Carrier localization in crystalline semiconductors subjected to hydrostatic compression

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The behavior of a crystalline semiconductor near a metal–insulator electronic phase transition induced by hydrostatic compression has been studied. Heavily doped, compensated p-$CdSnAs_2\langle Cu\rangle$ was selected as a model. There is a deep resonance acceptor band at the edge of the conduction band of this semiconductor. The behavior of interest was extracted from experimental data on the temperature dependence of the resistivity and the Hall coefficient in the temperature range 2–300 K, in fields up to 15 kOe, and at pressures up to 1.5 GPa. The results reveal the following behavior as the pressure is increased. (1) Near atmospheric pressure, p-$CdSnAs_2\langle Cu\rangle$ is in a metallic state. (2) A transition then occurs from an unactivated conductivity to a hopping conductivity of conduction-band electrons; i.e., holes of the deep acceptor band also localize in wells of the large-scale fluctuation potential. This is a resonance-hybridization version of a Mott transition. In the delocalization direction, this transition is accompanied by a "pulling" of the mobility of acceptor-band holes toward the mobility of conduction electrons. At the metal–insulator transition, the critical electron density decreases by several orders of magnitude as a result of the formation of ion clusters. The condition for a metal–insulator transition in a heavily doped, compensated semiconductor is refined. (3) The transition from metallic to hopping conductivity and from a heavily doped, compensated semiconductor to a heavily doped, completely compensated semiconductor is stretched out over $\simeq 10$ meV by the scatter in the density of states of the acceptor band. In this region, delocalized electrons coexist with localized electrons and with acceptor-band holes. (4) At pressures above 0.15 GPa, a modification of the model of a heavily doped, completely compensated semiconductor is realized in a semiconductor with an impurity band. (5) Finally, at very high pressures, the system consisting of the valence and acceptor bands corresponds to the model of a lightly doped, highly compensated semiconductor.

1. INTRODUCTION

In a lightly doped, lightly compensated semiconductor, a transition from an activated conductivity to a metallic conductivity usually occurs when a certain critical impurity concentration N_M is reached.[1,2] This critical concentration satisfies the condition

$$N_M^{1/3} a_B \simeq 0.25, \tag{1}$$

where $a_B=\chi\hbar^2/me^2$ is the effective Bohr radius of an electron at an isolated donor, χ is the dielectric constant of the crystal, and m and e are the effective mass and the charge of the electron. Here and below, we assume an n-type semiconductor for definiteness. The inverse metal–insulator transition in a heavily doped semiconductor occurs under the influence of compensation. A scanning of the Fermi level below the percolation level, with $N_A \to N_D$, where N_D and N_A are the concentrations of donors and acceptors, causes electrons to localize in the wells of the large-scale fluctuation potential.[3–10] The critical electron density corresponding to this transition is, according to Ref. 5,

$$n_c=\nu N^{2/3}/a_B \tag{2}$$

($N=N_A+N_D$). The value of the numerical coefficient ν is not yet known.[1,2] In a heavily doped semiconductor, a metal–insulator transition may be induced by a magnetic field, which compresses the electron wave functions and thereby promotes a localization of the electrons.[1,2] The threshold magnetic field is given by

$$H_M=\frac{64\hbar}{e} a_B N_D. \tag{3}$$

Hydrostatic compression reduces the distance between impurities in a semiconductor and thereby promotes the onset of a metallic state. The ensuing increase in the impurity concentration in the semiconductor does not, however, exceed 2% per 1 GPa (Ref. 11). The radius of the carrier state at an impurity changes more significantly as the pressure is varied. For definiteness we consider the diamond-like, direct-gap, n-type semiconductors InSb, InAs, $CdSnAs_2$, and $CdGeAs_2$, with a Kane dispersion law. For "hydrogen-like" impurities, for the two-band Kane model, and for the pressure dependence of the dielectric constant found empirically from existing data (Ref. 11, for example) for these semiconductors, we have

$$a_B=a_B^0[(1+\beta P/\varepsilon_{g_0})(1+\theta P/\varepsilon_{g_0})]^{-1}. \tag{4}$$

Here $\theta=0.025$ eV/GPa, ε_g is the width of the band gap, $\beta=d\varepsilon_g/dP$, and the subscript 0 means atmospheric pressure. According to (4), in n-InSb for example, an increase in the pressure to 1 GPa is accompanied by a 90% decrease

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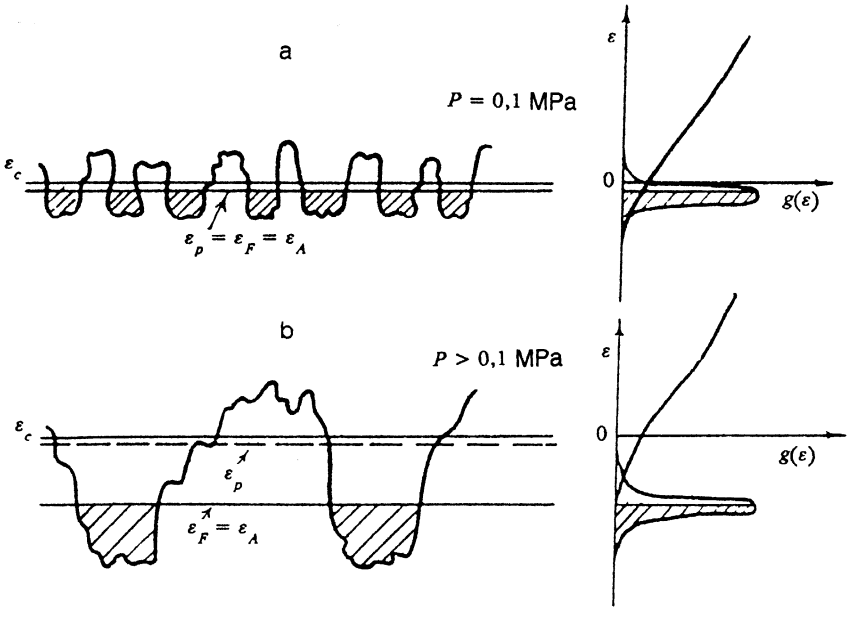

FIG. 1. Energy diagram of p-$CdSnAs_2\langle Cu\rangle$, a heavily doped, compensated semiconductor with a deep acceptor band. a: Atmospheric pressure. b: High hydrostatic pressure. Wavy line—curvature of the bottom of the conduction band; upper solid line—energy of the bottom of the conduction band in the absence of an impurity potential; lower solid line in frame a—coincident Fermi level, percolation level, and level of a deep acceptor; lower solid line in frame b—coincident Fermi level and level of a deep acceptor; dashed line—percolation level. Shown at the right are the density of states of the conduction band and that of the acceptor band. The regions occupied by electrons are hatched.

in the effective Bohr radius. It follows then from expressions (1)–(3) that N_M increases by a factor of 7, and n_c by a factor of 1.9, if we assume that the coefficient ν in (2) remains constant (see Sec. 3). The value of H_M decreases by a factor of 1.9. In other words, there is a well-expressed tendency toward localization. This tendency of the electrons to localize at a high pressure has been observed[12] in narrow-gap PbSnSe semiconductors, in which a pronounced increase in the density of states in the conduction band causes the Fermi level to shift toward the bottom of this band, from 37 to 2 meV, as the pressure is raised to 3 GPa. However, a metal–insulator transition does not occur: The Fermi level does not drop below the mobility threshold.

Another possibility of inducing a metal-insulator transition at a high pressure arises if there is a defect level near the edge of the band gap, as there is in the heavily doped, compensated semiconductor[13] p-$CdSnAs_2\langle Cu\rangle$. At a distance

$$\varepsilon_{AB}=\varepsilon^0_{AB}+\alpha T-\beta P \qquad (5)$$

from the unperturbed edge of the conduction band [$\varepsilon^0_{AB}=-30$ meV, $\alpha=4.6\cdot 10^{-2}$ meV/K, and $\beta=120$ meV/GPa], a deep acceptor level of an intrinsic Cd vacancy defect is observed in p-$CdSnAs_2\langle Cu\rangle$. Here and below, the energy is reckoned from the unperturbed bottom of the conduction band, and the positive direction is into the band. The acceptor band which forms as a result of concentration broadening effectively overlaps the bottom of the conduction band, which descends by an amount $\Delta\varepsilon_c=-\varepsilon^0_{AB}$ because of the heavy doping (Fig. 1). A gapless state forms. The acceptor band is related in energy to the valence band. As the pressure is increased, the conduction band moves away from the acceptor band and from the valence band at the same rate, $d\varepsilon_g/dP$. Even at 77.6 K, at pressures above atmospheric, the tail of the density of states of the conduction band has a noticeable effect on transport properties (this effect increases with increasing pressure). At $P>0.5$ GPa, the electrons are below the unperturbed edge of the conduction band. Simultaneously, electrons of the conduction band freeze out into the acceptor band, and the states of these bands separate from each other.

We thus see the value of an experimental study of electronic transport effects near liquid-helium temperatures when p-$CdSnAs_2\langle Cu\rangle$ is subjected to hydrostatic pressure. The purpose of such experiments is to obtain new data on the behavior of crystalline semiconductors near a metal-insulator electronic phase transition.

2. EXPERIMENTAL RESULTS

Data on the kinetic properties of heavily doped, compensated p-$CdSnAs_2\langle Cu\rangle$ semiconductors at $T>77.6$ K, both data obtained previously[13] and new data, make it possible to determine the characteristic properties of the carriers over a broad range of the concentration of excess acceptors ($N_\infty=N_A-N_D$), from 10^{13} to 10^{16} cm^{-3}. The concentration of deep acceptor centers (N_{AB}) is on the order of 10^{16} cm^{-3}. As N_∞ increases, the compensation coefficient ($K=N_D/N_A$) and the population coefficient of the acceptor band ($K_{AB}=I-N_\infty/N_{AB}$) decrease, from 0.999 99 to 0.99 and from 0.999 to 0, respectively. The extremely high compensation of p-$CdSnAs_2\langle Cu\rangle$ agrees with the Reis–Fuller theory, which attributes the high solubility of diffused copper in cadmium-tin diarsenide to a donor impurity.[14]

Two crystals, identical in properties ($N_\infty=1.6\cdot 10^{15}$ cm^{-3}, $N\simeq 10^{18}$ cm^{-3}, $N_{AB}=3.1\cdot 10^{16}$ cm^{-3}, $K=0.999$, $K_{AB}=0.92$, and $Na_B^3\simeq 100$), were selected for the low-temperature measurements. The resistivity ρ, the Hall coefficient R, and the transverse magnetoresistance $\Delta\rho/\rho_0$ were measured over the temperature range 2–300 K for hydrostatic pressures up to 1.5 GPa and in magnetic fields up to 15 kOe.

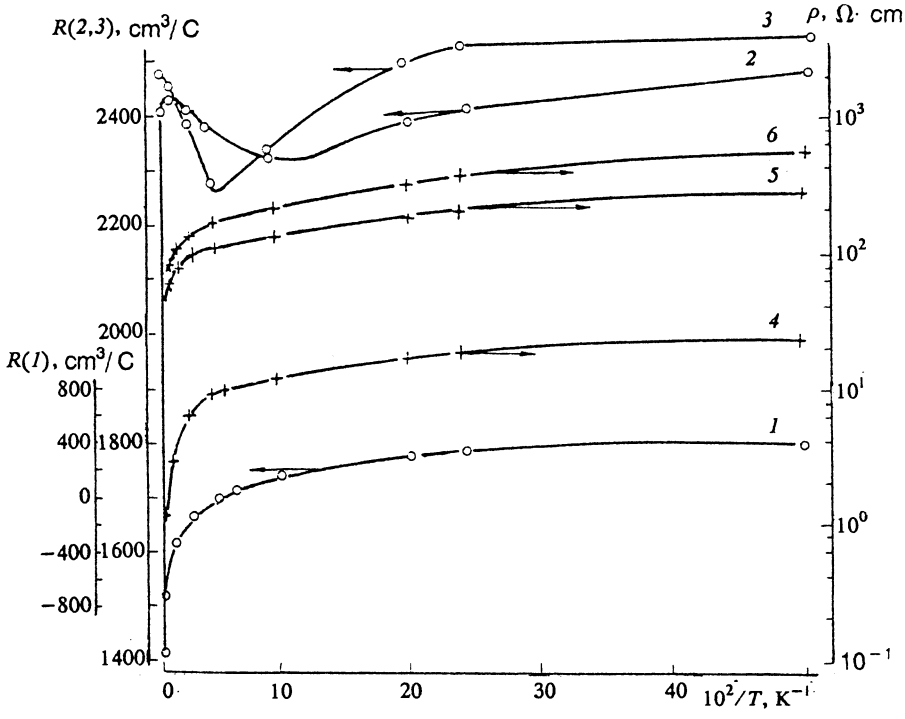

FIG. 2. Temperature dependence of the Hall coefficient R (curves *1–3*, $H=15$ kOe) and of the resistivity ρ (curves *4–6*) for sample 2. P, GPa: curves *1,4*—0.02; curves *2,5* —0.42; curves *3,6*—1.14. Scale $R(1)$ corresponds to curve *1*, scale $R(2,3)$ to curves *2,3*.

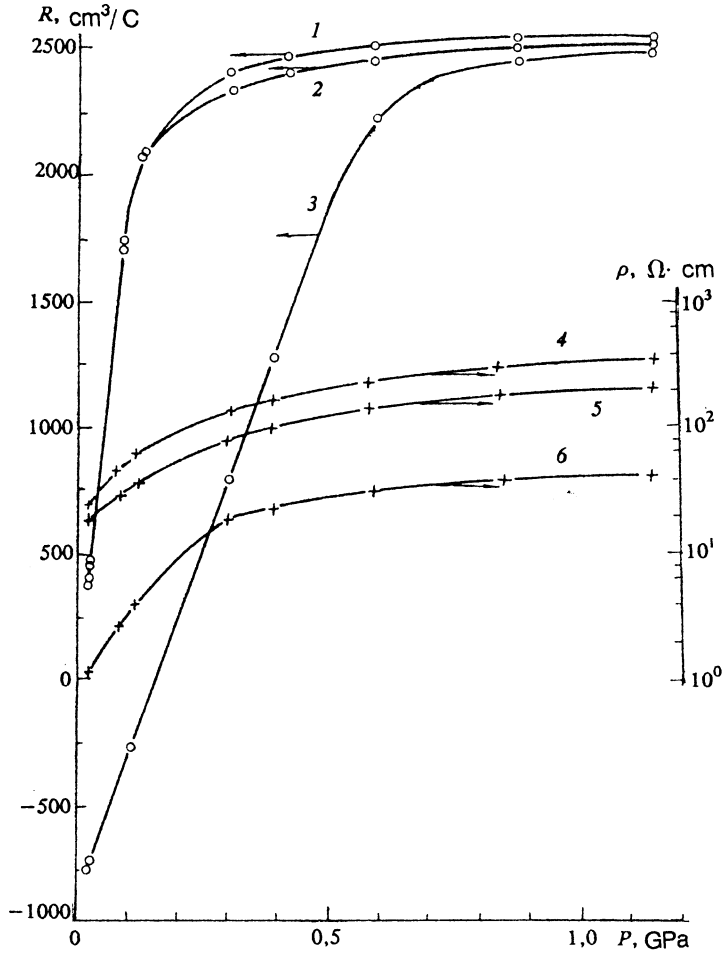

FIG. 3. Pressure dependence of the Hall coefficient R (curves *1–3*, $H=15$ kOe) and the resistivity ρ (curves *4–6*) for sample 2. T, K: curves *1,4*—2; curves *2,5*—4.2; curves *3,6* —77.6.

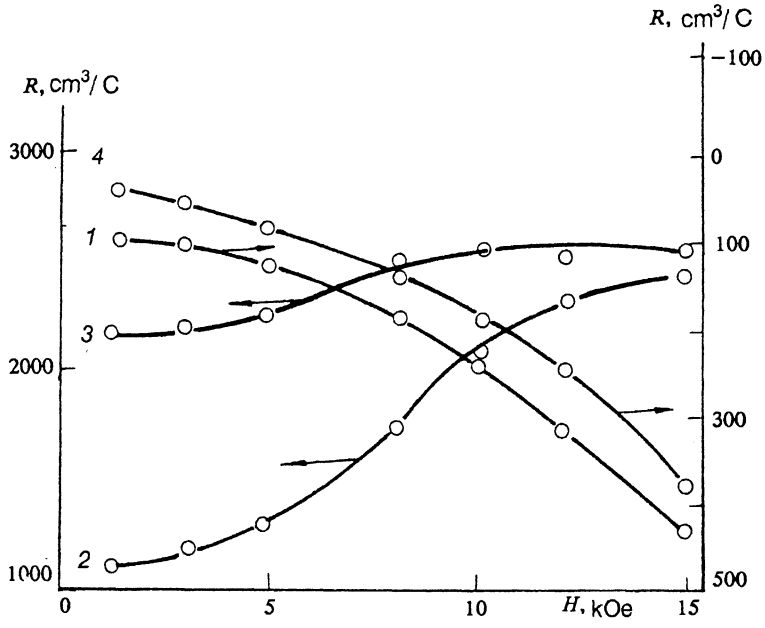

FIG. 4. Magnetic field dependence of the Hall coefficient R in sample 2. T, K: curves *1–3*—2; curve *4*—4.2. P, GPa: curves *1,4*—0.02; curve *2*—0.042; curve *3*—1.14.

Figures 2–4 and Table I show the data on sample 2. Control measurements on the other sample yielded essentially the same results. The $\rho(T,P)$ and $R(T,P,H)$ behavior is typical of a p-type semiconductor with two types of carrier: electrons and holes. An increase in the pressure and a lowering of the temperature increase the ratio $c=p/n$ of the hole density to the electron density, as can be seen from the P, T, and H dependence of the kinetic coefficients (Figs. 2–4). A negative $\Delta\rho/\rho_0$ was observed; its behavior was studied as a function of the hydrostatic pressure at 2, 4.2, and 77.6 K.

Measurements were first carried out on sample 1 in the temperature interval 4.2–77.6 K. The measurements were then continued, on a broader scale, on sample 2 over the range 2 K$\leqslant T\leqslant$300 K. We supplemented these measurements with measurements of the field dependence of R, in an effort to reach a systematic quantitative interpretation.

The effective characteristic properties of the conduction electrons and the acceptor-band holes—the densities n and p and the mobilities μ_e and μ_A—were extracted from $R(T,P,H)$ and $\sigma(T,P)$. For this purpose we made use of the existing phenomenological relations of a universal two-band model in which the contributions of the partial conductivities to the overall conductivity are assumed to be additive and in which the relaxation time is assumed to be independent of the energy.[1,2,11–13] We used the $R(H)$ dependence near $R_0=0$ ($R_0=\lim_{H\to 0} R$), where this dependence is most obvious, since at this point we have $R\sim H^2$ beginning at $H=0$. The effect is to improve the reliability of the estimates. Since $R_\infty=\lim_{H,P\to\infty} R=(N_\infty e)^{-1}$ can be determined by an approximate graphical procedure based directly on the experimental data (Figs. 3 and 4), we used the following expression for $R(H)$:

$$(R-R_\infty)^{-1}=(R_0-R_\infty)^{-1}+\beta_R(R_0-R_\infty)^{-1}H^2. \quad (6)$$

The coefficients R_0, R_∞, and β_R are determined by the characteristic properties of the charge carriers. If R_∞ is chosen correctly, the $(R-R_\infty)^{-1}=f(H^2)$ dependence is linear. It was linear in our case. From ρ and $R(H)$ near $R_0=0$, along with expression (6) (with $T=2$ and 4.2 K and $P=0.02$ GPa, and with $T=77.6$ K and $P=0.41$ GPa), we calculated the characteristic properties of the charge carriers (Table I and Figs. 5–7). Since we have $R_0>0$ at $T<77.6$ K, we have $c>b^2\gg 1$ ($b=\mu_e/\mu_A$). The acceptor-band components thus satisfy $\rho_A\simeq\rho$, $R_A\simeq R_\infty$, $p\simeq N_\infty$, and $\mu_A\simeq R_\infty\sigma$. Hence

TABLE I. Electrical conductivity, Hall coefficient, and some characteristic properties of the charge carriers of p-$CdSnAs_2\langle Cu\rangle$ sample 2.

T, K	P, GPa	R, cm³/C ($H=15$ kOe)	σ, S/cm	n, cm^{-3}	μ_e, cm²/(V·s)	μ_A, cm²/(V·s)	$b=\mu_e/\mu_A$	$c=p/n$
2	0,02	431	$4{,}33\cdot10^{-2}$	$3{,}6\cdot10^{12}$	2710	106	25,6	686
	1	2542	$2{,}15\cdot10^{-3}$			5,5		
4,2	0,02	380	$5{,}39\cdot10^{-2}$	$5{,}6\cdot10^{12}$	2730	131	20,8	441
	1	2520	$3{,}13\cdot10^{-3}$	$2{,}1\cdot10^{10}$	140	8	19,0	$1{,}2\cdot10^{5}$
77,6	0,02	−718	$9{,}42\cdot10^{-1}$	$1{,}2\cdot10^{15}$	2428	852	2,9	3,1
	1	2480	$1{,}73\cdot10^{-2}$			44,0		
300	10^{-4}	−203	38,1	$1{,}8\cdot10^{16}$	10450	2455	4,3	1,14
	1	−1070	4,04	$2\cdot10^{15}$	8050	2090	3,9	2,24

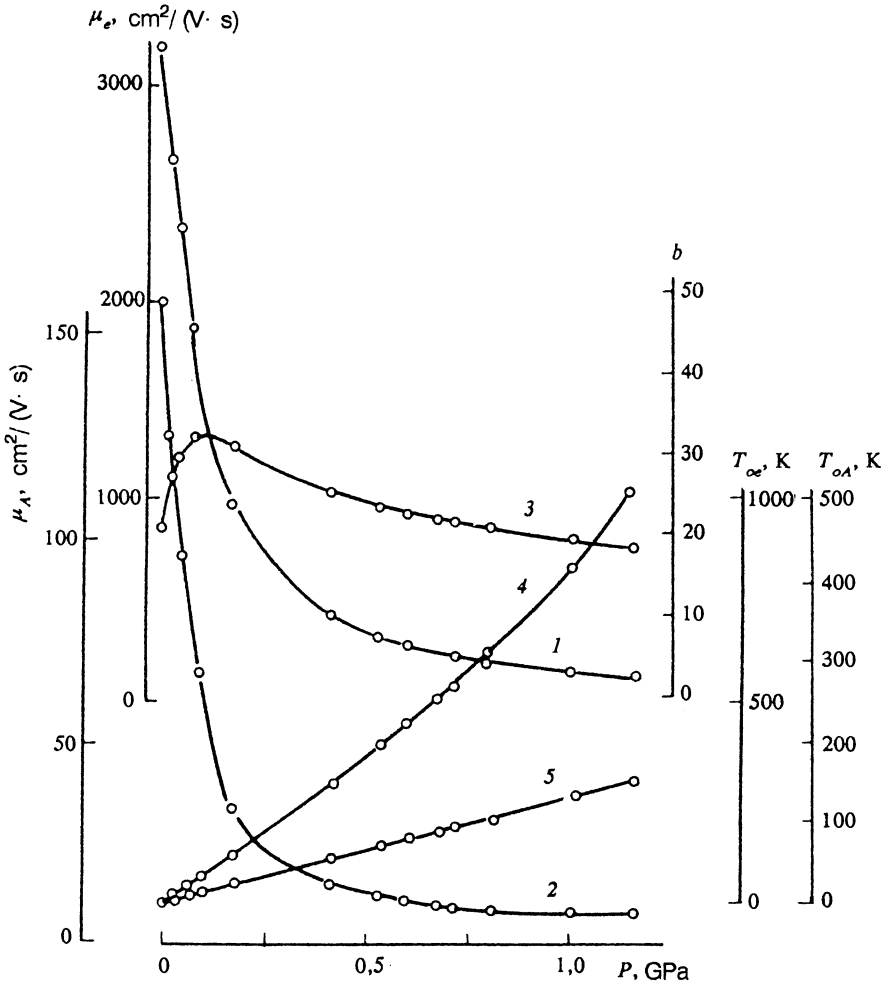

FIG. 5. Pressure dependence of the mobility of the conduction electrons, μ_e (*1*), and that of the holes of the acceptor band, μ_A (*2*), of their ratio $b=\mu_e/\mu_A$ (*3*), of the parameters of the Mott hopping conductivity of electrons, $T_{0e,A}$ (*4*), and of those of the holes of the acceptor band, T_{0A} (*5*), at 4.2 K in sample 2.

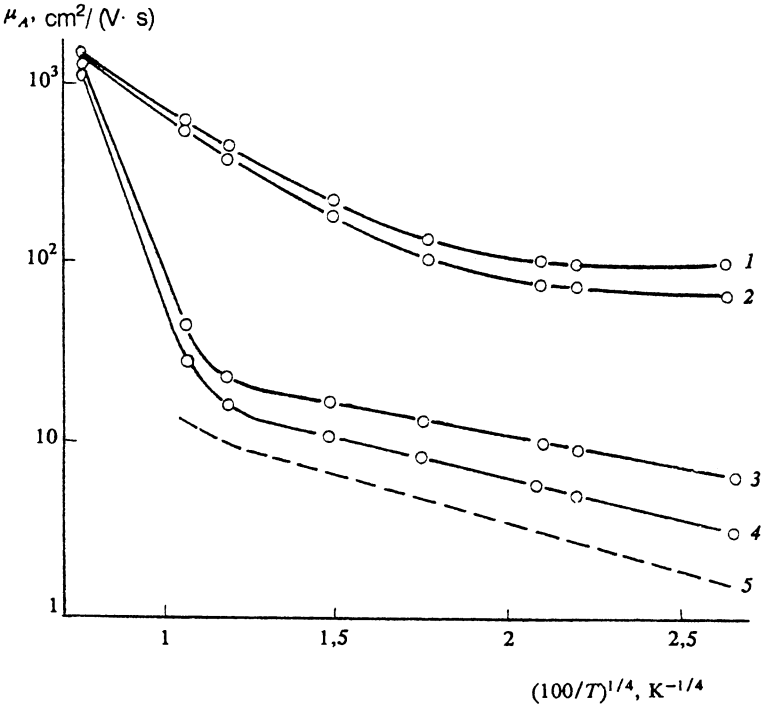

FIG. 6. Temperature dependence of the mobility of acceptor-band holes, μ_A, for sample 2. *P*, GPa: curve *1*—10^{-4}; curve *2*—0.02; curve *3*—0.42; curve *4*—1.14; curve *5*—$P\to\infty$.

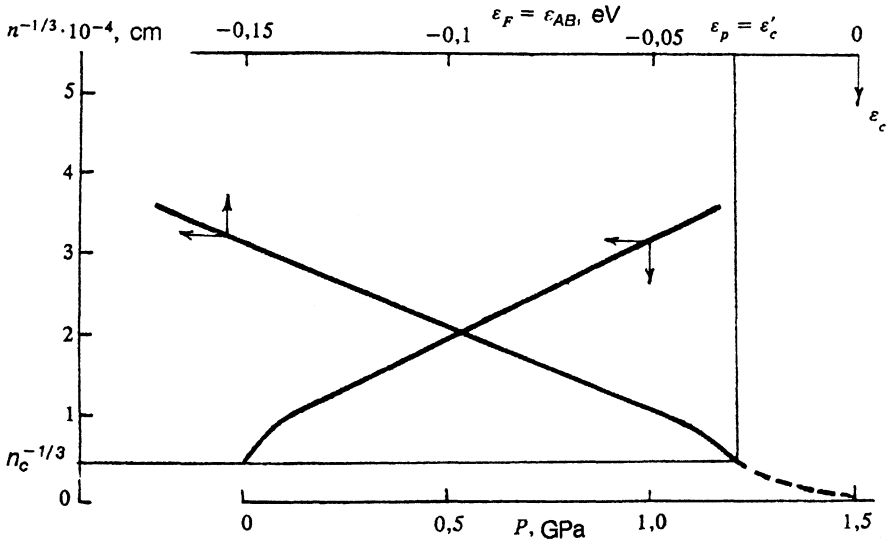

FIG. 7. Electron density n versus the pressure and the Fermi energy ε_F at 4.2 K for sample 2. The notation is explained in the text.

$$n=\frac{[1+(\mu_e H^2)](R_\infty - R)\sigma^2}{\mu_e^2 e}. \quad (7)$$

Since μ_e could be evaluated only near atmospheric pressure, we can work from (7) to estimate $n(P)$, within a coefficient[15] $[\mu_e(P)/\mu_e(P=0)]^2$. At sufficiently low temperatures and at $P>0.1$ GPa we have $(\varepsilon_p-\varepsilon_F)/kT \gg 1$, where ε_p and ε_F are the percolation energy and the Fermi energy, respectively. The electron density above the percolation level is thus negligibly low. In addition, the kinetic energy of the electrons in a droplet and also the size of the droplet are independent of the temperature; i.e., the electron gas in the droplet is degenerate.[1,16,17] We can thus assume that the electron density, on the average over the sample, is constant at sufficiently low temperatures and at a fixed pressure. Nevertheless, calculations from (7) in the approximation $\mu_e(P)=\mu_e(P=0)$ yield a Mott law (Fig. 6) for both $n(T)$ and $\mu_A(T)$. It is natural to ascribe this behavior to $\mu_e(T)$. We thus write

$$\mu_{e,A}=\mu_{e,A}^0 \exp\{-(T_{0e,A}/T)^{1/4}\}. \quad (8)$$

Taking this approach, we worked from the calculated $n(T)$, ignoring the temperature and pressure dependence of the pre-exponential factor, to determine the pressure dependence of T_{0e} and then $\mu_e(P)/\mu_e(P=0)$. In this manner we calculated the $\mu_e(T,P)$ dependences and a refined $n(P)$ dependence for 4.2 K in a p-$CdSnAs_2\langle Cu\rangle$ single crystal (Figs. 5–7; Ref. 18).

3. DISCUSSION

The $\mu_{e,A}(T)$ dependence can be described satisfactorily by expression (8) at temperatures from 2 K to $T_c(P)$. As the pressure is varied from atmospheric to 1.15 GPa, the high-temperature boundary of the interval increases to 40–50 K in both cases (Fig. 6; Ref. 18). According to the theory of Refs. 1, 6, 19, and 20, the transition to a hopping conductivity with a monotonically decreasing activation energy of the type in (8) should occur at temperatures below 4.2 K. Nevertheless, the temperature T_c varies from 10 to 60 K in heavily doped, compensated semiconductors, depending on N and K (see the papers cited in Refs. 1, 2, and 6). Furthermore, in all cases the $\rho(T)$ dependence is anomalously weak, to some extent or other, and estimates of the density of states at the Fermi level from the experimental value of T_{0e} yield results which are too high. This situation was discussed in Refs. 1, 2, 6, 8, and 9. It was attributed to either a correlation in the positions of impurities or the presence of highly conducting channels or local inhomogeneities which give rise to a significant scatter in the energy levels of the localized states. These particularities are also probable in p-$CdSnAs_2\langle Cu\rangle$ and can apparently be explained on the basis of the pronounced inhomogeneity of the crystals, which stems from the synthesis process itself:[14] The concentration of intrinsic structural defects in cadmium-tin diarsenide is greater than 10^{17} cm^{-3}. In addition, doping with copper atoms by diffusion leads to the formation of complexes with a concentration on the order of 10^{17} cm^{-3} (Ref. 14); i.e., there is a specific correlation. For this reason, we will make use of only qualitative data on the pressure dependence of the parameters $T_{0e,A}$, which characterize the activation energy.[21]

With increasing pressure, the properties $T_{0e,A}$ increase from zero levels, but in different ways (Fig. 5). An extrapolation from the measured pressure range to $P\to\infty$ at 4.2 K yields $T_{0e,A}\to\infty$, $\mu_e\to 0$, and $T_{0A}\to T_{0A}^\infty$, $\mu_A\to\mu_A^\infty$ (Ref. 18), in agreement with the pressure dependence of the density of states of conduction electrons at the Fermi level, $g_e(\varepsilon_F)\to 0$, and that of acceptor-band holes, $g_A(\varepsilon_F)$. An increase in $T_{0e,A}$ from zero with increasing magnetic field above the critical level has also been observed[17] in n-InSb. At the point $T_{0e,A}=0$, near atmospheric pressure, i.e., at the point of the metal-insulator transition, we find the following results for sample 2 by extrapolating from 2–5 K to absolute zero: $n_c\simeq 10^{13}$ cm^{-3}, $\mu_e=2750$ $cm^2/(V\cdot s)$, $\rho_e=230$ $\Omega\cdot cm$ and $p=2.45\cdot 10^{15}$ cm^{-3}, $\mu_A=155$ $cm^2/V\cdot s$), and $\rho_A=16.5$ $\Omega\cdot cm$. The pressure dependence of $b=\mu_e/\mu_A$ is not monotonic: There is a maximum near 0.1 GPa (Fig. 5). The increase in b with increasing pressure in the initial region is a consequence of the difference

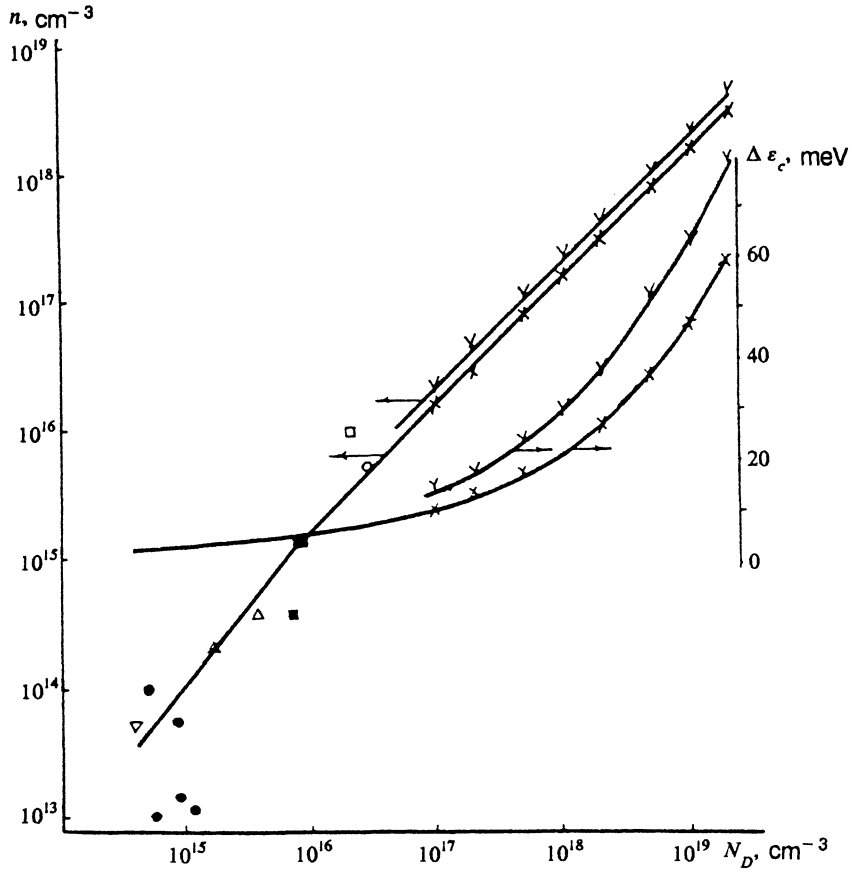

FIG. 8. Electron density near the metal-insulator transition in a heavily doped, compensated semiconductor and the energy $\Delta\varepsilon_c$, by which the bottom of the conduction band is lowered by the heavy doping, versus the donor concentration. v—InAs, theoretical;[22] ×—InSb, theoretical.[22] Open and filled circles, triangles, and squares—InSb, experimental; filled circles—Ref. 8; inverted triangles—Ref. 23; triangles—Ref. 24; squares—Ref. 10; filled circles—Ref. 18. Open symbols—$n > n_c$. The value $\delta = 1$ was used in (11) in the calculation of $n(N_D)$, since we have[8,10] $\delta > (\varepsilon_p - \varepsilon_F)/\gamma = 0.9 + 0.99$.

between the localization dynamics for conduction electrons and for holes of the acceptor band. It results from a pulling of μ_A toward μ_e (Ref. 18). The further decrease in b results from the decrease $\mu_e \to 0$.

The pressure dependence of n and, correspondingly $g_e(\varepsilon_F)$ at 4.2 K is characterized by two exponential regions, which can be approximated satisfactorily by

$$n = A \exp(\varepsilon_{AB}/\varepsilon_k), \qquad g_e(\varepsilon_F) = n/\varepsilon_k, \tag{9}$$

where A and ε_k are constants. For pressures between 0.1 MPa and 0.15 GPa we have $A = 6.84 \cdot 10^{15}$ cm^{-3} and $\varepsilon_k = 4.6$ meV. From 0.15 GPa to 1.15 GPa we have $A = 10^{12}$ cm^{-3} and $\varepsilon_k = 43.5$ meV (Fig. 3 in Ref. 18). The relation $g_e(\varepsilon_F) = n/\varepsilon_k$ has been derived for a heavily doped, compensated semiconductor and for a $\rho(T)$ dependence in (8) (Ref. 6); here $\varepsilon_k = \varepsilon_0 (N a_B)^{4/9}$ is the kinetic energy of the electrons in the droplet, and $\varepsilon_0 = e^2/(\chi a_B)$. According to the ideas which have been developed, the value found experimentally for the constant ε_k is the kinetic energy of the electrons in the droplet only near atmospheric pressure. This conclusion is supported by estimates below. At pressures above 0.1 GPa, where there is a state of a heavily doped, fully compensated semiconductor, the constant ε_k should apparently be treated as an adjustable parameter.

Let us examine the behavior of the carriers and their energy spectrum near the metal–insulator transition induced by pressure, at 4.2 K in p-$CdSnAs_2\langle Cu\rangle$ according to the data on sample 2. In the energy interval from the unperturbed edge of the conduction band to a depth of 40–50 meV, i.e., up to $P = 1.5$ GPa, the values of n and $g_e(\varepsilon_F)$ decrease dramatically, by four or five orders of magnitude, according to (9). The bottom of the conduction band, deformed by the random potential of the charged impurities, descends because of the heavy doping to a depth $\varepsilon_c' = \varepsilon_{AB}^0 = \varepsilon_p = -30$ meV. The value $\Delta\varepsilon_c = 30$ meV agrees satisfactorily with theoretical estimates.[4,22]

At the point of the metal–insulator transition in a heavily doped, compensated semiconductor, the coefficient ν in (2), which determines n_c, is on the order of unity.[5] However, when we substitute n_c and N into (2) for sample 2 at 4.2 K, we find[18] $\nu \simeq 10^{-5}$. According to the data[23,24] on an n-InSb sample (Fig. 8), the value is $\nu \simeq 0.01 \ll 1$. The condition for a disruption of the metallic conductivity in a heavily doped, compensated semiconductor was found from the equality $\gamma = \varepsilon_F$ in Ref. 5, where γ is the amplitude of the fluctuation potential. It was assumed at the outset that the density of states at the critical point is unperturbed. It follows that we have $\varepsilon_F > 0$ at the point of the metal–insulator transition. However, the exact condition for a metal–insulator transition in a semiconductor of this sort is $\varepsilon_F = \varepsilon_p < 0$, as was pointed out, in particular, in Ref. 2. As the condition for a disruption of the metallic conductivity in a semiconductor of this sort we should use

$$\varepsilon_p = -\Delta\varepsilon_c = \varepsilon_F = -\delta\gamma = -\delta e^2 N^{2/3} (\chi n_c^{1/3})^{-1}, \tag{10}$$

where δ is a numerical factor. Hence

$$n_c=\left(\frac{e^2}{\chi\Delta\varepsilon_c}\right)^3 N^2\delta^3,$$
$$n_c=\left(\frac{\delta\varepsilon_k}{\Delta\varepsilon_c}\right)^2\frac{N^{2/3}}{a_B}. \quad (11)$$

The coefficient $\nu=(\delta\varepsilon_k/\Delta\varepsilon_c)^3$ in (2) is thus not a constant.

Figure 8 shows calculated curves of $\Delta\varepsilon_c$ (Ref. 22) and of n_c from (11) for the n-type semiconductors InSb and InAs, along with curves of the electron density near the metal–insulator transition in the heavily doped, compensated semiconductor n-InSb, according to experimental data.[8,10,17,23,24] It follows from Fig. 8 that in n-InSb, with $N_D>10^{16}$ cm^{-3}, we have $n_c=0.17N_D$, and ν varies from 1.7 ($N_D=10^{19}$ cm^{-3}) to 0.2. In n-InAs, with $N_D>4\cdot10^{16}$ cm^{-3}, we have $n_c=0.22N_D$, and ν varies from 0.9 ($N_D=10^{19}$ cm^{-3}) to 0.2. According to experimental data on n-InSb (Fig. 8), as N_D decreases from 10^{16} to 10^{14} cm^{-3}, approaching N_M ($N_D^{1/3}\cdot a_B$ decreases from 1.5 to 0.3), the coefficient ν decreases to a few hundredths, possibly because electrons have begun to be frozen out. This behavior is evidence that the band and impurity states separate from each other over a finite interval along the N_D scale.

Since the characteristics of $CdSnAs_2$ (Ref. 11) occupy an intermediate position between those of InSb and InAs, we worked from the curves of $\Delta\varepsilon_c(N_D)$ (Fig. 8) and the value $\Delta\varepsilon_c=-\varepsilon_{AB}^0=30$ meV for p-$CdSnAs_2\langle Cu\rangle$ sample 2 to find N_D; the result is $N_D\simeq2\cdot10^{18}$ cm^{-3}. This value agrees with the self-doping level (see the Experimental Results). Working from refined condition (11), substituting in $n_c=10^{13}$ cm^{-3} for 4.2 K and $\Delta\varepsilon_c$, we find $\delta^{3/2}N_{\text{eff}}\simeq1.6\cdot10^{16}$ cm^{-3} and $\nu=6.5\ 10^{-4}\delta$. The parameter $\delta^{3/2}N_{\text{eff}}\simeq10^{16}$ cm^{-3} has also been determined from the dependences of $n^{-1/3}$ on ε_F and P on the insulator side of the metal–insulator transition (see Fig. 7 and the discussion below). A direct estimate of N_{eff} can be found from the value of ε_k at the critical point. The parameter ε_k appears as an adjustable parameter in the approximation (9). As a result we find $N_{\text{eff}}=5.7\cdot10^{16}$ cm^{-3} and a coefficient $\nu=3\cdot10^{-4}$. The parameters N, ν, and n_c thus turn out to be smaller than expected, by two, three, and four orders of magnitude, respectively. On the other hand, the value of N_D found from $\Delta\varepsilon_c=-\varepsilon_{AB}^0$ (Fig. 8) agrees with the experimental data, as was mentioned above.

The lowering of $N=N_{\text{eff}}$, ν, and n_c is due to formation of complexes as a consequence of the doping with copper atoms by diffusion. According to the estimates in Ref. 14, the concentration of these copper atoms approaches 10^{18} cm^{-3}, i.e., the initial self-doping level. The extent to which the edge of the conduction band lowers, $\Delta\varepsilon_c$, is determined by the self-doping condition $N_D\simeq10^{18}$ cm^{-3}, while the value of γ is determined by the residual concentration of charged centers which have not taken part of complex formation. The linear dependence of $n^{-1/3}$ on ε_F (see Fig. 7 and the discussion below) is evidence that the formation of complexes does not completely erase the large-scale fluctuations of the potential. It merely reduces the fraction of impurities which participate in the formation of the fluctuation potential, to a value N_{eff} (Ref. 1). The experimental data thus provide evidence that correlation has a strong effect on the amplitude of the fluctuation potential, while it has a negligible effect on $\varepsilon_p=-\Delta\varepsilon_c$. The percolation energy also depends weakly on the compensation,[8,10] the magnetic field,[2,17] and (apparently) the hydrostatic pressure.

The pressure interval from 0.1 MPa to 0.15 GPa (10–15 meV) is a region of transition for the conduction electrons, from a metallic conductivity to a hopping conductivity and from a heavily doped compensated semiconductor to a heavily doped fully compensated semiconductor[1,25] with an impurity band. The behavior of ε_F as a function of $n^{-1/3}$ in this region (Fig. 7) is affected by the scatter in the density of states in the acceptor band.[20] Delocalized electrons with $\varepsilon>\varepsilon_p$, acceptor-band holes, and electrons localized at wells of the fluctuation potential participate in the conductivity.

Above 0.1 GPa, the behavior of $n^{-1/3}$ as a function of P and ε_F is linear (Fig. 7). Since $\varepsilon_F<\varepsilon_p$ at $P>0.1$ MPa, the electron density should be zero near absolute zero and under the condition $(\varepsilon_p-\varepsilon_F)>\Delta$ (Δ is the width of the acceptor band) in the absence of an impurity potential. However, fluctuations of the impurity concentration bend the edge of the conduction band to the point that it intersects the Fermi level (which is frozen into the acceptor band) repeatedly, by an amount on the order of ε_{AB}. As a result, electrons appear. The electrons collect in droplets which screen the fluctuation potential. Here we have a version of the model of a heavily doped, fully compensated semiconductor[1,25] in a semiconductor with an impurity band. In contrast with ordinary heavily doped, compensated semiconductors with $N_A\neq N_D$, the smallest dimension (R_g) of a typical fluctuation which bends the band by an amount $\gamma(R_g)$ in the model of a heavily doped, fully compensated semiconductor is on the order of the width of the band gap, and the carrier density is determined not by the degree of compensation but by the value of ε_g (Refs. 1 and 25):

$$\gamma(R_g)=\varepsilon_g,\quad R_g=(\varepsilon_g\chi)^2/(Ne^4),$$
$$n=(N^2e^6)/(\varepsilon_g^3\chi^3). \quad (12)$$

In the case at hand, ε_g is to be understood as $\varepsilon_{AB}=\varepsilon_F$, where, according to (12), we have

$$\varepsilon_F=-\delta\frac{e^2N^{2/3}}{\chi n^{1/3}}=-Bn^{-1/3}. \quad (13)$$

Expression (13) can be rewritten as

$$n^{-1/3}=\frac{\beta}{B}P-\frac{\varepsilon_{AB}^0}{B},$$
$$S=\left(n^{-1/3}+\frac{\varepsilon_{AB}^0}{B}\right)^{-1}=\frac{B}{\beta}P^{-1}. \quad (14)$$

The plots of $n^{-1/3}(P)$ (Fig. 7) and $S(P^{-1})$ (Ref. 18) for $P>0.1$ GPa are linear, in agreement with the theory. In the limit $P\to\infty$ we have $S\to0$. From these curves we have $\varepsilon_{AB}^0=(-30\pm7)$ meV and $N_{\text{eff}}\delta^{3/2}=10^{16}$ cm^{-3}. The values

of ε_{AB}^0 found for $T \geqslant 77.6$ K (Ref. 13) and 4.2 K, from (14), are thus the same. This agreement is evidence that the models used here correspond to the actual situation. The value of N_{eff}, two orders of magnitude lower than N, is due to the formation of complexes as a result of the doping with copper atoms by diffusion, as was mentioned above.

In the limit $P \to \infty$, the states of the conduction band and those of the acceptor band are completely separated. The system consisting of the valence band and the deep acceptor band, separated by an energy interval $\varepsilon_i = \varepsilon_g - |\varepsilon_{AB}^0| \simeq 0.25$ eV (Ref. 11), corresponds to the model of a lightly doped, highly compensated semiconductor.[19,20] Actually we have $N_{AB}\alpha_{hl}^3 = 4 \cdot 10^{-3} \ll 1$ [$\alpha_{hl} = \hbar/\sqrt{2m_{hl}\varepsilon_i}$ is the length scale over which the wave function of the impurity state of an isolated acceptor decays, and $m_{hl} = 0.027 m_0$ (Ref. 11) is the effective mass of a light hole]. The compensation coefficient (the population coefficient serves as the compensation coefficient in this case) is 0.92 (see the discussion above). Using the results of numerical calculations,[20] we can estimate the characteristics of the acceptor band. The Fermi level ε_F^{AB}, reckoned from the energy of an isolated acceptor in the direction of the conduction band, is 15 meV, and the density of states at the Fermi level is $g_A(\varepsilon_F) = 3.2 \cdot 10^{17}$ eV^{-1} cm^{-3}. The value of $g_A(\varepsilon_F)$ has been used to calculate the hopping length and the activation energy ε_M (Ref. 21) at $T = T_c \simeq 40$ K, at the transition to a conductivity of the type in (8), and also at 4.2 K. It was found that near 40 K the values of ε_M and R_M are close to $\varepsilon_{AB} \simeq \varepsilon_F^{AB}$ and $N_{AB}^{-1/3}$. At 4.2 K, we have $\varepsilon_M = 5$ meV $< \varepsilon_F^{AB}$ and $R_M = 5.2 \cdot 10^{-6}$ cm $> N_{AB}^{-1/3}$.

As the pressure is lowered, as states of the acceptor band reach a resonance with states of the conduction band, and as the distance between the edge of the conduction band and ε_F decreases, the distances from ε_F to the percolation levels of the conduction band and of the acceptor band also decrease, falling to zero near atmospheric pressure. At the same time, the parameters $T_{0e,A}$ decrease to zero (Fig. 5). The quantity T_{0e} decreases from an infinitely high value, while T_{0A} decreases from a finite value. A metal–insulator transition begins. In terms of the acceptor band, the transition sets in at $N_{AB} = 3.1 \cdot 10^{16}$ cm$^{-3} \ll N_M = 10^{18}$ cm^{-3}. It results from the superposition of acceptor-band states on the band continuum and is a version of the Mott model. This version of the metal–insulator transition was called a "resonance-hybridization version of the Mott transition" in Ref. 18. This resonance-hybridization transition in the delocalization direction is accompanied by a pulling of μ_A toward μ_e. The limiting case ($b = \mu_A/\mu_e = I$) is realized when band states are superimposed on impurities previously split off from the same band by the defect potential, as is observed in (for example) n-InSb. In p-CdSnAs$_2$⟨Cu⟩, the value of b decreases to 3–4 (Ref. 13). This effect probably explains the anomalously high mobility of the carriers of the resonance impurity band in PbSnSe (Ref. 12).

The Ge⟨Sb,Au⟩, InSb⟨Cr⟩, and apparently InAs (Ref. 26) systems and also gapless semiconductors look promising for a study of these effects at high pressures.[2,12]

4. CONCLUSION

Metal–insulator transitions have been induced by hydrostatic pressure in a heavily doped, compensated semiconductor through a localization of electrons in the large-scale fluctuation potential and in the impurity band as the result of a separation of states of the band continuum from impurity states. The compound p-CdSnAs$_2$⟨Cu⟩ was used as a model. The resonance-hybridization version of the Mott transition is accompanied by a pulling of the mobility of the impurity carriers toward the mobility of the band carriers. A modification of the state of a heavily doped, fully compensated semiconductor has been observed in a semiconductor with an impurity band. The model of a heavily doped, fully compensated semiconductor has been compared with experimental data for the first time, and a satisfactory quantitative agreement has been found. This model has been used previously for a qualitative description of the temperature dependence of the resistivity of n-Ge compensated by fast neutrons.[7] The condition for a metal–insulator transition in a heavily doped, compensated semiconductor has been refined, and the influence of complex formation on the nature of the localization has been identified. A material like p-CdSnAs$_2$⟨Cu⟩ is a model amorphous semiconductor which can be effectively controlled by high pressure. The high pressure makes it possible to scan the Fermi level under the percolation level of the heavily doped, compensated semiconductor, by an amount one or two orders of magnitude greater than the values which can be reached by compensation or a quantizing magnetic field.[8,10,17,27]

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