Semimetal–semiconductor transition in p-type $Hg_{0.91}Cd_{0.09}Te$ under pressure

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A systematic study is made of the semimetal–semiconductor transition under pressure in p-type $Hg_{0.91}Cd_{0.09}Te$ at liquid-helium temperatures. The classical galvanomagnetic effects and the Shubnikov–de Haas effect are measured at pressures to 17 kbar and magnetic fields to 60 kOe. The cross section of the electron Fermi surface at the Γ point and the electron cyclotron mass are determined as functions of the gap parameter ε_g. It is shown that the activation energy ε_a of the acceptor band is practically independent of ε_g. Data are obtained which indicate that there is no appreciable renormalization of the electron spectrum in the p-type alloys for energies in the resonance region $\varepsilon_F \simeq \varepsilon_a$. It is shown that at liquid-helium temperatures there are three groups of carriers involved in transport phenomena in the p-type semimetal alloys: "light" electrons in the conduction band, holes in the acceptor band, and thermally excited holes at the top of the valence band. The features appearing in the field dependence of the magnetoresistivity $\rho(H)$ and Hall coefficient $R_x(H)$ are explained on the basis of a semimetal–semiconductor transition in the magnetic field H.

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INTRODUCTION

The compounds HgTe and CdTe form a continuous series of solid solutions throughout the entire range of compositions $0 \leqslant x \leqslant 1$ (Refs. 1, 2). A peculiarity of the restructuring of the energy bands in $Hg_{1-x}Cd_xTe$ alloys is the presence of a semimetal–semiconductor (SM–SC) transition due to the inversion of the Γ_6 and Γ_8 terms. At a certain value of x, which depends on the pressure p and temperature T, the gap parameter $\varepsilon_g \equiv \varepsilon_{\Gamma_6} - \varepsilon_{\Gamma_8}$ goes to zero (at atmospheric pressure and $T = 4.2$ K, one has[3] $\varepsilon_g = 0$ at $x = 0.165$). In $Hg_{1-x}Cd_xTe$ alloys with $\varepsilon_g < 0$ the SM–SC transition can be observed by applying a pressure p (Refs. 4–7), a quantizing magnetic field H (Refs. 4, 8, 9), or a uniaxial stress (Ref. 10).

Owing to the strong $\mathbf{k}\cdot\mathbf{p}$ interaction of the conduction band with the Γ_6 band, the electron dispersion relation is nonparabolic. The overall character of the dispersion curves $\varepsilon(k)$ in the vicinity of Γ is well described by the complete Kane model incorporating both the interaction of the three closest bands Γ_6, Γ_7, and Γ_8 and the influence of the distant bands.[2]

In the region of the inverted spectrum ($\varepsilon_g < 0$) the electron and hole dispersion relations (Γ_8) near the Γ point can be obtained by the Luttinger method.[1] The interaction of the bands Γ_6 and Γ_8 is taken into account by introducing additional terms in the Luttinger parameters γ_i^L:

$$\gamma_1^L = \gamma_1^0 + \frac{E_p}{3\varepsilon_g}, \quad \gamma_2^L = \gamma_2^0 + \frac{E_p}{6\varepsilon_g}, \quad \gamma_3^L = \gamma_3^0 + \frac{E_p}{6\varepsilon_g}.$$

Here $\varepsilon_g < 0$ is the gap parameter, $E_p = 2m_0\mathscr{P}^2/\hbar^2$ is the energy equivalent of the matrix element $\mathscr{P}$ specifying the Γ_6–Γ_8 interaction, and γ_i^0 are the parameters characterizing the interaction with the distant bands.

In HgTe and the semimetallic $Hg_{1-x}Cd_xTe$ alloys the terms containing E_p are dominant, so that the Luttinger parameters are negative and increasing in absolute value as $\varepsilon_g \to 0$. The values of E_p and γ_i^0 have been calculated in a number of papers.[3,11] According to the data of Weiler *et al.*,[11] E_p is equal to 17.9 eV ($\mathscr{P} = 8.26 \cdot 10^{-8}$ eV·cm) and does not depend on x (at least for compositions up to $x = 0.27$). The parameters γ_i^0, which take into account the influence of the distant bands, are of nearly unit order and have been determined only to extremely low accuracy. Evidently, near the point of inversion of the bands Γ_6 and Γ_8, where the Γ_6–Γ_8 interaction plays the dominant role, the function $\varepsilon(k)$ for the electrons is described satisfactorily by the simplified Kane dispersion relation, which is obtained without allowance for the effect of the distant bands, in neglect of the free-electron energy, and under the condition $\varepsilon, \varepsilon_g \ll \Delta$, where Δ is the spin–orbit splitting. In this approximation one obtains a gap dependence of the effective mass $m^*(0)$ at the bottom of the conduction band which is linear, dependent on a single parameter $\mathscr{P}$, and symmetric about $\varepsilon_g = 0$ (despite the change in the symmetry of the term forming the conduction band: $\Gamma_8 \to \Gamma_6$). We note that when the effect of the distant bands is taken into account ($\gamma_i^0 \neq 0$), the gap dependence of $m^*(0)$ becomes weakly nonlinear and is asymmetric about $\varepsilon_g = 0$ (Ref. 3).

The interaction with the distant bands has a substantial influence on spin effects in a quantizing magnetic field and on the nature of the SM–SC transition for magnetic fields in the extreme quantum region. The calculations of Kowalski and Zawadzki[8] have shown that the shift in a magnetic field of the Landau level O^+, which determines the bottom of the conduction band, is much slower than would be expected on the basis of a simple quasiclassical treatment.

It follows from Refs. 4–7 and 12 that the specifics of the SM–SC transition under pressure at liquid-helium tempera-

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tures are determined by the defects in the $Hg_{1-x}Cd_xTe$ alloy. In n-type alloys ($N_D - N_A > 10^{16}$ cm^{-3}) the Fermi level at liquid-helium temperatures lies above the completely filled acceptor band (level), and the SM–SC transition under pressure occurs at a fixed electron density N (Ref. 12). The Fermi energy in this case passes through a sharp peak at the point of inversion of the bands ($\varepsilon_g = 0$). In the p-type alloys ($N_A > N_D$) investigated in Refs. 4-7 the Fermi level ε_F is pinned in the acceptor band. In this latter case the study of the SM–SC transition presents a unique possibility for a most direct determination of how the activation energy ε_a of the acceptor band (level) depends on the gap parameter ε_g, which can vary under pressure over wide limits. This problem is of interest in connection with a number of theoretical studies[13–17] which have yielded a nontrivial gap dependence $\varepsilon_a(\varepsilon_g)$ of the activation energy of the quasidiscrete acceptor level that overlaps with the conduction band in semimetallic $Hg_{1-x}Cd_xTe$ alloys. It has shown[15] that in the case of a Coulomb impurity potential (with allowance for the nonlocality of the exchange interaction) the energy of the quasidiscrete acceptor level ε_a increases by a factor of 2.6 upon the transition from the inverted spectrum to the normal spectrum. Calculations with a highly localized potential of the vacancy type imply that the activation energy ε_a of the acceptor level depends strongly on the density of states in the conduction band, i.e., on the size of the gap ε_g (Refs. 13, 14, 16-18). In the SM–SC transition the acceptor level moves upward on the energy scale behind the rising bottom of the conduction band and becomes pinned in the forbidden band far beyond the inversion point of the bands, in the region $\varepsilon_g > 0$ (Ref. 14).

It should be noted that most of the calculations done in the impurity-potential approximation are of a semi-empirical nature and must be fitted to the experiment. At the present time, however, there is essentially only one experimental study[19] in which a strong growth of the activation energy ε_a of the acceptor defect was detected in $Hg_{1-x}Cd_xTe$ alloys at the transition to the semiconducting phase. In Ref. 19 the value of ε_a was determined in an indirect way [from the features in the temperature dependence of the resistivity $\rho(T)$] and, in our view, cannot be considered reliable. At the same time, other studies[4–7] have not revealed any appreciable dependence of ε_a on the gap parameter. Those results have since been reconfirmed.[20]

It should be noted that the theoretical calculations (with the exception of Ref. 17) have not incorporated the possible overlap of the wave functions corresponding to neighboring impurity centers. The presence of such an overlap greatly complicates comparison of theory and experiment, since real single crystals of $Hg_{1-x}Cd_xTe$ alloys, as a rule, are highly compensated, and in the majority of cases the integrated concentration of defects remains unknown. In the semiconducting phase, experiment has shown[21] that ε_a depends strongly on the defect concentration. Evidently a similar dependence should also exist in alloys with inverted spectra (the semimetallic phase). The concentration dependence of the activation energy of the acceptor levels complicates their classification; the disagreement between the values of the activation energy ε_a in Refs. 4 and 5–7 is possibly due to a difference in the integrated defect concentration of the investigated $Hg_{1-x}Cd_xTe$ alloys.

A number of questions remain in regard to the features of the electron and hole dispersion relations in the neighborhood of the point of contact Γ of the bands for $\varepsilon_g < 0$. It has been shown theoretically[22,23] that many-particle effects should lead to a renormalization of the electron and hole spectra near the Γ point in pure materials with inverted spectra. Mekhtiev[13] has indicated the possibility of a resonant renormalization of the electron spectrum in p-type materials at electron energies $\varepsilon \sim \varepsilon_a$.

There is still no unified point of view on the character of the acceptor-band conductivity at liquid-helium temperatures (in particular, Arapov *et al.*[20,24] assume an n-type acceptor-band conductivity in $Hg_{1-x}Cd_xTe$ alloys in order to explain the negative sign of the Hall coefficient $R_x(H)$ in the saturation region). Finally, the total number of groups of charge carriers involved in transport phenomena in p-type alloys at liquid-helium temperatures has not been definitively established.

In the present paper we systematically investigate the features of the SM–SC transition under pressure in p-type $Hg_{0.91}Cd_{0.09}Te$. We show that for a difference $N_A - N_D \gtrsim 10^{16}$ cm^{-3} in the acceptor and donor defect concentrations the activation energy ε_a of the acceptor band is practically independent of the size of the gap parameter ε_g. We establish that the value $\mathscr{P} = (8.4 \pm 0.3)\cdot 10^{-8}$ eV·cm of the Kane matrix element in the p-type alloy under study agrees within the error limits with the value obtained for n-type $Hg_{1-x}Cd_xTe$ alloys,[12] indicating that there is no appreciable renormalization of the electron spectrum in the p-type alloys for energies in the resonance region $\varepsilon_F \simeq \varepsilon_A$. We show that three groups of carriers participate in the transport phenomena in the semimetallic p-type alloys at $T = 4.2$ K: "light" electrons in the conduction band, holes in the acceptor band, and thermally excited holes at the top of the valence band. We explain the features in field dependence of the magnetoresistivity $\rho_{\parallel}(H)$ and Hall coefficient $R_x(H)$ on the basis of an SM–SC transition in the magnetic field H (Ref. 4).

MEASUREMENT PROCEDURES

To study the Shubnikov–de Haas effect we devised an apparatus capable of automatically recording the Shubnikov oscillations of the magnetoresistivity $\rho(H)$ and its derivative $\partial\rho(H)/\partial H$ in the field of a superconducting solenoid (up to 60 kOe) at liquid-helium temperatures. To eliminate the monotonic component of the $\sim\rho(H)$ signal we used an analog computer with Hall-effect transducers to generate a voltage $\sim(\alpha H \pm \beta H^2)$. A $\sim 1/H$ signal was generated by an analog computer using a Hall-effect transducer with a photoamplifier in the feedback circuit. The $\sim H$ or $\sim 1/H$ voltage was fed to the x coordinate of an xy recorder.

For measurement of the galvanomagnetic coefficients, the signal from the sample (with the magnetic field directed opposite to the current through the sample), the signal from a reference resistance R_{ref} and the $\sim H$ signal were recorded

in digital form with the aid of an FZO voltmeter with digital printout. The weak-field ($H < 2$ kOe) measurements of the galvanomagnetic coefficients were made in the field of a modulation coil to avoid the characteristic hysteresis effects of the main solenoid.

Pressures of up to 17 kbar were generated by a standard booster made of heat-treated beryllium bronze.[25] A pentane-kerosene-oil mixture was used as the pressure medium. The pressure at liquid-helium temperatures was determined from the temperature shift, which was measured by an induction method,[26] of the superconducting transition in a tin washer.

The measurements were made on an unoriented rectangular single-crystal sample of $Hg_{1-x}Cd_xTe$ ($x = 0.09$) with dimensions of $2.4 \times 0.85 \times 0.85$ mm. The distance between the potential contacts was 1 mm. The current and potential leads were gold wires with a diameter of 20 μm. The leads were soldered to the surface of the sample with pure indium.

MEASUREMENT RESULTS

The quantum oscillations of the magnetoresistance in a single crystal of $Hg_{0.91}Cd_{0.09}Te$ under pressure were studied in a longitudinal geometry ($\mathbf{H} \| \mathbf{j}$; the sample was mounted along the working channel of the high-pressure chamber). The Shubnikov–de Haas oscillations of $\rho_{\|}(H)$ were reliably recorded at pressures to 15 kbar.

Quantum oscillations of an unusually large amplitude were also detected in the field dependence of the Hall emf. This effect is an indirect indication that the Fermi level in the investigated alloy is pinned in the acceptor band. In fact, for $\varepsilon_F = \text{const}$ the carrier density and, hence, the Hall coefficient R_x will oscillate in a magnetic field.

In the case of a longitudinal orientation the conductivity $\rho_{\|}(H)$ is known to pass through a minimum when the next Landau quantum tube separates from the Fermi level; here the longitudinal magnetoresistivity $\rho_{\|}(H) = 1/\sigma_{\|}(H)$ passes through a maximum.[27]

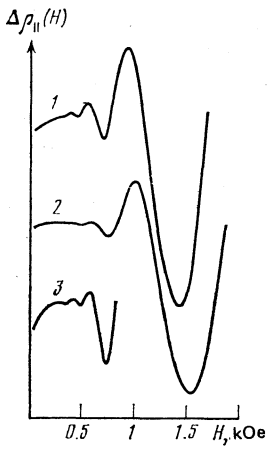

FIG. 1. Shubnikov–de Haas oscillations of the longitudinal magnetoresistivity $\Delta\rho_{\|}(H)$ in p-type $Hg_{0.91}Cd_{0.09}Te$ at $p = 11$ kbar; 1) $T = 2.1$ K; 2, 3) $T = 4.2$ K (curve 3 was recorded with a five-times greater amplification than curve 2). For ease of viewing, curves 2 and 3 have been shifted an arbitrary amount along the vertical axis.

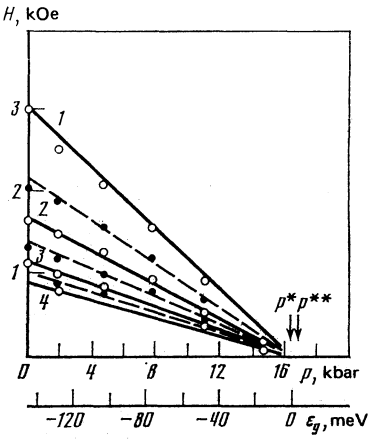

FIG. 2. The pressure and gap dependence of the fields at which the extrema of $\rho_{\|}(H)$ occur for $T = 2.1$ K: ○) the fields at the oscillatory peaks, ●) the fields at the minima. The solid lines are the theoretical curves for the fields corresponding to the emergence of the a series Landau levels with quantum numbers 1) 1^+ (a_1); 2) 2^+ (a_2); 3) 3^+ (a_3); 4) 4^+ (a_4).

It is established in the present study that the oscillatory peaks in $\rho_{\|}(H)$ are systematically shifted to weaker magnetic fields by the application of pressure. Figure 1 shows examples of the Shubnikov oscillations of $\rho_{\|}(H)$ from a spherical electron Fermi surface at the Γ point, recorded with the monotonic background suppressed for two temperatures, $T = 4.2$ and 2.1 K, at a pressure $p = 11.0$ kbar. The pressure dependence of the fields at which the oscillatory maxima and minima of $\rho_{\|}(H)$ occur for $T = 2.1$ K is given in Fig. 2. It is seen in Fig. 2 that the electron Fermi surface in the alloy under study contracts to a point at $p \simeq 16.5$ kbar.

The cyclotron mass m_c and the Dingle temperature T_D were determined from the temperature and field dependence of the amplitude of the Shubnikov oscillations.[27]

A number of the characteristic features of $\rho_{\|}(H)$ in the alloy under study complicate the calculation of m_c and T_D. First, the resistivity ρ_0 in zero magnetic field decreases appreciably as the temperature is lowered (Fig. 3), and this change must be taken into account. Second, the oscillatory peaks in $\rho_{\|}(H)$ are shifted to weaker magnetic fields as the temperature is lowered (Fig. 1). The latter effect is due to the shift of the Fermi level with temperature, which is observed in the semimetallic $Hg_{1-x}Cd_xTe$ alloys even at liquid-helium temperatures.[7,28]

We denote by $(\rho_0)_i$ and H_i the resistivity in zero magnetic field and the field of the selected oscillatory peak at T_i. In first approximation the corresponding Fermi energy is given by $\varepsilon_F \sim H_i$. If the Dingle temperature T_D is independent of T, the ratio $(b_1)_{T=T_2}/(b_1)_{T=T_1}$ of the amplitudes of a given oscillatory peak measured at temperatures T_2 and $T_1 (T_2 < T_1)$ will be[27]

$$\frac{(b_1)_{T=T_2}}{(b_1)_{T=T_1}} = \frac{\rho_{02}}{\rho_{01}} \frac{T_2 H_1}{T_1 H_2} \frac{\operatorname{sh}(2\pi^2 k T_1 m_c c/\hbar e H_1)}{\operatorname{sh}(2\pi^2 k T_2 m_c c/\hbar e H_2)} \times \exp\left[-\frac{2\pi^2 k T_D m_c c}{\hbar e}\left(\frac{1}{H_2} - \frac{1}{H_1}\right)\right]. \quad (1)$$

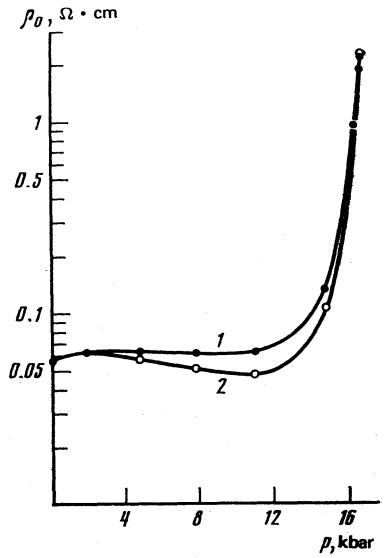

FIG. 3. Pressure dependence of the resistivity ρ_0 of p-type $Hg_{0.91}Cd_{0.09}Te$ at: 1) $T = 4.2$ K; 2) $T = 2.1$ K.

Relation (1) was used to calculate m_c on a computer. The cross section S of the electron Fermi surface was found from the period $\Delta(1/H) = eh/cS$ of the Shubnikov oscillations in the reciprocal magnetic field for fields far from the quantum limit. The electron density N was calculated from the expression

$$N = \frac{1}{3\pi^2}\left(\frac{2e}{c\hbar\Delta(1/H)}\right)^{3/2}, \quad (2)$$

which holds for a spherical Fermi surface.

Figure 3 shows the pressure dependence of the resistivity ρ_0 of the alloy under study in zero magnetic field at temperatures $T = 4.2$ and 2.1 K. A characteristic feature of the pressure dependence of $\rho_0(p)$ is the sharp growth of the resistivity at pressures $p \sim 16$ kbar. Step-like functions $\rho_0(p)$ such as these are usually observed at first-order phase transitions. In our case, however, the phase transition to the hexagonal cinnabar structure occurs at much higher pressures.[29]

The step-like behavior of $\rho_0(p)$ observed in the present study is due to a semimetal-semiconductor phase transition and can be explained qualitatively in the following way. The Fermi level, which determines the density of light electrons at liquid-helium temperatures, is "frozen into" the acceptor band, which overlaps the conduction band. As the pressure rises, the density of states at the bottom of the conduction band falls ($\varepsilon_g \to 0$), and the volume enclosed by the electron Fermi surface at the Γ point systematically decreases (Fig. 2). At the same time, the effective mass of the electrons decreases and their mobility increases sharply, reaching a maximum in the region of the inversion point of the bands Γ_6 and Γ_8. Over a wide range of pressures, the growth of the electron mobility μ as the inversion point is approached turns out to be stronger than the decrease in the electron density N. Therefore, at pressures in this range the resistivity ρ_0 not only fails to increase, it even falls off somewhat with increasing pressure at $T = 2.1$ K (Fig. 3). Near $\varepsilon_g = 0$ the decrease of the electron density N becomes the dominant factor, and ρ_0 begins to increase sharply. The size of the "jump" in $\rho_0(p)$ is governed by the relative contribution to the conductivity from carriers of the hole group. The growth of $\rho_0(p)$ should go to completion in the transinversion region ($\varepsilon_g > 0$) after the conduction band Γ_6 ceases to overlap with the acceptor band, leading to the complete disappearance (for $T \to 0$ K) of the electron group of carriers. In this case the conductivity at liquid-helium temperatures will be due entirely to the holes.[4-7]

In the present study we measured the field dependence of the transverse $\rho_\perp(H)$ and longitudinal $\rho_\parallel(H)$ magnetoresistivities (Fig. 4) and Hall coefficient $R_x(H)$ (Fig. 5) of $Hg_{0.91}Cd_{0.09}Te$ at liquid helium temperatures for pressures up to 17 kbar. We established that upon the transition to the extreme quantum region of magnetic fields the magnetoresistance increases anomalously rapidly with increasing field, this effect being especially strong near the point of inversion of the bands (Fig. 4). At high enough pressures (near boundary of the SM–SC transition) the functions $\rho(H)$ and $\rho_\perp(H)$ come together at the maximum attainable magnetic field (Fig. 4). The characteristic growth of the magnetoresistance beyond the quantum limit can be explained by the onset of a gap at Γ in a magnetic field and the lifting of the overlap between the conduction and acceptor bands (the magnetic "freeze-out" of the electrons at acceptor defects). The magnetic "freeze-out" model for the electrons in $Hg_{1-x}Cd_xTe$ alloys in a strong quantizing magnetic field was first proposed[4] in 1972.

A distinctive feature of the field dependence $R_x(H)$ of the Hall coefficient at liquid-helium temperatures over a wide range of pressures is an inversion of the sign of R_x as H increases (Fig. 5).

As the pressure is raised, the inversion field H^* at which R_x changes sign from " $-$ " to " $+$ " shifts rapidly toward

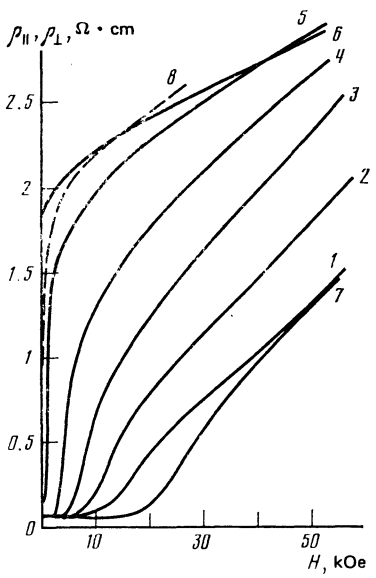

FIG. 4. Longitudinal magnetoresistivity $\rho_\parallel(H)$ (solid curves) and transverse magnetoresistivity $\rho_\perp(H)$ (dashed curve) in the investigated alloy at $T = 4.2$ K for pressures p: 1) 1.9; 2) 4.8, 3) 7.8; 4) 11; 5) 14.8; 6) 16.7; 7) 0.001; 8) 16.4 kbar.

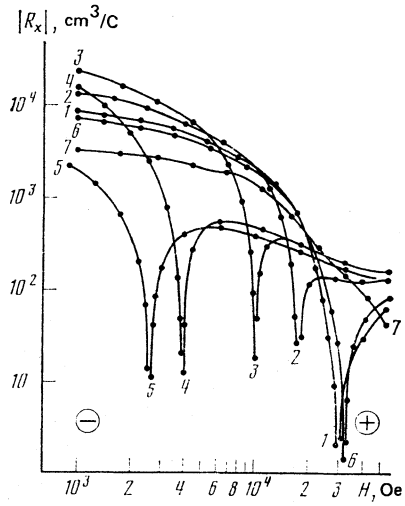

FIG. 5. Field dependence of the Hall coefficient $|R_x(H)|$ in the investigated alloy at $T = 4.2$ K for pressure p: 1) 5; 2) 7.8; 3) 11; 4) 14.6; 5) 16.8; 6) 4.7; 7) 0.001 kbar. The sign of $R_x(H)$ before and after the inversion is indicated in the figure.

weaker magnetic fields (Fig. 6). For purely technical reasons, the inversion field H^* was not reached at atmospheric pressure in the present study.

The $R_x(H)$ curves obtained in this study (Fig. 5) constitute direct proof of the existence of an acceptor band with p-type conductivity in $Hg_{0.91}Cd_{0.09}Te$ at liquid-helium temperature. On the basis of a qualitative analysis of the $R_x(H)$ curves in Fig. 5 one can conclude the following. The mobility of the electrons in the conduction band is substantially higher than that of the holes in the acceptor band. Therefore, in spite of the significantly higher density of the holes ($P \gg N$), the sign and magnitude of R_x in weak magnetic fields are predominantly governed by the electron group of charge carriers. With increasing pressure the electron density decreases, leading to the growth of $|R_x|$ in weak magnetic fields. It is only near the point of inversion of the bands that the growth in $|R_x|$ changes to a sharp drop. Evidently, the Hall coefficient R_x in weak magnetic fields changes sign during the SM–SC transition under pressure as a result of the complete disappearance of the electron group of carriers.[4–7]

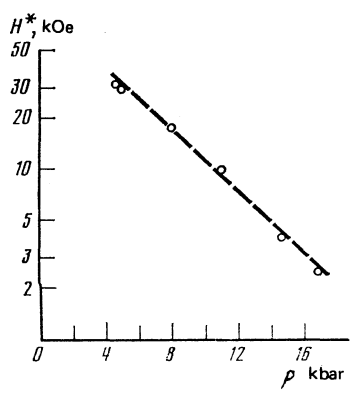

FIG. 6. Pressure dependence of the inversion field H^* of the Hall coefficient $R_x(H)$ (Fig. 5) at $T = 4.2$ K.

A noteworthy feature of the curves in Fig. 5 is the presence of a local maximum in $|R_x(H)|$ which appears immediately following the inversion of the sign with increasing H. We believe that this maximum indicates the presence of two groups of holes at liquid-helium temperatures in the investigated alloy, with highly different mobilities: holes in the acceptor band, and thermally activated holes at the top of the valence band Γ_8.

DISCUSSION OF RESULTS

Our studies of the oscillatory and classical galvanomagnetic effects in $Hg_{0.91}Cd_{0.09}Te$ at the transition from the semimetal to the semiconductor phase at liquid-helium temperatures enable us to describe unambiguously the nature of the restructuring of the bands in this alloy.

Certain of the experimental data indicate that there is an acceptor band in this alloy that is split off from the top of the valence band Γ_8 and overlaps the conduction band.

These data include: 1) the inversion of the Hall coefficient $R_x(H)$ in a magnetic field H (Fig. 5); 2) the anomalously large amplitude of the Shubnikov oscillations of the Hall emf at atmospheric pressure [these oscillations are practically unnoticeable in Fig. 5 because of the logarithmic scale used in plotting $R_x(H)$]; 3) the sharp decrease with pressure of the cyclotron mass of the electrons and the frequency of the Shubnikov oscillations from the electron Fermi surface, which results from the pinning of the Fermi level at the SM–SC transition under pressure (in the case of a free Fermi level the frequency of the Shubnikov oscillations from the electron Fermi surface at the SC–SM transition remains strictly constant[12]).

Using the pressure dependence of both the cross section of the electron Fermi surface and the electron cyclotron mass, one can calculate the Fermi energy ε_F over a wide range of pressures and thus determine to good accuracy the position of the acceptor band at the SM–SC transition under pressure (making use of the obvious condition $\varepsilon_F \simeq \varepsilon_a$).

Our analysis has shown that the density of states in the acceptor band in the alloy under study is high enough for the Fermi level to be pinned in the acceptor band both under pressure p and in a magnetic field H. This circumstance substantially simplifies the problem of identifying the Landau quantum levels. The curves of the quantum numbers of the oscillations versus the reciprocal of the field ($1/H$) obtained for various pressures p imply that the peaks in $\rho_{\parallel}(H)$ for all pressures correspond to the a series of Landau levels[1] [for $(1/H) \to 0$ all the straight lines extrapolate to the same value, $n = -1/4$]. At atmospheric pressure we also observed a peak in $\rho_{\parallel}(H)$ corresponding to the emergence of the O^- level (the b series),[1] but the amplitude of this peak fell off sharply under pressure. The reasons for the depression of the amplitude of the oscillatory peaks due to the b series of Landau quantum levels remains unclear.

The value of the spin-splitting factor $\nu = \Delta_{spin}/\Delta_{orb}$ determined from the position of the O^- peak in $\rho_{\parallel}(H)$ at atmospheric pressure turned out to be close to its limiting value[1] 0.5. We note that in a case where oscillatory peaks from the b series of Landau levels are present the frequency of the Shub-

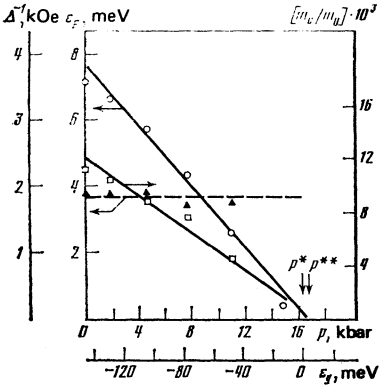

FIG. 7. The pressure and gap dependence of: ○) the frequency Δ^{-1} of the Shubnikov oscillations; □) the electron mass $m_c(\varepsilon_F)$; ▲) the electron Fermi energy ε_F in the investigated alloy at $T = 2.1$ K. The solid lines are constructed from the theory for $\varepsilon_F = 3.7$ meV and $\mathscr{P} = 8.4\cdot10^{-8}$ eV·cm.

nikov oscillations would be practically doubled.

To convert from the pressure dependence of the carrier parameters to the gap dependence, one must know the starting value ε_g^0 of the gap in the alloy at atmospheric pressure and the pressure coefficient of the gap $\partial\varepsilon_g/\partial p$. The absolute value of the gap parameter ε_g decreases linearly with pressure, reaching zero at the point of inversion of the Γ_6 and Γ_8 bands,

$$p^* = |\varepsilon_g^0|\,(\partial\varepsilon_g/\partial p)^{-1},$$

and then increases. At a pressure

$$p^{**} = (|\varepsilon_g^0| + \varepsilon_a)\,(\partial\varepsilon_g/\partial p)^{-1}$$

the overlap of the conduction band (Γ_6) with the acceptor band is lifted, leading to the disappearance of the electron group of charge carriers for $T \to 0$ K. At liquid helium temperatures one has[12] $\partial\varepsilon_g/\partial p = (8.8 \pm 0.3)$ meV/kbar. The value of ε_g^0 can, in principle, be obtained from empirical expressions relating the value of the gap parameter to the composition x and temperature T at atmospheric pressure,[1] but the accuracy with which ε_g^0 is determined in this case is manifestly inadequate. In the present study we determined the starting gap ε_g^0 (or p^*), the electron Fermi energy ε_F, and the matrix element $\mathscr{P}$ by comparing the experimental pressure dependence of the Shubnikov oscillation frequency $\Delta^{-1}(1/H)$ and cyclotron mass m_c with the theoretical values calculated in the two-band Kane model[1] (ε, $\varepsilon_g \ll \Delta$) using the known value[12] of $\partial\varepsilon_g/\partial p$ and assuming that the matrix element $\mathscr{P}$ does not depend on the pressure (Fig. 7). It should be noted that the use of the two-band version of the Kane dispersion relation, which does not allow for the influence of the distant bands, is completely justified in the present case, since in our alloy, even at atmospheric pressure, the corrections γ_i^0 for the interaction with the distant bands constitute no more than a few percent of the Luttinger parameters γ_i^L.

The straight lines in Fig. 7 are given by the theory. The calculations show that the Fermi energy ε_F and, hence, the activation energy of the acceptor band ε_a are independent the gap parameter ε_g to within the accuracy of the experiment (Fig. 7). The values of ε_g^0 and p^* come to -145 ± 5 meV and 16.5 ± 0.5 kbar, respectively. The vanishing of the electron group of carriers for $T \to 0$ should occur at a pressure $p^{**} = 16.9$ kbar.

The matrix element $\mathscr{P}$ is equal to $(8.4 \pm 0.3)\cdot10^{-8}$ eV·cm and agrees within the error limits with the value of $\mathscr{P}$ calculated[12] for n-type $Hg_{1-x}Cd_xTe$ alloys with a "free" Fermi energy ε_F. This agreement indicates that there is no appreciable renormalization of the electron energy spectrum for energies in the resonance region $\varepsilon_F \simeq \varepsilon_a$ in the p-type alloys.

Calculations of the Dingle temperature T_D from the field dependence of the amplitude of the Shubnikov oscillations show that in first approximation the Dingle temperature, which characterizes the nonthermal broadening of the Landau levels, does not depend on ε_g.

At liquid-helium temperatures the conductivity of the alloy $Hg_{0.91}Cd_{0.09}Te$ is equal to the sum of the electron and hole contributions: $\sigma = \sigma_e + \sigma_h$. As we shall see, the integrated hole contribution σ_h to the conductivity is independent of the pressure p and, for pressures $p > p^{**}$, practically coincides with the conductivity of the alloy: $\sigma \simeq \sigma_h$. The change in the conductivity σ of the alloy with pressure p is completely determined by the pressure dependence of the electron contribution $\sigma_e(p) = \sigma(p) - \sigma_h$, which can easily be calculated from the experimental data (Fig. 3; at atmospheric pressure σ_h comprises ~2.5% of the total conductivity σ). In this paper we have used the data of the oscillation measurements [$N(\varepsilon_g)$, $m_c(\varepsilon_g)$] and the gap dependence $\sigma_e(\varepsilon_g)$ of the electronic contribution to the conductivity to calculate the electron mobility

$$\mu_e(\varepsilon_g) = \sigma_e(\varepsilon_g)/eN(\varepsilon_g)$$

and the relaxation time $\tau^* = \mu_e m^*/e$, where

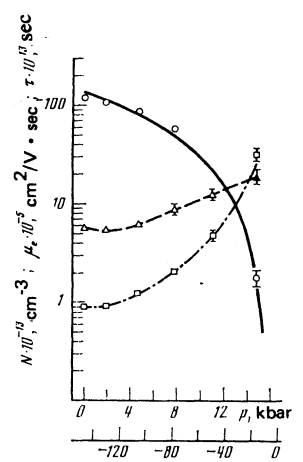

FIG. 8. The pressure and gap dependence of: ○) the electron density N; □) the electron mobility μ_e; △, ▲) the relaxation time τ in the investigated alloy at $T = 2.1$ K. The solid curve is given by the theory. The value of τ indicated by the filled triangle (▲) was calculated using an extrapolated value of the effective mass.

$$m^* \equiv m_c = m^*(0)\,(1+2\varepsilon_F/\varepsilon_g)$$

and $m^*(0)$ is the effective mass at the bottom of the conduction band. The results of the calculation are shown in Fig. 8. Near the point of inversion of the bands the electron mobility μ_e reaches values $\sim 10^6$ cm^2/V·sec, which agree in order of magnitude with the theoretical estimates.[18]

Important information on the nature of the hole conductivity at liquid-helium temperature in p-type $Hg_{0.91}Cd_{0.09}Te$ was obtained by studying the field dependence of the Hall coefficient $R_x(H)$ under pressure (Fig. 5). The sample was mounted at right angles to the working channel of the chamber. We note that a pressure drop took place at the partition of the high-pressure chamber, resulting in an increase in the integrated hole density P from $\sim 2\cdot 10^{16}$ cm^{-3} to $\sim 5\cdot 10^{16}$, in an increase in the hole contribution σ_h to the conductivity by a factor of ~ 2.5, in a drop in the electron mobility μ_e, and in a decrease in the activation energy of the acceptor band from ~ 3.7 meV (Fig. 8) to ~ 2 meV (see Table I).

It must be kept in mind that for a p-type semimetallic $Hg_{1-x}Cd_xTe$ alloy, an analysis of the field dependence of $R_x(H)$ (Fig. 5) based on a purely classical model, which assumes that the carrier density and the relaxation time are independent of the magnetic field H is only a crude approximation. For $T \to 0$ the lifting of the degeneracy of the bands at Γ in a magnetic field results in the complete outflow of electrons from the conduction band into the acceptor band at magnetic fields in the extreme quantum region ("magnetic freeze-out").[4] Near the point of inversion of the bands Γ_6 and Γ_8, the sharp drop in the electron density with increasing magnetic field H gives rise to an anomalously large longitudinal magnetoresistivity $\rho_{\parallel}(H)$ (Fig. 4).[4]

In the case of three independent groups of carriers the Hall coefficient $R_x(H)$ is given in the classical model (n_i = const, τ_i = const) by

$$R_x(H)/R_x(0) = (1+\alpha H^2+\beta H^4)/(1+\gamma H^2+\delta H^4), \qquad (3)$$

where

$$\alpha = \frac{(en_1+en_2)\mu_1^2\mu_2^2+(en_2+en_3)\mu_2^2\mu_3^2+(en_1+en_3)\mu_1^2\mu_3^2}{(en_1\mu_1^2+en_2\mu_2^2+en_3\mu_3^2)},$$

$$\beta = \frac{(en_1+en_2+en_3)\mu_1^2\mu_2^2\mu_3^2}{(en_1\mu_1^2+en_2\mu_2^2+en_3\mu_3^2)}$$

$$\gamma = \frac{[(en_1+en_2)\mu_1\mu_2+(en_2+en_3)\mu_2\mu_3+(en_1+en_3)\mu_1\mu_3]^2}{(en_1\mu_1+en_2\mu_2+en_3\mu_3)^2} > 0,$$

$$\delta = \frac{(en_1+en_2+en_3)^2\mu_1^2\mu_2^2\mu_3^2}{(en_1\mu_1+en_2\mu_2+en_3\mu_3)^2} > 0,$$

$$R_x(0) = \frac{(en_1\mu_1^2+en_2\mu_2^2+en_3\mu_3^2)}{(en_1\mu_1+en_2\mu_2+en_3\mu_3)^2}$$

is the Hall coefficient for $H \to 0$. Here e, $\mu_i < 0$ for electrons and e, $\mu_i > 0$ for holes.

To obtain unambiguous results in calculating n_i and μ_i from $R_x(H)$, one must use the experimental values of the conductivity in zero magnetic field ($H = 0$):

$$\sigma_0 = 1/\rho_0 = (en_1\mu_1+en_2\mu_2+en_3\mu_3).$$

The parameters α, β, γ, and δ are found from the system of linear equation (3) under the condition $\gamma, \delta > 0$. Equations (3) contain the experimental values $[R_x(H)/R_x(0)]_m$ determined in the fields H_m (m = 1, 2, 3, 4). The choice of the four pairs of experimental values of H_m and $[R_x(H)/R_x(0)]_m$ was varied during the calculation.

We used the values of $\alpha, \beta, \gamma, \delta, R_x(0)$, and ρ_0 for a given pressure to find the mobilities μ_i and carrier densities n_i (i = 1, 2, 3). Three independent values of the mobility μ_i were obtained from the cubic equation. The carrier densities n_i were calculated from the three linear equations with the known values of the mobilities μ_i substituted in. The calculations based on the classical model showed that one of the three groups of carriers consists of electrons and the other two consist of holes with highly different mobilities at

TABLE I. Electron and hole parameters in the investigated alloy at $T = 4.2$ K and at various pressures, as calculated from the field dependence of the Hall coefficient $R_x(H)$ and resistivity ρ_0; N is the electron density, μ_e is the electron mobility, P_H is the density of holes in the impurity band, μ_{hH} is the hole mobility in the impurity band, P_L is the density of thermally activated holes in the valence band, μ_{hL} is the hole mobility in the valence band, and ν is the spin-splitting factor.

p, kbar	ε_g, meV	ε^*_F, meV	ε^{***}_F, meV	ν	$(N)_{H\to 0}$, [10^{14} cm^{-3}]	μ_e, 10^5 cm^2/V·sec	P_H, 10^{16} cm^{-3}	μ_{hH}, 10^3 cm^2/V·sec	P_L, 10^{18} cm^{-3}	μ_{hL}, 10^4 cm^2/V·sec	Notes
7.8	−77	2.0	2.2	0.8	2.4	1.2	5.4±0.5	1.5	3.0±2.0	1.0	*
11.0	−48	1.9	2.0	0.79	1.15	2.5	4.8±0.4	1.5	6.2±0.5	1.0	*
14.6	−17	1.7	2.0	0.82	0.24	5.5	4.8±0.4	1.5	6.2±0.5	1.0	*
16.8	+3	–	2.0	–	0.04	1.2	5.7±0.3	1.2	5.6±0.5	0.9	**

*Calculated by formula (3) with allowance for the dependence of the electron density N on the magnetic field H [formula (4)].
**Calculated by formula (3) for n_i = const, τ_i = const (the classical model).
***Fermi energy ε_F calculated by formula (5).

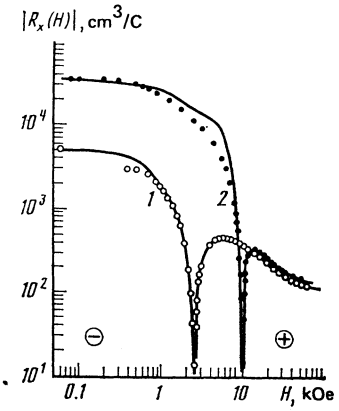

FIG. 9. Experimental (○, ●) and theoretical (solid curves) field dependence of the Hall coefficient $|R_x(H)|$ in the investigated alloy at $T = 4.2$ K for pressures p: 1) 16.8; 2) 11 kbar. The theoretical curve for $p = 16.8$ kbar is constructed with the classical model of Eq. 3 ($n_i = \text{const}$, $\tau_i = \text{const}$). The theoretical curve for $p = 11$ kbar is constructed with allowance for the dependence of the electron density on the magnetic field (Eq. 4; see Table I and Fig. 10).

$T = 4.2$ K (see Table I). According to the model we have adopted here, the holes with the lower mobility $\mu_{hH} \sim 10^2$ cm^2/V·sec are found in the acceptor band, while those with the higher mobility $\mu_{hL} \sim 10^4$ cm^2/V·sec are thermally activated holes at the top of the valence band (the "heavy" branch Γ_8).

Near the point of inversion of the bands ($p = 16.8$ kbar) we obtained good agreement between the theoretical and experimental dependence of R_x over a wide range of magnetic fields (Fig. 9). The theoretical curve in Fig. 9 ($p = 16.8$ kbar) was calculated from (3) with the parameters given in Table I. In the region of the SM–SC transition the electron density N even at $H = 0$ is three to four orders of magnitude smaller than the integrated hole density $P = P_H + P_L$, while the electron mobility μ_e reaches its peak value (Fig. 8). Under these conditions the dependence of N on the magnetic field H does not have a substantial effect on the form of $R_x(H)$, and the classical model can be used. Quantum effects become appreciable at pressures $p < 16$ kbar, since here the electron group of carriers gives only an insignificant contribution to the field dependence $R_x(H)$ of the Hall coefficient. In this case one cannot obtain good agreement between theory and experiment over the entire range of magnetic fields on the basis of a purely classical model. The results can be improved significantly by introducing a field-dependent electron density $N(H)$ in Eq. (3) (Fig. 9, theoretical curve 2 for $p = 11$ kbar). The density $N(H)$ was calculated by numerical methods on a computer (without allowance for the collision broadening of the Landau levels) with the aid of the expression ($\varepsilon_F = \text{const}$)

$$N(H) = \frac{2^{3/2} eH}{h^2 ckT} [m^*(0)]^{1/2} \sum_{n,s} \int_{\varepsilon^*}^{\infty} \frac{\{\varepsilon(1+\varepsilon/\varepsilon_g) - \varepsilon_{n,s}\}^{1/2} e^{(\varepsilon-\varepsilon_F)/kT}}{(1+e^{(\varepsilon-\varepsilon_F)/kT})^2} d\varepsilon, \tag{4}$$

where

$$\varepsilon_{n,s} = (n+1/2 - sv/2)\hbar\omega_c(0), \qquad \omega_c(0) = eH/m^*(0)c$$

is the cyclotron frequency corresponding to the bottom of the band, $m^*(0)$ is the effective mass at the bottom of the band, ν is the spin-splitting factor, $s = \pm 1$, and

$$\varepsilon^* = -\varepsilon_g/2 + [(\varepsilon_g/2)^2 + \varepsilon_{n,s}\varepsilon_g]^{1/2}.$$

The functions $N(H)$ which yielded the best agreement between the experimental and theoretical $R_x(H)$ curves for $p = 7.8$, 11, and 14.6 kbar are shown in Fig. 10. In the framework of the simplified Kane model [formula (4)], the rate of

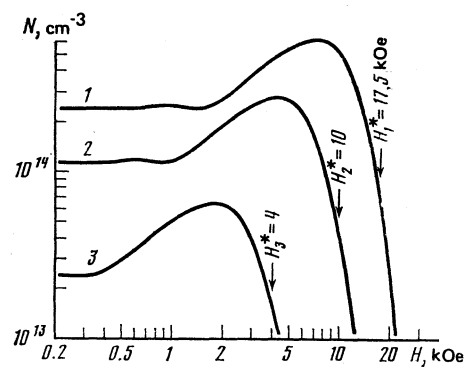

FIG. 10. Theoretical dependence of the electron density N on the magnetic field H at $T = 4.2$ K, calculated according to Eq. (4) (see Table I). 1) $p = 7.8$; 2) 11; 3) 14.6 kbar. H_i^* is the field at which the inversion of R_x occurs.

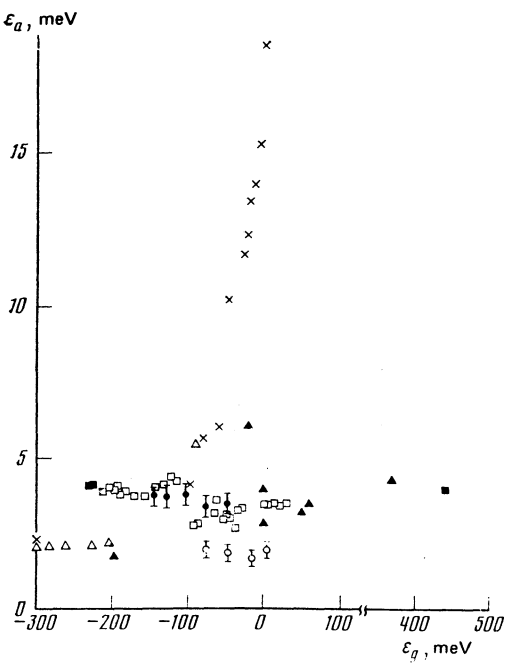

FIG. 11. The dependence of the activation energy ε_a of the acceptor band (level) on the gap parameter ε_g in the alloy system $Hg_{1-x}Cd_xTe$. The data are taken from: ○, ●) the present study; □) Refs. 5-7; ■) Ref. 21 ($N_A - N_D = 8 \cdot 10^{16}$ cm^{-3}); △) Ref. 3; ▲) Ref. 20; ×) Refs. 14 and 19.

motion of the lowest Landau level (the O^+ level), which determines the rate of growth of the direct gap at Γ, is governed by the values of the gap parameter ε_g and ν factor.[1] A theoretical analysis disregarding the influence of the distant bands[1] has shown that for $\varepsilon_g < 0$ the ν factor at the bottom of the conduction band is independent of ε_g and is equal to 0.5. Our calculations have shown, however, that for $\nu = 0.5$ the inversion of the Hall coefficient $R_x(H)$ occurs at considerably weaker fields than implied by experiment. Agreement between the theoretical and experimental functions $R_x(H)$ is obtained for $\nu \simeq 0.8$ (see Table I and Fig. 9). Thus the shift (to higher energies) of the bottom of the conduction band in a magnetic field occurs much more slowly than predicted by the simple model of Ref. 1. It follows from what we have said that the use of expression (4) for small quantum numbers n requires serious justification even for $\varepsilon_g \to 0$.

It is of interest to consider the characteristic local growth of the electron density (Fig. 10). This growth, which is due to the increase of the density of states at the Landau level O^+ in the magnetic field H, can be important in slowing the upward shift of the O^+ level in the magnetic field [the electron density N falls sharply only when the bottom of the Landau subband O^+ approaches ε_F (Fig. 10)].

It follows from the data given in Table I that the parameters of the holes of the impurity and thermally activated bands are practically independent of the pressure, i.e., of the gap parameter ε_g.

The Fermi energy ε_F of the investigated alloy in the semimetallic phase can be estimated from the density P_L of thermally activated holes in the valence band with the aid of the expression

$$P_{\text{л}} = \frac{(2m_h kT)^{3/2}}{4\pi^{3/2}\hbar^3} e^{-\varepsilon_F/kT}. \qquad (5)$$

At $T = 4.2$ K and for a band-hole mass $m_h = 0.5m_0$ (Ref. 3), relation (5) gives a value $\varepsilon_F \simeq 2$ meV (see Table I). This pressure-independent value of ε_F is in good agreement with the value of ε_F determined from the calculations of $R_x(H)$ according to Eqs. (3) and (4) (see Table I).

We have used the results of this study and the data of other authors to construct the gap dependence of the activation energy ε_a of the acceptor band in $Hg_{1-x}Cd_xTe$ alloys over a wide interval of values of the gap parameter ε_g (Fig. 11), both in the region of the inverted spectrum ($\varepsilon_g < 0$) and in the region of the normal spectrum ($\varepsilon_g > 0$). The sharp growth in ε_a for $\varepsilon_g \to 0$ detected in the experiment of Finck *et al.*[5] is not supported by the results of the present work or by the data of other authors. We have established that, at least for $N_A - N_D > 10^{16}$ cm^{-3}, the activation energy ε_a of the acceptor band does not depend in an appreciable way on the size of the gap parameter ε_g in the region of the transition of $Hg_{1-x}Cd_xTe$ alloys from the semimetal to the semiconductor phase. This result is in disagreement with the theoretical Refs. 14–17.

It should be pointed out in conclusion that the absence of reliable information about the degree of compensation of the defects in the actual $Hg_{1-x}Cd_xTe$ single crystals used in the experimental studies makes it very difficult to analyze the data (Fig. 11) on the basis of the existing theories.

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