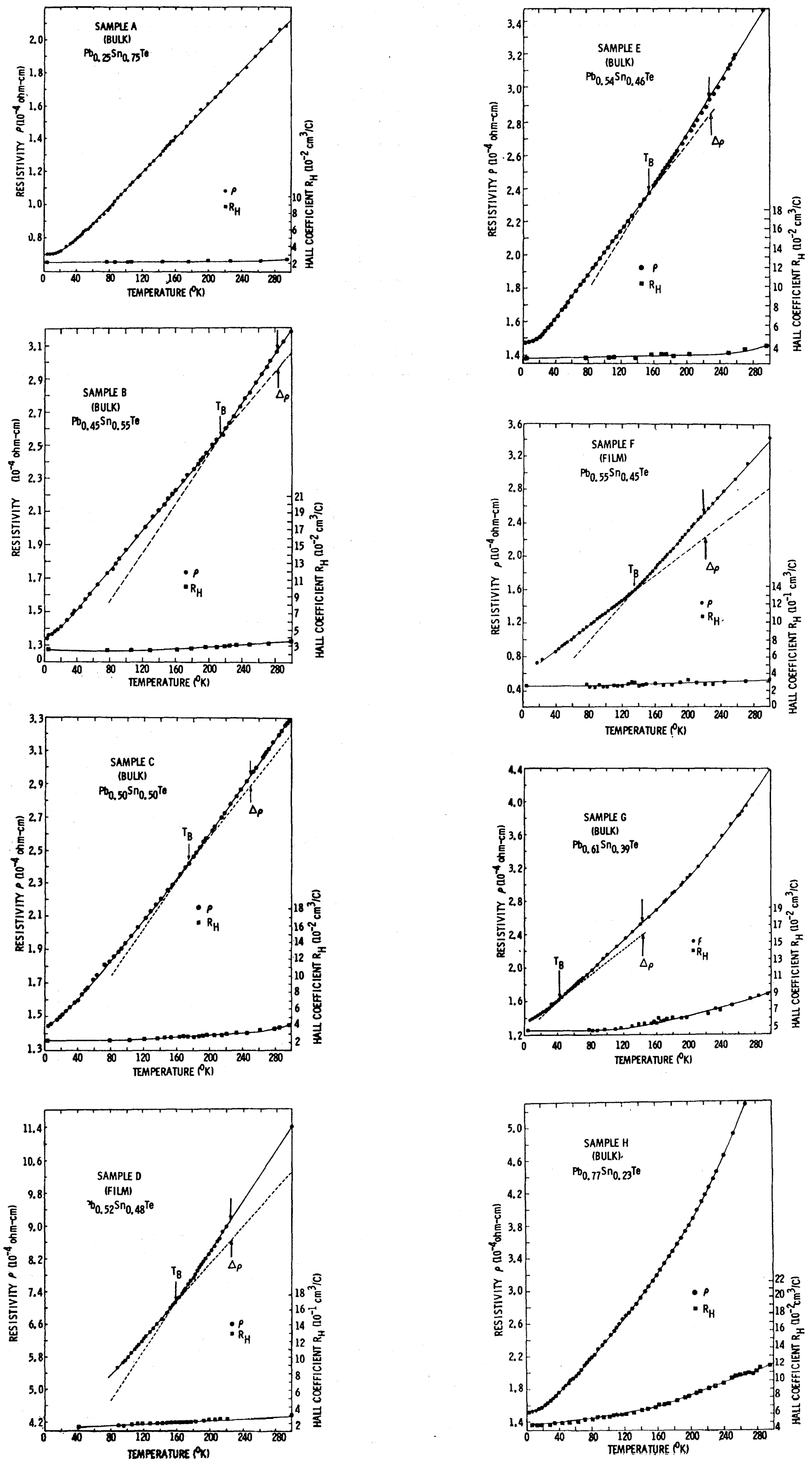

FIG. 2. Temperature dependence of the resistivity ρ and Hall coefficient R_H for the alloys described in Table I.

shown to be carrier-concentration-dependent.[18–21] We have taken this fact into account in applying Vegard's law, as discussed elsewhere.[17] Sharpness of the Bragg diffraction peaks indicated good crystalline quality for both films. Samples employed in the electrical measurements were formed during the evaporation process by the use of a mask. They consisted of a rectangular central section 0.318×0.953 cm^2 from which arms extended for electrical contact. Gold was applied to these arms by vacuum evaporation, after which electrical leads were attached with air-dry silver paste. Film thicknesses were 0.16 and 1.6 μ for samples D and F, respectively.

Bulk material was prepared and characterized by the Bell and Howell Research Laboratory.[16,18] These high-quality single crystals were grown under liquid B_2O_3, using the Czochralski technique. Electrical samples were cut from slices taken perpendicular to the direction of growth, which was approximately $\langle 111 \rangle$. They were in the form of rectangular parallelepipeds having dimensions of approximately $0.500 \times 0.076 \times 0.050$ cm^3. Pointed tungsten wires served as Hall and resistivity probes, while the current was supplied through spring-loaded pressure contacts.

Standard dc potentiometric methods were used to determine the resistivity ρ and the weak-field Hall coefficient R_H. The carrier concentrations given in Table I were calculated from low-temperature values of R_H and the relation $p = 1/R_H e$. A gas-exchange Dewar was used to control sample temperatures over the range 5–300°K. Below 20°K, temperatures were measured with a (gold +3% iron)-copper thermocouple,[22] while at higher temperatures a copper-constantan couple was employed. The uncertainty in the sample temperatures determined in these ways is believed to be less than ±0.5°K.

III. RESULTS AND DISCUSSION

A. Resistivity and Hall Coefficient

Values of ρ and R_H measured as a function of temperature are presented in Fig. 2. The resistivity is characterized by its linear dependence upon T over wide ranges and by the distinct breaks which occur in this dependence at the temperatures designated as T_B. The well-defined nature of these breaks is illustrated in Fig. 3, where we have plotted resistivity differences $\Delta\rho$ applying to sample F. As indicated in Fig. 2, $\Delta\rho$ is the difference between the observed resistivity and values defined by extrapolation of the linear dependence of ρ observed below the break. This method of differences was applied to all of our data so as to take advantage of the relatively high precision of these measurements (<1%). Well-defined breaks were observed in this way for alloys B–G, but no breaks were detected for alloys A and H. In contrast, the Hall-coefficient data presented at the bottom of each plot in Fig. 2 do not display unusual behavior in the vicinity of the resistivity break. This may be attributable to the fact that these latter measurements were considerably less precise (<5%) than the resistivity determinations. In addition, one would not expect the Hall coefficient to be as sensitive to changes in the band structure and scattering mechanisms.

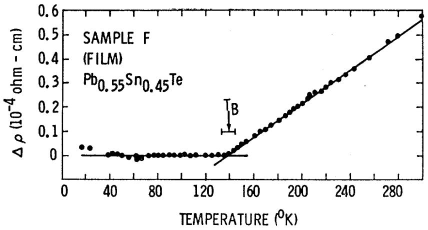

FIG. 3. Resistivity differences $\Delta\rho$ for sample F, as defined in Fig. 2. Such plots were employed to determine the temperature of the resistivity break T_B for all samples.

The results applying to samples G and H in Fig. 2 differ from the others in two respects. For these alloys, the resistivity deviates strongly from linearity with temperature in the high-temperature region. In addition, the Hall coefficient increases with temperature considerably more rapidly than for the other alloys. Both variations are typical of the behavior observed previously for PbTe and SnTe, a behavior which has been attributed to multiple band effects.[23,24] It is likely that this mechanism is also involved in the alloys like G and H.

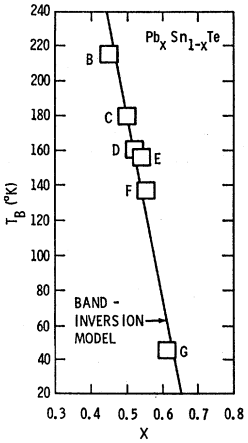

FIG. 4. Temperature of the resistivity break T_B as a function of alloy fraction x. The solid line represents temperatures of band crossing predicted on the basis of the band-inversion model and the data of Fig. 1.

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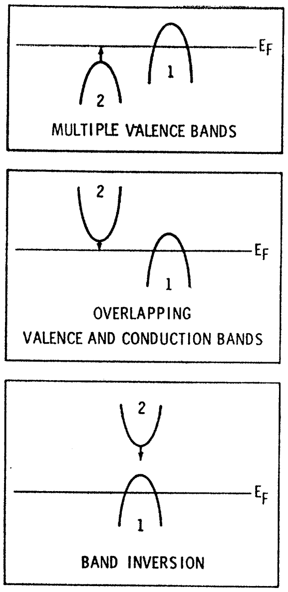

FIG. 5. Features of various band models that have been proposed for PbTe, SnTe, and their alloys. Arrows indicate relative motion of bands with increasing temperature.

B. Band-Model Considerations

The dependence of T_B upon alloy fraction x is presented in Fig. 4. The data are in excellent agreement with the solid line representing the band-crossing temperatures predicted on the basis of the band-inversion model and the data of Fig. 1. Note that our failure to observe breaks in the resistivities of alloys A and H is consistent with this model, since it specifies that band crossing for these two materials will take place outside of our range of temperatures. We consider these facts as strong evidence for the validity of the band-inversion model. In this regard, several other features of the data presented in Fig. 4 are of significance. These data apply to bulk and film samples differing widely in their carrier concentrations and carrier mobilities. Since these differences are not reflected as irregularities in the observed dependence of T_B upon x, we conclude that T_B is relatively independent of these variables. This suggests that T_B is dependent only upon the intrinsic nature of the band structure, a result which would be expected on the basis of the DMS model.

Even though our results are consistent with the band-inversion model in several respects, they do not prove that it is the only possible explanation. Consequently, it is of value to consider whether or not the breaks observed in the resistivity could be accounted for in terms of other band phenomena. Various band structures have been proposed to explain the electrical, optical, and thermal properties of these materials. These have included such features as multiple valence bands,[23–32] overlapping valence and conduction bands,[21,32,33] and the band-inversion phenomenon discussed above. The arrows in Fig. 5 show how each of these features might shift and produce a break in a ρ-versus-T curve. The upper two models in the figure would involve transfer of carriers from one band to another commencing at the temperature for which the second band first contacts the Fermi energy E_F. The question that we have considered is whether or not these models could account for the observed behavior of ρ and R_H in the neighborhood of T_B. An elementary analysis indicates that for any reasonable combination of band masses, neither model is consistent with our experimental results. The overlapping valence-conduction band model leads to variations in ρ which are opposite to those observed, while the multiple-valence-band model yields nonlinear variations of ρ. In addition, both models fail to account for the very abrupt nature of the resistivity break and the fact that T_B appears to be independent of carrier concentration over a wide range. The latter failure is a particularly significant one, since both models lead to large variations of T_B with carrier concentration. Thus, we conclude that our results are not describable in terms of either the overlapping valence-conduction or multiple-valence-band models. It follows that the agreement with the band-inversion model is unique at least to this extent.

Breaks of the type observed in the temperature dependence of the resistivity could result also from phase changes. One of the reasons for considering this possibility is that evidence for a phase change in SnTe has been reported.[34,35] We do not believe, however, that such a phenomenon is involved in producing our results, since x-ray studies of these materials at room temperature have shown that the cubic NaCl type of structure prevails throughout the entire system.[1,16,18,36,37] Such a result would not be expected if a phase change were taking place at T_B. This follows from the fact that an extrapolation of the T_B-versus-x curve of Fig. 4 indicates that the alloy fraction x corresponding to room temperature is 0.38. Thus, if a phase change were occurring, the alloy system at room temperature would be divided into two crystallographic species about this value of x. The fact that only a single species is observed indicates that phase changes are not involved. However,

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such evidence is indirect and cannot be considered conclusive. Additional experimental studies will be required before the possibility of a phase change can be definitely ruled out. A desirable study for this purpose would be detailed crystallographic determinations as a function of temperature in the neighborhood of T_B.

C. Carrier Scattering Mechanisms

The data of Fig. 2 are not extensive enough to serve as a basis for a detailed evaluation of the carrier scattering mechanisms in these materials. However, a considerable amount of useful information concerning the general characteristics of carrier scattering can be inferred from the simple nature of our experimental results.

An unusual feature of the data presented in Fig. 2 is the linearity of ρ with T over wide temperature ranges. An impressive example of this is the result applying to sample A, for which the linearity extends from approximately 30 to 300°K. Such a temperature dependence is characteristic of many metals, for which it is attributed to lattice scattering. The results for metals can often be described by applying Matthiessen's rule[38,39]

$$\rho(T)=\rho_R+\rho_L(T), \tag{1}$$

where ρ_R is a residual, temperature-independent resistivity and $\rho_L(T)$ represents the lattice resistivity given by the Grüneisen-Bloch formula[40]

$$\rho_L(T)=(\kappa T/\Theta_R^2)G(\Theta_R/T). \tag{2}$$

Here Θ_R is a characteristic temperature normally approximating the Debye temperature, κ is a constant, and $G(\Theta_R/T)$ is the Grüneisen function. Despite the fact that the Grüneisen-Bloch relation is based upon assumptions that are often unrealistic, it describes the resistivity of a large number of metals.[41] Since our materials are degenerate semiconductors, and in this sense metallic in nature, it seemed appropriate to compare our results with those predicted on the basis of Eqs. (1) and (2). Such a comparison applying to sample A is presented in Fig. 6. The parameters given in the figure were determined by straightforward curve-fitting procedures. The Debye temperature for this alloy has not been reported. However, the value of 190°K that we have obtained for Θ_R compares favorably with the zero-degree Debye temperature of 175°K determined by Houston *et al.* for PbTe.[42] The excellent agreement between experiment and calculation suggests that lattice scattering is a dominant mechanism determining the resistivity in these alloys.

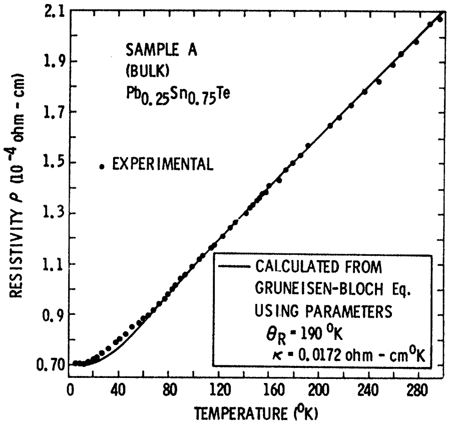

FIG. 6. Temperature dependence of the resistivity ρ of sample A. The solid curve represents values calculated on the basis of Matthiessen's rule and the Grüneisen-Bloch relation for lattice resistivity.

Additional information regarding the scattering mechanisms can be obtained most conveniently by plotting our data in terms of the conductivity mobility μ_c. We define this quantity as

$$\mu_c \equiv R_H(4°\mathrm{K})/\rho. \tag{3}$$

The temperature dependences of μ_c applying to our samples A–H are presented in Fig. 7, along with the results for PbTe and SnTe reported by Allgaier and Houston.[24] One-phonon acoustic lattice scattering is believed to be dominant in determining the temperature dependence of μ_c for PbTe and SnTe of high carrier concentration.[24] This fact, along with the similarities in the shapes of all the curves of Fig. 7, supports our assertion that lattice scattering is also important for the

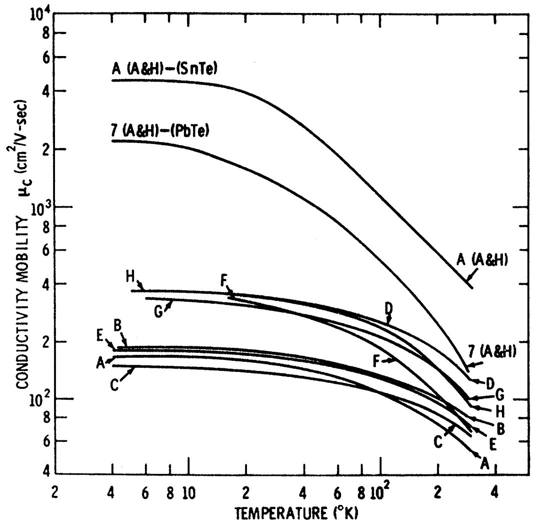

FIG. 7. Temperature dependence of the conductivity mobility, defined by Eq. (3), for alloy samples A–H. Data of Allgaier and Houston for PbTe and SnTe are also presented for comparison. All the materials are described in Table I.

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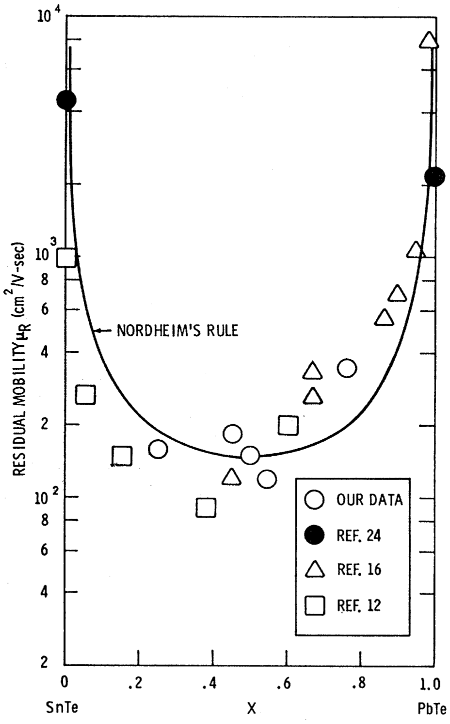

FIG. 8. Residual mobilities as a function of alloy fraction. The solid curve represents Nordheim's rule normalized to a mobility of 150 cm^2/V sec at $x=0.5$.

alloys. As one would expect when this type of scattering is involved, differences between the curves become smaller at high temperatures. At low temperatures, the mobilities applying to the alloys form two distinct groups and become temperature-independent. By referring to Table I, it can be seen that these groupings correlate with carrier concentration, the smaller concentrations being associated with the group of higher mobility. We conclude from this that the residual, temperature-independent mobility depends upon carrier-related imperfections. There is considerable evidence that these imperfections are lattice vacancies,[19,20] which suggests that this component of the residual mobility is of the ionized-impurity type. The fact that the correlation mentioned above does not apply to the PbTe and SnTe results shown in Fig. 7 indicates that the degree of alloying is also significant in determining the residual mobility, as one would expect. This dependence can be more clearly seen by plotting the residual mobility μ_R as a function of alloy fraction x, as in Fig. 8. The data apply to our materials as well as to those of others, as indicated. We have selected data applying only to the limited range of carrier concentration from 1×10^{20} to 5×10^{20} cm^{-3}. This was done to de-emphasize variations due to the carrier-related imperfections discussed above. Despite some scatter in the results, a relationship to the degree of alloying is evident. This second component of the residual mobility is believed to arise from a form of neutral impurity scattering. The solid curve in Fig. 8 represents Nordheim's rule[43] for such scattering, given by

$$\mu_R \propto 1/x(1-x). \tag{4}$$

The curve is normalized to a mobility of 150 cm^2/V sec at $x=0.5$. This rule describes the dependence of residual mobility upon alloying for many simple, binary metal alloy systems. However, the conditions under which it can be applied to a system like ours have not been established. Therefore its use here should be considered only as an empirical means to emphasize the correlation of our results to alloy fraction.

In summary, our results indicate that the resistivity in these materials is dependent upon lattice scattering and upon scattering from imperfections related to carrier concentration and to the degree of alloying.

D. General Relationships between Resistivity and the Band-Inversion Model

In order to test thoroughly the band-inversion model on the basis of our experimental results, one would require detailed information concerning the carrier scattering phenomena and band structure in these materials. Since such information is not available, the desirable analysis of our data in terms of this band model could not be carried out. However, some useful general relationships follow directly from our results.

As indicated in the Introduction, breaks in the temperature dependence of the resistivity could result from the change in sign of dE_g/dT, which is an inherent part of the band-inversion model. Such an hypothesis is based upon the assumption that the resistivity is dependent upon E_g. This is not an unreasonable assumption, since carrier-scattering phenomena often depend upon parameters which vary appreciably with the forbidden energy gap. Examples of such parameters are the carrier effective mass and dielectric constant, both of which are involved in the theoretical description of the scattering mechanisms described in Sec. III C. These assertions can be formalized in terms of the following expression for the total derivative of resistivity with respect to temperature:

$$\frac{d\rho(T,\beta)}{dT}=\frac{\partial\rho(T,\beta)}{\partial T}+\frac{\partial\rho(T,\beta)}{\partial\beta}\,\frac{\partial\beta}{\partial E_g}\,\frac{dE_g}{dT}. \tag{5}$$

In this relation, β represents a scattering parameter dependent upon the forbidden energy gap E_g, and T stands for the explicit dependence of ρ upon the temperature. It follows from this relation that a change in sign of dE_g/dT at the point of band crossing would produce an abrupt change in the temperature dependence of ρ, as discussed above. The experimental fact that the breaks occur within regions where the resistivity varies linearly with T leads to the requirement that Eq. (5) be equal to a constant throughout these ranges of linearity.

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[43] Reference 38, p. 337; Ref. 39, p. 113.

Whether or not this very stringent condition is satisfied for these alloys cannot be determined until more details of the scattering mechanisms and band structure are known.

Despite our incomplete knowledge of scattering mechanisms and band structure, we have carried out an elementary analysis using Eq. (5) which we believe is of sufficient general interest to warrant a brief description. This analysis was based upon a form of Eq. (1) given by

$$\rho(T,m^*)=\rho_R(m^*)+\rho_L(T,m^*)\,, \qquad (6)$$

in which the implicit temperature dependence is assumed to arise from the carrier effective mass m^*. In applying this relation to Eq. (5), we have assumed that $\rho_R(m^*)$ is due to ionized impurity scattering, $\rho_L(T,m^*)$ is given by the Grüneisen-Bloch formula, and the temperature dependence of E_g is as indicated in Fig. 1. The results of the analysis were in good qualitative agreement with all but one of our observations described in Secs. III A and III B. The exception was that the analysis predicts a nonlinear dependence of ρ upon T, in contrast to the strict linearity of our experimental results. Even though these findings are suggestive, they cannot be used as a basis for accepting or rejecting the role of carrier effective mass in producing the resistivity breaks. This limitation arises from the speculative nature of the assumptions on which the analysis is based.

As an aid to future analyses of our data in terms of Eq. (5), we have tabulated in Table I the slopes of the linear portions of our experimental curves above and below T_B. The percentage change in these slopes in passing through T_B increases regularly with decreasing carrier concentration and is relatively independent of alloy composition, as shown in Fig. 9. This dependence should serve as useful evidence in future efforts to identify details of the mechanisms involved in producing the resistivity breaks.

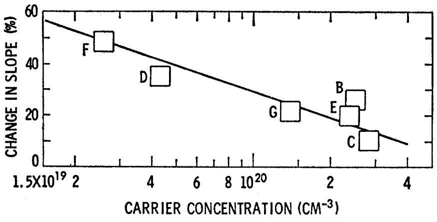

FIG. 9. Percentage change in slope of the ρ-versus-T relations occurring at the break temperature T_B. The changes apply to the data presented in Fig. 2 for alloys *B–G*.

IV. SUMMARY

Distinct breaks have been observed in the linear temperature dependence of the resistivity of $Pb_xSn_{1-x}Te$ alloys. They occur at temperatures that vary with alloy fraction x. These break temperatures T_B are in excellent agreement with the band-crossing temperatures predicted on the basis of the band-inversion model of Dimmock, Melngailis, and Strauss. In addition, T_B is found to be relatively independent of carrier concentration and carrier mobility, characteristics that are also consistent with the band-inversion model. We consider these findings to be strong supporting evidence for the validity of the band-inversion model. On the basis of this model, the measurements represent the first observation of an effect due to band inversion at the immediate point of band crossing.

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