Study of impurity donor states in GaSb⟨Se⟩

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Galvanomagnetic and oscillatory effects have been investigated in single-crystal samples of GaSb⟨Se⟩ with a selenium concentration $2\cdot10^{17}$–10^{18} cm^{-3}, subjected to a hydrostatic pressure p up to 12 kbar in a magnetic field up to 50 kOe in the temperature range $0.07\text{K}\leqslant T\leqslant 300\text{K}$. The parameters of the impurity band $\varepsilon_L^{\text{Se}}$ split off from the L-extremum were determined from the pressure dependence of the Fermi energy $\varepsilon_{F\Gamma}(p)$ of the Γ electrons. It is shown that, in comparison with Te, Se in gallium antimonide forms a deeper and narrower $\varepsilon_L^{\text{Se}}$ level separated from the bottom of the L band by 26 ± 2 meV. The width of the $\varepsilon_L^{\text{Se}}$ level is $\gamma\sim 0.5$ meV. Using pressure as the external parameter to vary continuously the position of the Fermi level ε_F relative to the mobility threshold ε_c in the Γ band, we studied the behavior of galvanomagnetic effects in GaSb⟨Se⟩ near ε_c. It was found that the mobility threshold ε_c was located approximately 25 meV above the undistorted boundary ε_c^0 of the Γ band. This result indicates that the classical percolation approach, in which $\varepsilon_c<\varepsilon_c^0$, cannot be used to determine ε_c and can be attributed to multiple above-barrier reflection from the potential relief of the bottom of the Γ band, giving rise to electron localization at $\varepsilon_c>\varepsilon_c^0$. As the transition from $\varepsilon_F>\varepsilon_c$ to $\varepsilon_F<\varepsilon_c$ proceeds, the temperature dependence of the resistivity $\rho(T)$ undergoes a qualitative change: from a metallic behavior, through a power-law dependence $\rho\sim 1/T^{\beta}$ ($\beta=0.28$), to an exponential dependence, $\rho(T)\sim\exp\{(T_0/T)^{\alpha}\}$, with the exponent α taking on the values $0.25\lesssim\alpha\lesssim 0.4$. The quantity α exhibits a nonmonotonic dependence on the position of ε_F in relation to ε_c: it has a maximum $\alpha=0.4$–0.33 near ε_c, and then at $\varepsilon_F\ll\varepsilon_c$ it approaches the Mott value $\alpha=0.25$. The data obtained make it possible to take a new look at the problem of the metal-insulator transition in scaling theory.

1. INTRODUCTION

Recently, a method of studying electron states has been widely applied in experiments where pressure is used as the external parameter that varies the relative arrangement of the bands. This technique was named pressure spectroscopy.[1–3] Such experiments can yield a large amount of information on both the structure of the energy spectrum of initially undoped semiconductors and the character of the impurity states associated with different extrema.

In studying impurity donor states in semiconductors, of major importance is the material investigated. If the semiconductor employed, for example InSb, has a distance of about 800 meV between neighboring extrema in the conduction band,[4] a hydrostatic pressure $p\geqslant 80$ kbar is necessary for inversion of these terms, since the pressure rates of closer approach of the bands are approximately 10 meV/kbar for semiconductors of the $\text{A}^{\text{III}}\text{B}^{\text{V}}$ group.

At the same time, by selecting gallium antimonide as the semiconductor matrix, in which the distance $\Delta\varepsilon_{\Gamma L}$ between the Γ and L conduction bands is unusually small and amounts to 93 meV,[5] one can observe an inversion of the Γ and L terms at pressures 9–10 kbar.

In GaSb, the impurity donor level split off from the L extremum lies in the region of allowed energy values and is a resonance level. The effective masses corresponding to the Γ and L valleys in the conduction band of GaSb differ markedly: $m_\Gamma=0.043\,m_0$ (Ref. 6) and $m_L^d=0.3\,m_0$ (Ref. 7) (here m_Γ is the effective mass of the electron at the bottom of the Γ band, m_L^d is the mass of the density of states corresponding to the L band, and m_0 is the mass of the free electron). Therefore, there exists a range of donor densities N_d in which the conditions of high doping for the Γ band and low doping for the L band are satisfied simultaneously:

$$(a_{\text{B}}^{\Gamma})^{-3}\ll N_d\ll(a_{\text{B}}^{L})^{-3}, \tag{1}$$

where a_B^Γ and a_B^L are the Bohr radii for the Γ and L bands: $a_B^\Gamma=190$ Å, $a_B^L=20$ Å.

In the case of a hydrogenlike impurity, for example Te in GaSb, the Γ electrons can be used as a kind of reference for studying the structure of the $\varepsilon_L^{\text{Te}}$ impurity states split off from the L extremum,[5] since hydrostatic compression causes Γ electrons to overflow into the impurity band. In such a situation, by using the condition of conservation of charge, from the filling of the Γ extremum at different pressures one can determine the amount of electrons which have overflowed into the $\varepsilon_L^{\text{Te}}$ band, and in final analysis, to reconstruct the behavior of the density of states in this band.

As we turn to deeper impurities (Se, S) in GaSb, which cause an appreciable distortion of the potential relief of the bottom of the Γ band, it is of interest to study the $\varepsilon_\Gamma^{\text{Se}}$ impurity states in the tail of the Γ band as the Fermi level ε_F passes smoothly from delocalized states ($\varepsilon_F>\varepsilon_c$) to localized ones ($\varepsilon_F<\varepsilon_c$) through the mobility threshold ε_c.

To this end, we studied oscillatory and galvanomagnetic effects in single-crystal samples of GaSb⟨Se⟩ ($N_{\text{Se}}=2\cdot10^{17}$–$10^{18}$ cm^{-3}) over a wide range of temperatures, $0.07\text{K}\leqslant T\leqslant 300\text{K}$, at a pressure $p\leqslant 12$ kbar in a magnetic field up to 50 kOe.

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The experimental technique is described in detail in Refs. 8 and 9. The single-crystal samples of GaSb⟨Se⟩ were prepared at the A. A. Baĭkov Institute of Metallurgy of the Academy of Sciences of the USSR (Moscow) and at the A. F. Ioffe Physicotechnical Institute of the Academy of Sciences of the USSR (Leningrad).

2. DETERMINATION OF THE DENSITY OF STATES IN THE IMPURITY BAND SPLIT OFF FROM THE L EXTREMUM IN GaSb⟨Se⟩

Under hydrostatic compression, the Γ band shifts upward relative to the L extremum at a rate $d\Delta\varepsilon_{\Gamma L}/dp = 10.1$ meV/kbar.[5] Therefore, starting at a certain pressure p_0, when the Fermi level lands in the impurity ε_L^{Se} band split off from the L extremum, the Γ electrons overflow into the impurity level. From the period $\Delta(1/H)$ of the quantum oscillations of the Shubnikov–de Haas (SdH) magnetoresistance, one can find[5,8] for the spherical Fermi surface in the Γ band the Fermi energy $\varepsilon_{F\Gamma}$, measured from the undistorted bottom ε_c^0 of the Γ band at different pressures p (Fig. 1), using the reliably established law of dispersion for the Γ band.

The plateau at $p < p_0$ on the $\varepsilon_{F\Gamma}(p)$ curve corresponds to the case $\varepsilon_F < \varepsilon_L^{Se}$, and the descending sections of $\varepsilon_{F\Gamma}(p)$ correspond to the overflow of Γ electrons into the ε_L^{Se} band. As the initial carrier density in the Γ band increases (see Table I, which gives data for $T = 4.2$K), the pressure p_0 decreases (Fig. 1).

A qualitative comparison of the two samples GaSb⟨Te⟩ and GaSb⟨Se⟩ (respectively, dot-dash line and black circles in Fig. 1), with the same density $n_\Gamma(0)$ in the Γ band at $p = 0$, shows that the overflow to the ε_L^{Se} level begins earlier than in ε_L^{Te}, and the transition portion of $\varepsilon_{F\Gamma}(p)$ from the plateau to the region of linear $\varepsilon_{F\Gamma}(p)$ decrease that characterizes the width of the impurity band is more extended in GaSe⟨Te⟩ than in GaSb⟨Se⟩. These data indicate the selenium in gallium antimonide gives a deeper and narrower impurity level than tellurium, this being in accord with the result of Ref. 3.

The parameters determining the behavior of the density of states in the impurity band can be found from the equation of electrical neutrality:

$$N_d = N_a + n_\Gamma + n_i, \tag{2}$$

which is based on the assumption that N_d electrons supplied by the donors compensate for N_a acceptors and fill the Γ band, as well as the ε_L^{Se} impurity band in the case of $p > p_0$. The density n_i of electrons in the impurity band is determined in terms of the density of states $g(\varepsilon)$:

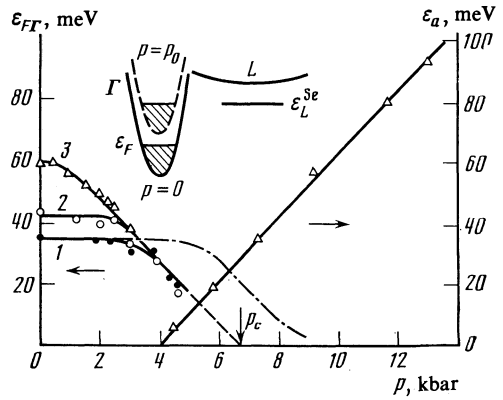

FIG. 1. Pressure dependences of Fermi energy $\varepsilon_{F\Gamma}(p)$ of Γ electrons for different samples of GaSb⟨Se⟩ at $T = 4.2$ K. Numbers of curves correspond to the numbers of samples in Table I. Dot-dash line indicates the $\varepsilon_{F\Gamma}(p)$ curve for a GaSb sample doped with tellurium. Also shown is the pressure dependence of activation energy ε_a for sample No. 3.

$$n_i = \int_{-\infty}^{\varepsilon_F} g(\varepsilon - \varepsilon_0(p))\, d\varepsilon \tag{3}$$

[$\varepsilon_0(p)$ gives the position of the ε_L^{Se} level under pressure], which in the case of low doping [see Eq. (1)] can be represented as follows:[10]

$$g(\varepsilon) = (kN_d/\pi^{1/2}\gamma_0)\exp(-\varepsilon^2/\gamma_0^2), \tag{4}$$

where γ_0 is the halfwidth of the impurity band with degeneracy multiplicity k.

From Eq. (2), taking Eqs. (3) and (4) into consideration, one can obtain the theoretical pressure dependence of the density of Γ electrons $n_\Gamma(p, N_d, N_a, \varepsilon_0(0), \gamma_0, k)$ and the corresponding dependence $\varepsilon_F^{th}(p, N_d, N_a, \varepsilon_0(0), \gamma_0, k)$.

After comparing $\varepsilon_{F\Gamma}^{th}(p, N_d, N_a\ \varepsilon_0(0), \gamma_0, k)$ with the determined experimental dependence $\varepsilon_{F\Gamma}(p)$ obtained for values of $\varepsilon_{F\Gamma}$ such taht the Fermi level is fairly high relative to ε_c (Fig. 1), and after determining in the space of variables $N_d, N_a, \varepsilon_0(0), \gamma_0$ the minimum of the functional

$$\Phi(N_d, N_a, \varepsilon_0(0), \gamma_0, k) = \sum_{p_i} |\varepsilon_{F\Gamma}(p_i) - \varepsilon_F^{th}(p_i, N_d, N_a, \varepsilon_0(0), \gamma_0, k)|, \tag{5}$$

one can find the parameters $N_d, N_a, \varepsilon_0(0), \gamma_0$ which produce this minimum. This problem was solved by the method of

TABLE I.

Number of sample	$n_\Gamma(0)$, 10^{17} cm^{-3}	$\varepsilon_{F\Gamma}(0)$, meV	$\rho_{4.2}$, 10^{-2} Ω·cm	μ, cm^2/V·s
1	2.86	35.5	1.01	1850
2	3.79	41.6	0.58	2330
3	6.65	55.0	0.57	2020
4	8.39	69.8	0.60	1220
5	8.55	70.7	0.71	930
6	8.65	71.1	0.83	730
7	9.47	75.2	0.85	490

TABLE II.

Number of sample	N_d, 10^{17} cm^{-3}	γ_0, meV	N_a, 10^{17} cm^{-3}
1	3.35	0.60	0.49
2	5.17	0.99	1.38
3	6.87	0.41	0.22

coordinate-by-coordinate descent[11] with a Nord 10-S computer.

The computer calculation showed that the values of the functional Φ are most sensitive to a change in variables N_d, N_a, $\varepsilon_0(0)$, and the error of these parameters was 3–10%. At the same time, the level width γ_0 may be calculated with a large error (15–20%), since γ_0 determines the transition portion of the $\varepsilon_{F\Gamma}(p)$ curve in the region $p \sim p_0$ from the plateau $\varepsilon_{F\Gamma}(p) \approx$ constant at $p < p_0$ to the decreasing portion of $\varepsilon_{F\Gamma}(p)$ at $p > p_0$.

The dependence of Φ on $\varepsilon_0(0)$ is substantially more pronounced, since the amount $\Delta\varepsilon_0(0)$ by which it is permissible to change $\varepsilon_0(0)$ without any appreciable variation of Φ is given by the relation $\Delta\varepsilon_0(0) \approx 2\gamma_0$. For GaSb⟨Se⟩, $\gamma_0 \sim 0.4$–1 meV (see Table II), and the error of $\varepsilon_0(0)$ is $\Delta\varepsilon_0(0) = 1$–2 meV.

Let us note that the position of the $\varepsilon_0(0)$ level can be found by linear extrapolation of the decreasing portion of the $\varepsilon_{F\Gamma}(p)$ curve to the value $p = 0$. In this case, the error of $\varepsilon_0(0)$ calculated by the method of least squares is substantially greater and lies in the 5–6 meV range. It was found that the position $\varepsilon_0(0)$ of the ε_L^{Se} level relative to the undistorted bottom of the Γ band ε_c^0 amounted to 67 ± 2 meV for all samples with density $n_\Gamma(0) \lesssim 7 \cdot 10^{17}$ cm^{-3}. The independence of $\varepsilon_0(0)$ from $n_\Gamma(0)$ in this density range is consistent with the condition (1) of low doping for the L band.

The pressure rate of motion of the ε_L^{Se} level relative to the Γ band is 10.1 ± 0.2 meV/kbar, which is the same as the corresponding rate for GaSb⟨Te⟩. This indicates that the ε_L^{Se} level, although deeper than ε_L^{Te}, nevertheless does not shift under pressure relative to the bottom of the L band, i.e., the position of ε_L^{Se} is chiefly determined by an expansion in Bloch functions in some small neighborhood of point L of the Brillouin zone.

The ε_L^{Se} level is nondegenerate ($k = 1$), and its width, which amounts to 0.4–1.0 meV, is consistent with the value of the acceptor density (see Table II, which lists data on the most typical samples). The behavior of the reconstructed density of states in the ε_L^{Se} band is shown in Fig. 2 (Curves 3 and 4).

Thus the computer calculation confirms the results of the above qualitative comparison of the impurity states of Te and Se in GaSb: for GaSb⟨Te⟩, the value of γ_0 is ~ 5 meV (Ref. 5) and $\Delta\varepsilon_{\Gamma L} - \varepsilon_0(0) \approx 14$ meV, where for GaSb⟨Se⟩ $\gamma_0 \sim 0.5$ meV and $\Delta\varepsilon_{\Gamma L} - \varepsilon_0(0) \approx 26$ meV, i.e., when GaSb is doped with selenium, a narrower and deeper impurity level is formed. It can be expected, therefore, that the bottom of the Γ band itself in GaSb⟨Se⟩ will also be distorted much more than in GaSb⟨Te⟩.

This conclusion is confirmed by the behavior of the SdH amplitude of oscillations near ε_c: whereas SdH oscillations can be observed in GaSb⟨Te⟩, up to the values $\varepsilon_{F\Gamma} \sim 5$ meV, SdH oscillations in GaSb⟨Se⟩, are already suppressed at $\varepsilon_{F\Gamma} \sim 20$ meV.

3. DEPENDENCE OF THE MOBILITY OF Γ ELECTRONS ON THE POSITION OF THE FERMI LEVEL IN GaSb⟨Se⟩

As the electron density increases, the temperature dependences of the resistivity $\rho(T)$ of GaSb⟨Se⟩ (Fig. 3) change in the following manner. The values of ρ at $T = 200$ K decrease as $n_\Gamma(0)$ increases. At the same time, the resistivity at low temperatures is essentially a nonmonotonic function of

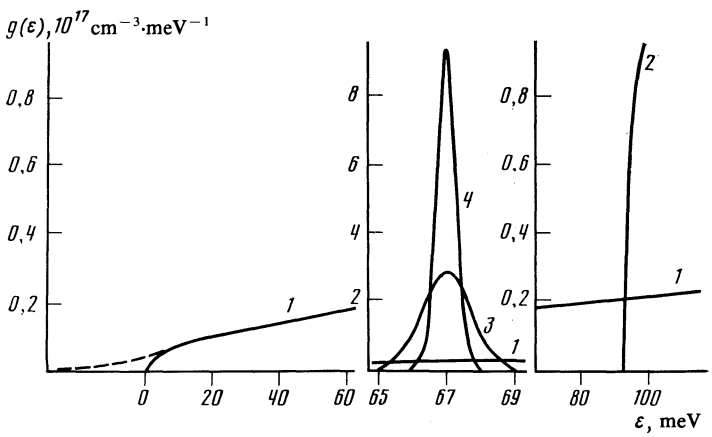

FIG. 2. Density of states $g(\varepsilon)$ in the conduction band of GaSb⟨Se⟩: curves 1—Γ band; 2—L band (for one extremum); 3—impurity band, sample No. 1; 4—impurity band, sample No. 3. The dashed line is a schematic representation of the variation of the density of localized states in the tail of the Γ band.

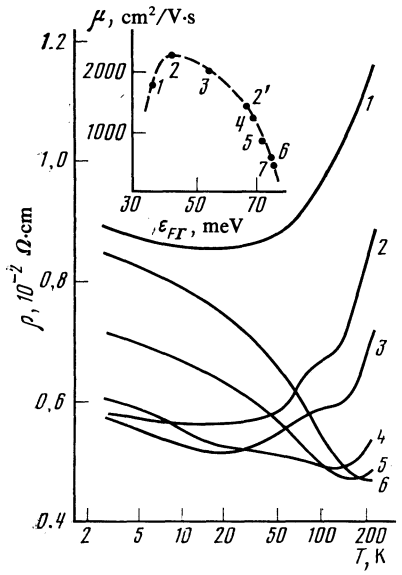

FIG. 3. Temperature dependences of resistivity $\rho(T)$ for samples of GaSb⟨Se⟩ at $p = 0$: Curve 1—sample No. 1; 2—No. 2; 3—No. 3; 4—No. 4; 5—No. 5; 6—No. 7. The numbers at the points on the μ vs $\varepsilon_{F\Gamma}$ curve correspond to the numbers of samples.

$n_\Gamma(0)$: initially (Curves 1–3 in Fig. 3), $\rho(T\to 0)$ decreases, then increases (Curves 4–6 in Fig. 3).

By determining from the oscillation data the position $\varepsilon_{F\Gamma}$ of the Fermi level in the Γ band, one can compare the value of the Hall mobility μ in a weak field ($\mu H \ll 1$) at low temperatures with the relative location of ε_F and of the ε_L^{Se} impurity level (see inset in Fig. 3). The increase of $\varepsilon_{F\Gamma}$ corresponding to the approach of ε_F to ε_L^{Se} initially leads to a slight increase of μ, and then, for $\varepsilon_{F\Gamma} \gtrsim 45$ meV, to an appreciable decrease of the Hall mobility.

Since the electron mobility at low temperatures is chiefly determined by scattering from impurities, it is necessary in the case of GaSb⟨Se⟩ to determine precisely which impurity states, ε_L^{Se} or ε_Γ^{Se}, are responsible for the specific features of the scattering of Γ electrons.

The data obtained (Fig. 3) show that in GaSb⟨Se⟩, the $\mu(\varepsilon_F)$ dependence is apparently due to the fact that the occupation boundary approaches the resonance impurity level ε_L^{Se}. However, in experiments at $p = 0$ in samples with different densities $n_\Gamma(0)$ of Γ electrons, both the distance from the tail of the Γ band and the potential relief of the Γ band, as well as the energy interval between ε_F and ε_L^{Se}, change, so that it is impossible to establish with confidence precisely which impurity states, ε_L^{Se} or ε_Γ^{Se}, determine the characteristics of the mobility μ in GaSb⟨Se⟩ at low temperatures.

It is of interest in this connection to determine the character of the change in mobility under pressure, when at $p < p_0$ the overflow of Γ electrons to the ε_L^{Se} level has not yet started, and only the location of $\varepsilon_{F\Gamma}$ relative to ε_L^{Se} varies (Fig. 4). The plotted dependence of μ on the difference $\varepsilon_L^{Se} - \varepsilon_{F\Gamma}$ shows that as ε_F approaches the resonance impurity band, and the Fermi energy ε_F measured from the bottom of the undistorted Γ band does not yet change, i.e., $\varepsilon_{F\Gamma}$ is a constant (see the

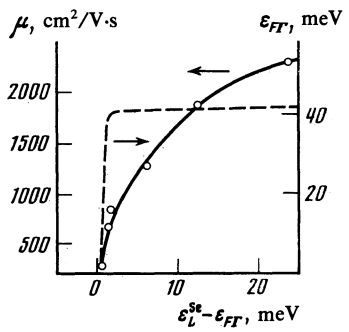

FIG. 4. Hall mobility μ and Fermi energy $\varepsilon_{F\Gamma}$ of Γ electrons vs difference $\varepsilon_L^{Se} - \varepsilon_{F\Gamma}$ at $T = 4.2$ K for sample No. 2.

dashed line in Fig. 4), the mobility $\mu(\varepsilon_L^{Se} - \varepsilon_{F\Gamma})$ decreases by a factor of more than two.

These data make it possible to attribute the behavior of $\mu(\varepsilon_F)$ precisely to scattering in the ε_L^{Se} impurity level, as is also confirmed by the change in the temperature dependences of mobility $\mu(T)$ under pressure: the markedly different Curves 1 and 2 in Fig. 5 correspond to the same filling of the Γ band and differ only in the distance from the ε_L^{Se} impurity level. A characteristic feature of the $\mu(T)$ curves for different pressures is the presence of a maximum. The mobility μ_{max} changes little with pressure, so that for convenience of comparison of curves with different μ, the $\mu(T)$ curves are shown in Fig. 5 in the form of the ratio $\mu(T)/\mu_{max}$. Let us note that the similarly shaped Curves 2 and 4 can be obtained both with the aid of pressure (Curve 2) and by varying the filling of the Γ band at $p = 0$ (Curve 4). Moreover, the mobility $\mu(\varepsilon_F)$, which decreases under pressure (point 2′ in Fig. 3), shows a correlation with the arrangement of the points on the $\mu - \varepsilon_{F\Gamma}$ curve plotted for $p = 0$. The value of μ for point 2′ was obtained from the experimental value of μ ($p = 2.6$ kbar) (Fig. 5, Curve 2), and the abscissa $\varepsilon_{F\Gamma}$ was plotted from the Fermi energy of point 2, increased by the amount 2.6 kbar·10.1 meV/kbar$\approx$26 meV, corresponding to the closer approach of ε_F and ε_L^{Se} as the pressure is increased by 2.6 kbar.

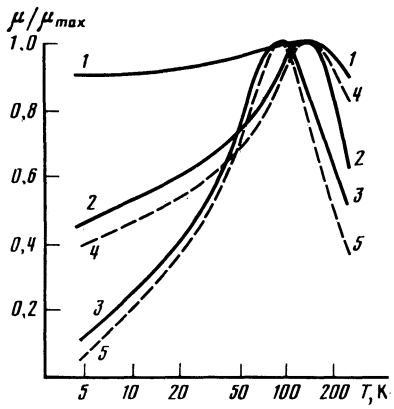

FIG. 5. Temperature dependences of Hall mobility $\mu(T)$ at different pressures for samples No. 2 (continuous line) and No. 7 (dashed line): Curve 1—0; 2—2.6; 3—4.86; 4—0; 5—5 kbar.

The body of data obtained (Figs. 3–5) indicate that the mechanism responsible for the suppression of μ as the ε_L^{Se} impurity level is approached may be resonant scattering of Γ electrons in this level. Since the resonant scattering in the ε_L^{Se} level for semiconductors of groups A^{III} B^{V} has not, to our knowledge been calculated, the following relationship can be used for the analysis of the $\mu(\varepsilon_F)$ curve (Fig. 4):

$$\mu_{res} \sim (1-(\varepsilon_0/\varepsilon_F)^{1/2})^2, \quad (6)$$

obtained in Ref. 12 for the resonant scattering of electrons in type HgTe zero-gap semiconductors. Qualitatively, the curve shape (see inset in Figs. 3 and 4) corresponds to the relation (6), but any quantitative comparison with (6) is scarcely justified, since expression (6), although derived under fairly general assumptions concerning the nature of the energy spectrum, cannot be directly applied to the calculation of the effectiveness of resonance scattering in the ε_L^{Se} level in GaSb⟨Se⟩.

It should be noted that the resonant scattering model can only be used for a Fermi level sufficiently distant from the mobility threshold ε_c in the tail of the Γ band, since the approach used in the derivation of formula (6) is inapplicable near ε_c.

In this connection, the situation in the range of pressures $p > p_0$, when ε_F is located in the vicinity of ε_c, is more complex, since the mobility μ is limited not only by scattering in the ε_L^{Se} level, but also by the interaction of Γ electrons with the impurity states in the tail of the Γ band itself. This question is discussed in detail in the next two sections.

4. FEATURES OF GALVANOMAGNETIC EFFECTS IN GaSb⟨Se⟩ UNDER PRESSURE

The instant of passage of the Fermi level ε_F through the unperturbed boundary ε_c^0 of the Γ band can be determined from the critical pressure p_c obtained by extrapolating the linear portion of the $\varepsilon_{F\Gamma}(p)$ curve to the value $\varepsilon_{F\Gamma} = 0$ (Fig. 1). For samples Nos. 1–3, which satisfy the condition $n_\Gamma(0) \lesssim 7\cdot10^{17}$ cm^{-3}, $\varepsilon_0(0) \approx$ const and p_c amounts to 6.7 ± 0.2 kbar. In the region of the high densities $n_\Gamma(0)$ (samples Nos. 4–7), the segment $\varepsilon_{F\Gamma}(p) =$ const does not occur, and the decrease of Fermi energy begins with the value $p_0 = 0$.

Because of the resonant scattering in the ε_L^{Se} level and the related depression of the amplitude of SdH oscillations in the region $n_\Gamma(0) \gtrsim 7\cdot10^{17}$ cm^{-3}, the $\varepsilon_{F\Gamma}(p)$ dependence can be tracked only up to pressures $p \leqslant 1$–1.5 kbar; this makes it difficult to determine p_c accurately. An estimate of the position of the level at $p = 0$ for samples Nos. 4–7 gives values of $\varepsilon_0(0)$ in the range 70–75 meV, to which correspond p_c in the 7–7.5 kbar range.

With increasing p, the resistivity ρ at low temperatures increases substantially (Fig. 6). Typical values of the ratio $\rho(p=0)/\rho(p=p_c)$ amount to approximately 10^4 at $T = 4.2$ K, and to 10^6 at $T = 1$ K. In addition, the $\rho(p)$ curves for GaSb⟨Se⟩ are characterized by a much broader region of variation of ρ in the vicinity of p_c in comparison with the curve for GaSb⟨Te⟩ (Fig. 6, dashed curve). Since Se gives a deeper level than does Te, it is natural to attribute the difference described to the presence in GaSb⟨Se⟩ of a more extended tail of localized states in the Γ band.

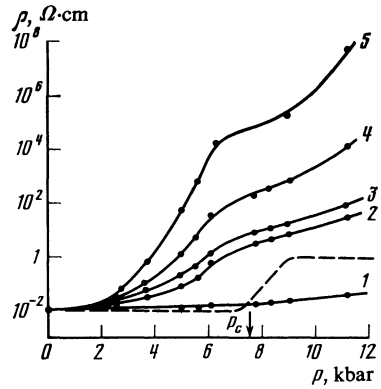

FIG. 6. Pressure dependences of resistivity $\rho(p)$ for samples No. 7 at different temperatures: Curve 1—300; 2—50; 3—20; 4—4.2; 5—1 K. The dashed line represents the curve of $\rho(p)$ at $T = 4.2$ K for the GaSb⟨Te⟩ sample.

As $p \to p_c$, the form of the temperature curves $\rho(T)$ undergoes a qualitative change: from quasi-metallic behavior $\rho(T) \approx$ const ($p \lesssim 2$ kbar) to a power law dependence, $\rho \sim T^{-\beta}$ with $\beta = 0.28 \pm 0.02$ ($2 \lesssim p \lesssim 3$ kbar), to an exponential dependence

$$\rho = \rho_0 \exp\{(T_0/T)^\alpha\}, \quad (7)$$

observed in the region $p \gtrsim 4$ kbar (Fig. 7).

The method of numerical differentiation of the curves $\ln\rho = f(1/T)$ is usually[13] employed to determine the exponent α. However, it is well known[11] that the operation of numerical differentiation of a function whose values are given with a certain error is generally incorrect and therefore requires regularization. The differentiation result obtained can be substantially dependent on the choice of the regularization algorithm, but this question was not discussed in Ref. 13, and apparently has not been studied at all.

At the same time, the values of α can be determined by a simpler method free of this disadvantage. An identity trans-

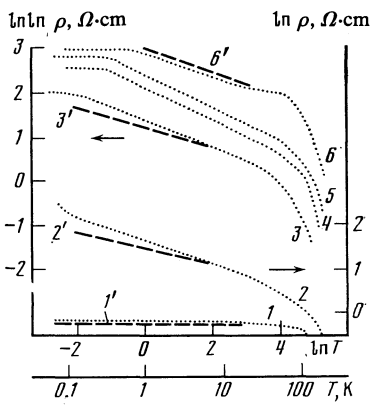

FIG. 7. Temperature dependences of resistivity $\rho(T)$ for sample No. 7 at different pressures (in kbar) in the absence of magnetic field (dotted curves 1–6) and in a field $H = 50$ kOe (dashed curves 1′, 2′, 3′, 6′); Curves 1, 1′—$p = 0$; 2, 2′—2.28; 3, 3′—3.7; 4—5.0; 5—5.7; 6, 6′—9.0.

formation of Eq. (7) yields

$$\ln \ln\rho=\alpha \ln T_0-\alpha \ln T+\ln(1+(T/T_0)^{\alpha} \ln \rho_0). \qquad (8)$$

The last term in Eq. (8) can be neglected when $|ln\rho_0| \ll (T_0/T)^{\alpha}$, which is always the case at sufficiently low temperatures. Thus, by plotting a relation of the type of Eq. (7) in the coordinates $\ln \ln \rho = f(\ln T)$, one can determine α, from the slope of the linear segments and T_0 from the intercept. By replotting $\rho(T)$ once again in the coordinates $\ln \rho = f(1/T^{\alpha})$, one can estimate the value of the pre-exponential factor ρ_0.

The condition for applicability of this approach to the determination of α is that $|\ln \rho_0|$ be small compared to $|\ln \rho|$. If, however, the condition $|\ln \rho| \gg |\ln \rho_0|$ is not met, preference should be given to the method of differentiation of the curves.

In processing the data obtained in the study of GaSb⟨Se⟩, we used both methods of determination of α. The validity of the calculation of α from the slope of the linear segments in the coordinates $\ln \ln \rho = f(\ln T)$ was checked by subsequent replotting in the coordinates $\ln \rho = f(1/T^{\alpha})$. The simplest regularization along the length of the step was used in the numerical differentiation of the curves.[11] For GaSb⟨Se⟩, the two methods were found to give practically the same values of α (to within 5%).

It should be noted that for GaSb⟨Se⟩ samples, in the coordinates $\ln \ln \rho = f(\ln T)$, extended linear segments are observed (Fig. 7) that correspond to a 60 to 120-fold change in temperature. The values of α, T_0 and ρ_0 obtained for sample 7 are listed in Table III. It is evident from Fig. 7 and Table III that $\ln \rho_0 \ll (T_0/T)^{\alpha}$ in the entire range of temperatures where, in the coordinates $\ln \ln \rho = f(\ln T)$, linear segments are observed having slopes which determine the exponent α (when the logarithms were taken, the value of ρ was taken in units of 10^{-2} Ω·cm). Values of α calculated for GaSb⟨Se⟩ samples for different pressures are shown in Fig. 8.

Attention is drawn to the fact that the exponential $\rho(T)$ dependence appears at considerably lower pressures (by approximately 2.5 kbar) than p_c, i.e., when ε_F is separated from ε_c^0 by 25 meV and the electron density in the Γ band is $\sim 2 \cdot 10^{17}$ cm^{-3}.

The transition from the quasi-metallic behavior of $\rho(T)$ through a power-law dependence to an exponential dependence can naturally be attributed to the displacement of the Fermi level into the region of localized states under pressure. It should be emphasized that such behavior of the temperature dependences of resistivity in the region $p \sim p_c$ cannot be explained by a comparable contribution of two groups of carriers—Γ electrons and electrons in the ε_L^{Se} band—to the current transport.

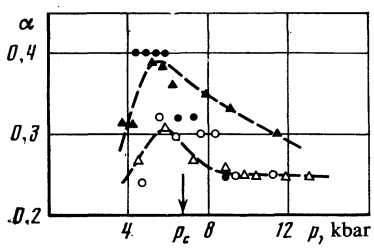

FIG. 8. Exponent α in Eq. (7) at different pressures for GaSb⟨Se⟩ samples: ●—sample No. 1, ○—sample No. 2, △—sample No. 3, ▲—sample No. 7. The dashed lines characterize the change in α under pressure. The error of determination of α is no greater than 0.02 for the data cited.

We shall estimate the upper conductivity limit in the ε_L^{Se} impurity band as follows: we compare the resistivity in the region $p \sim p_c$ (Fig. 6) with the resistivity in the region $p \gtrsim 11$ kbar, when the Γ extremum is located 20 meV above the bottom of the L band. At temperatures below 20 K, when the $\rho(T)$ curves are described by Eq. (7), the resistivity ρ increases by more than two orders of magnitude during the transition from $p \sim p_c$ to $p \gtrsim 11$ kbar. Thus the conductivity in the ε_L^{Se} impurity band, predominant at $p \gg p_c$, is at least 100 times lower than that in the Γ band in the pressure range $0 < p < 7$–8 kbar. Therefore, the characteristics of the galvanomagnetic effects near p_c are related to the conductivity precisely in the Γ band and cannot be caused by current transport over ε_L^{Se} impurity states.

Hence, the above-described transformation of the temperature dependences can apparently be attributed to the passage of ε_F through the mobility threshold ε_c in the Γ band. This assumption is confirmed by the dependence of activation energy ε_a on pressure, determined from the slope of the curves $\ln \rho = f(1/T)$ in the temperature range 100 K $\lesssim T \lesssim$ 150 K. The activation energy ε_a increases with pressure at a rate $\partial \varepsilon_a / \partial p = 10.1 \pm 0.5$ meV/kbar, becoming zero at $p \sim 4$ kbar (Fig. 1), i.e., considerably before ε_F intersects ε_c^0.

We should also like to emphasize that ε_a is actually determined by the activation energy of the carriers to the mobility threshold, since the pressure rates $\partial \varepsilon_a / \partial p$ and $\partial \varepsilon_F / \partial p = \partial \varepsilon_0 / \partial p = 10.1 \pm 0.2$ meV/kbar are practically the same.

Since the level ε_c lies substantially above the undistort-

TABLE III.

p, kbar	α	T_0, K	ρ_0, 10^{-2} Ω·cm
3,7	0.31	78	1,25
4.0	0.31	100	1,25
5,0	0,39	250	1,42
5,7	0,38	570	1,67
6.2	0.36	1710	1,67
7,8	0.35	3160	1.67
9.0	0,33	6960	1.67
11,2	0.30	33980	1.67

ed boundary ε_c^0 of the Γ band (Fig. 1), $\varepsilon_c - \varepsilon_c^0 \approx 25$ meV, the position of ε_c cannot be determined by classical percolation level ε_c^{cl} over a system of regions with metallic conduction, since the most general consideration of the problem of the percolation threshold in the three-dimensional case[14-16] suggests that ε_c^{cl} is located below ε_c^0.

At the same time, in the case of the quantum-mechanical treatment of the metal-insulator transition, the interference of partial waves, caused by above-barrier reflection from the potential relief of the bottom of the Γ band, may lead to localization of electronic states for $\varepsilon_c^q > \varepsilon_c^0$.[17] For example, when electrons of energy ε are scattered from a rectangular potential barrier of height U and width a, the transmission coefficient differs from unity over a fairly wide range of energies $U < \varepsilon < U + \pi^2\hbar^2/2m_0a^2$.[18,19] Thus it can be expected that also in the case of small-scale distortion of the bottom relief of the band (small a) of large amplitude (U is large), localization will be due to above-barrier reflection.

5. THE METAL-INSULATOR TRANSITION IN GaSb⟨Se⟩

A theoretical study of the curves of ρ vs T as the Fermi level passes smoothly through the mobility threshold constitutes a complex problem that apparently has not been fully solved. On the metal side of the transition, where $\varepsilon_F \to \varepsilon_c + 0$, the kinetic equation of Ref. 20 proves inapplicable, and in the dielectric region, where $\varepsilon_F \to \varepsilon_c - 0$, consideration of Mott type hops is inadmissible because of the divergence of the localization radius of the wave function. Therefore, the only approach applicable to the description of the entire metal-insulator transition, including the vicinity of ε_c, is scaling theory.

The characteristic parameters of this theory are the mean free path, the characteristic length of inelastic collisions $L_T = (D\tau_{in})^{1/2}$ (here D is the diffusion coefficient, and τ_{in} is the time of inelastic collisions), the localization radius γ^{-1}, and the Mott length of the hop $R_{opt} \sim 1/T^{1/4}$.[17,20-22]

Depending on the relative positions of ε_F and ε_c, the different types of temperature dependences of the conductivity $\sigma(T)$ will be determined by some characteristic parameter. In this section we shall compare the $\sigma(T)$ predictions of the scaling theory, for different values of the difference $\varepsilon_F - \varepsilon_c$, with the experimental results (Figs. 7 and 8).

From the standpoint of the scaling theory of a metal-insulator transition, which uses the technique of calculating the quantum corrections to the conductivity,[23] the dimensionless conductivity $G = \sigma L^{d-2}\hbar/e^2$ is described by the one-parameter scaling equation (also applicable when electron-electron interaction is taken into account[20]):

$$d\ln G/d\ln L = W(G), \tag{9}$$

where L is the characteristic length, d is the number of space dimensions, and $W(G)$ is a smooth function which in the three-dimensional case has the asymptotic behavior $W \to 1$, as $G \to \infty$ and $W \to \ln G$ as $G \to 0$ (Ref. 21).

The form of the solution of Eq. (9) for $d = 3$ is substantially dependent on the position of ε_F relative to ε_c. Far from the mobility threshold when $\varepsilon_F \gg \varepsilon_c$, the solution of Eq. (9) can be represented in the form $\sigma = \sigma_0 + \Delta\sigma$.[20-22] In this case one must add to the conductivity σ_0 determined from the kinetic equation a correction $\Delta\sigma$, proportional to L_T^{-1}, which for $\tau_{in} \sim \hbar/T$ and $D = \text{const}$ will vary with temperature like $\Delta\sigma \sim T^{1/2}$.

In the vicinity of the mobility threshold $\varepsilon_F \geqslant \varepsilon_c$ on the metal side of the transition, Eq. (9) gives[20]

$$\sigma \approx e^2/\hbar L_T. \tag{10}$$

Using Einstein's relation $\sigma = e^2 D g(\varepsilon_F)$ ($g(\varepsilon_F) = \partial n_\Gamma/\partial\varepsilon_F$) as well as the expression for L_Γ in the form $L_T = (D\hbar/T)^{1/2}$, we find from (10)

$$L_T \approx (1/Tg(\varepsilon_F))^{1/3} \tag{11}$$

and $\sigma \sim T^{1/3}$.[20]

According to Ref. 17, for $\varepsilon_F \lesssim \varepsilon_c$ as well, provided $\gamma L_T \ll 1$, the solution of Eq. (9) is described as before by a formula similar to (10): $\sigma \sim 1/L_T$. The temperature dependence of L_T retains the form (11), since the length L_T determined from (11) has the meaning of the average distance by which the electron is displaced between two events of phonon absorption. Therefore, in a certain vicinity of ε_c –on both the metallic and the dielectric sides of the transition– there exists a critical region in which $\sigma \sim T^{1/3}$.

In the experiment (Fig. 7), the power law dependence $\sigma = 1/\rho \sim T^\beta$ occurs at a pressure $p \sim 3$ kbar, and the exponent $\beta = 0.28 \pm 0.02$ is close to the theoretical value $\beta = 1/3$.

On the dielectric side of the transition for $\varepsilon_F < \varepsilon_c$ and $\gamma L_T \gg 1$, i.e., when the length L_T considerably exceeds the localization radius, an asymptotically exact solution of Eq. (9) is given by the relation

$$\sigma \approx (e^2/\hbar L_T)\exp(-\gamma L_T). \tag{12}$$

It should be noted that in contrast to the region $\varepsilon_F \sim \varepsilon_c$, when L_T is described by formula (11), with $\varepsilon_F < \varepsilon_c$ and $\gamma L_T \gg 1$, the length L_T has the meaning of coherence length, on which the "memory" of the phase of the wave function is preserved.[17] In this case, in the treatment of the hopping conduction between localized states, Mott's approach[24] to finding the optimum distance R_{opt} is applicable, provided the hop length $R_{opt} \sim 1/T^{1/4}$ does not exceed the coherence length L_T. Otherwise, when $L_T < R_{opt}$, Mott's optimization procedure is incorrect, since in hops over a distance in excess of L_T, a phase change will inevitably take place, and hence, the average matrix element of such a transition between localized states will become zero.

For $L_T < R_{opt}$, it is necessary to consider a modified Miller-Abrahams random resistance grid, for which the maximum resistance of the element is proportional to $\exp(\gamma L_T)$. Then the temperature dependence of the conductivity will be described by formula (12), in which L_T can be estimated as $L_T \sim 1/T^{1/2}$.[17] This is associated with the exponential dependence of the resistivity (7) with exponent $\alpha = 0.5$.

On the dielectric side of the transition ($\varepsilon_F < \varepsilon_c$) over a wide temperature range (Figs. 7 and 8), exponential dependences of ρ on T are experimentally observed, and most likely correspond to the above-discussed modified model of hopping conduction, although the experimental values

$\alpha = 0.33$–0.4 differ from the theoretical value $\alpha = 0.5$. As ε_F shifts further downward relative to ε_c, the exponential dependence (12) is preserved, but R_{opt} should be substituted for L_T in (12), owing to the transition to hopping conduction between electronic states localized on impurity centers.

A monotonic decrease of exponent α from 0.33–0.4 to 0.25 takes place in the pressure region $p \gtrsim 7$ kbar (Fig. 8), and the Mott conductivity for $p \gg p_c$ can be due to states in the tail of the Γ band as well as to those in the ε_L^{Se} impurity band.

An additional argument in favor of the applicability of scaling theory to the description of the metal-dielectric transition in GaSb⟨Se⟩ is the character of the change in the temperature dependence of ρ on T in a magnetic field (Fig. 7). In the metallic region far from the mobility threshold (Fig. 7, Curves 1 and 1′), a weak $[\Delta\rho(H = 50\ \text{kOe})/\rho(H = 0) \sim -1.5\%]$ negative magnetoresistance (NegMR) is observed. In a certain critical region near ε_c, the NegMR effect turns out to be appreciable: in a field of 50 kOe, the exponent β decreases in comparison with the value at $H = 0$ and amounts to 0.18 (Fig. 7, Curve 2′). The exponent α in Eq. (7) also decreases in a magnetic field (Fig. 7, Curve 3′): $\alpha = 0.25$ ($H = 50$ kOe).

It is known[25] that a magnetic field detunes the interference of wave functions during backscattering and therefore results in NegMR when $\varepsilon_F \gg \varepsilon_c$. Near ε_c, the NegMR effect will apparently be most appreciable, since the phase shift in the magnetic field will decrease the degree of localization and hence ρ.

In the region $p \gg p_c$, a transition takes place from NegMR to positive magnetoresistance (Fig. 7), which is naturally explained in terms of ordinary models of hopping conduction.[10] Nevertheless, the exponent α remains greater than 0.25 (Fig. 7, curves 6 and 6′). This fact can be interpreted in terms of the Mott hopping conduction, account being taken of the fact that the potential of the center on which the electron is localized may differ from the potential of a point charge. Let us assume that in GaSb⟨Se⟩ at the indicated pressures, the electron is localized not on an individual donor, but on a cluster of characteristic dimension a, the potential of which can be approximately represented in the form of the potential $V(R)$ of a uniformly charged sphere.

In the case $\gamma a \sim 1$, the potential $V(R)$ is proportional to R (Ref. 19), and then the solution $\psi(R)$ of Schrödinger's equation is an Airy function having the asymptotic form $\psi(R) \sim \exp\{-(\gamma R)^{3/2}\}$.[26] According to the results of Ref. 17, the value of α calculated by taking into account this asymptotic form of the wave function is equal to 1/3, which is in good agreement with the experimental value $\alpha = 0.33$ (Fig. 7, Curve 6).

In the framework of scaling theory, it is of interest to analyze the possible mechanisms responsible for the downward deviation of the dependence $\rho(T)$ from linear, in the coordinates $\ln\ln\rho = f(\ln T)$, in the region of the lowest temperatures (see curves 3-6 in Fig. 7 at $T \lesssim 0.2$–0.3K). It is natural to attribute this behavior of $\rho(T)$ to the transition from the relation $L_T < R_{opt}$ to the opposite relation $L_T > R_{opt}$ as the temperature decreases.

Actually, both characteristic parameters, L_T and R_{opt}, vary as the square root of the reciprocal temperatures: $L_T \sim 1/T^{1/2}$ (Ref. 17) and $R_{opt} \sim 1/T^{1/4}$.[24] Therefore, at not too low temperatures, when $1/T$ is small, the fourth root is greater than the square root, and the inequality $R_{opt} > L_T$ is satisfied; this inequality becomes reversed $R_{opt} < L_T$, when $1/T$ is large. From this point of view, the experimental exponential dependence (7) with $\alpha = 0.33$–0.4 (Curves 3–6 for $0.2 \lesssim T \lesssim 20$ K in Fig. 7) corresponds to the condition $R_{opt} > L_T$, and the tendency toward saturation at $T \leqslant 0.2$ K corresponds to the transition to the regime $L_T > R_{opt}$.

Let us note that the transition from the exponential dependence of ρ and T to a weaker dependence takes place in a region of fairly low temperatures ($T \lesssim 0.2$ K), where a more effective mechanism of charge transfer in comparison with one-electron hops over a distance R_{opt} may prove to be cascade multielectron hops,[28,29] for which the dependence of ρ on T is not exponential, but rather a power-law dependence.

An analogous change of regime may also occur in the region $\varepsilon_F \lesssim \varepsilon_c$, where $\sigma \sim T^{1/3}$ if the condition $\gamma L_T \ll 1$ is met, and $\sigma \sim \exp(-\gamma L_T)$ if the reverse relation $\gamma L_T \gg 1$ is true. Since L_T increases as the temperature decreases, in the temperature range defined by the condition $\gamma L_T \sim 1$, a transition will occur from the power-law dependence $\sigma(T)$ [formula (10)] to an exponential dependence [formula (12)]. In the experiment (Fig. 7, Curve 2), it is probable that this is what causes the transition from the dependence $\sigma \sim T^{\beta}$ [straight line 2 in Fig. 7 in the coordinates $\ln \rho = f(\ln T)$] for $0.12 \lesssim T \lesssim 15$ K to the more pronounced dependence for $T \lesssim 0.12$ K.

An important characteristic of the metal-insulator transition observed in GaSb⟨Se⟩ is the critical behavior of the low-temperature conductivity values in the metallic phase. According to scaling theory, at $T = 0$ the dependence of σ on ε_F for $\varepsilon_F > \varepsilon_c$ is given by the equation[21]

$$\sigma(\varepsilon_F) = \sigma_0(\varepsilon_F/\varepsilon_c - 1)^t, \tag{13}$$

where the exponent t is in the range $0.5 \leqslant t \leqslant 1.25$.[30]

The experimental $\sigma(\varepsilon_F)$ curve for $T \lesssim 2$ K, as $\varepsilon_F \to \varepsilon_c$, is satisfactorily described by Eq. (13). The value of t for the samples studied is $t = 0.6 \pm 0.1$. The value of σ_0 in Eq. (13) is approximately 100 $(\Omega\cdot\text{cm})^{-1}$, and the spread of the values for different samples does not exceed 10%, whereas the density N_{Se} in these samples changes from $3\cdot10^{17}$ to $\sim 10^{18}$ cm^{-3}. Let us note that the value of σ_0 is within 20% of ρ_0^{-1} in Eq. (7), which describes the dependence $\rho(T)$ in the dielectric phase.

The data obtained are in good agreement with the results of Ref. 31, in which the critical behavior of $\delta(\varepsilon_F)$ was investigated for samples of n-Si at $T = 1$ mK, and the value of the exponent obtained was $t = 0.55 \pm 0.1$.

Let us note that the experimental values of t cannot be matched to the predictions of percolation theory, for which $t \approx 1.6$.[10]

Thus by studying the kinetic phenomena near the mobility threshold ε_c in GaSb⟨Se⟩ in a continuous transition from the metal ($\varepsilon_F \gg \varepsilon_c$) to the dielectric ($\varepsilon_F \ll \varepsilon_c$), we were able to show the following: the metal-insulator transition takes place not via a monotonic increase in the exponent α from 0 to the Mott value $\alpha = 0.25$, as predicted in Ref. 24, but via a gradual transformation of dependences $\rho(T)$ from

metallic behavior ($\varepsilon_F \gg \varepsilon_c$) to a power-law dependence, $\rho(T) \sim 1/T^{\beta}$ ($\varepsilon_F \sim \varepsilon_c$), to an exponential ($\varepsilon_F < \varepsilon_c$) dependence $\rho \sim \exp\{(T_0/T)^{\alpha}\}$, with exponent α dependent nonmonotonically on the difference $\varepsilon_F - \varepsilon_c$ and taking on a whole series of values from the interval $0.25 \leqslant \alpha \leqslant 0.4$. The exponent α initially increases to the value $\alpha = 0.33$–0.4 and only then, with $p \gg p_c$, monotonically decreases, approaching the value $\alpha = 0.25$.

From the standpoint of scaling theory,[20] the power law dependence of $\rho(T)$ should be attributed to the contribution to the conductivity made by quantum corrections which increase sharply as ε_c is approached, and starting from certain values of ε_F, make a decisive contribution to the current transport and in this sense cease to play the role of corrections, but for $\varepsilon_F = \varepsilon_c > \varepsilon_c^0$ lead to quantum localization of electrons, caused by interference of partial waves reflected from distortions of the potential relief of the bottom of the Γ band.

In the region $\varepsilon_F < \varepsilon_c$, in accordance with the scaling approach, one should expect temperature dependences of ρ of the type of Eq. (7) with exponent $\alpha = 0.33$ or 0.5; this is in satisfactory agreement with experiment (Figs. 7 and 8).

The above-barrier reflection leading to localization above the bottom of the undistorted Γ band is substantially dependent on the parameters [for example, a and U (Refs. 18 and 19)] characterizing the potential barrier. One could therefore expect an appreciable change in the picture of the metal-insulator transition upon the introduction of impurities which distort less the bottom relief of the band.

In particular, for shallow hydrogenlike impurities [for example, Te in GaSb (Ref. 5)], the role of quantum corrections will evidently be substantially less important, the interval $\varepsilon_c^q - \varepsilon_c^0$ will become narrower, and the classical percolation description of the metal-insulator transition with mobility threshold ε_c^{cl} may turn out to be more adequate.

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