Pressure-induced restructuring of energy spectrum of GaSb:Te

N. B. Brandt, S. V. Demishev, V. V. Moshchalkov, A. S. Rylik, and S. M. Chudinov

Moscow State University
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The effect of hydrostatic pressure p up to 15 kbar on the Shubnikov–de Haas oscillations and the galvanomagnetic effects in tellurium-doped single crystals of GaSb with tellurium density 2×10^{17}–2.2×18^{18} cm^{-3} is investigated. Hydrostatic compression decreases the energy gap $\varepsilon_{\Gamma L}$ between the Γ and L minima in the conduction band and induces transfer of the electrons from the Γ band into the impurity band that is split away from the L-minimum. This makes it possible to determine the behavior of the state density in this band by using, as a reference of sorts, the Γ electrons whose dispersion law has been reliably established. The following is shown: 1) the energy gap $\varepsilon_{\Gamma L}$ at $p=0$ amounts to 93 ± 4 meV, is independent of the density N_d of the introduced tellurium, and decreases under pressure at a rate 10.1 ± 0.2 meV/kbar. 2) The formation of an impurity band split away from the L extremum is due mainly to overlap of the wave functions of the donor centers, and not to transitions into the continuous spectrum (into the Γ band). 3) The impurity band is not degenerate—its capacity is equal to the number of donors N_d, and its width is determined by the density N_d and by the degree of compensation; the width of the impurity band is practically independent of pressure.

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INTRODUCTION

The electronic properties of various disordered systems are now being intensively investigated, particularly the electronic states in doped semiconductors,[1] in which the carriers are subjected simultaneously to the periodic field of the crystal atoms and to the random field of the chaotically distributed impurity atoms. The very fact that impurity and Bloch states coexist makes it possible in principle to study disordered systems by investigating the properties of the band electrons, using the effective experimental methods of the physics of crystalline solids.

From the point of view of this approach to the problem of disordered systems, gallium antimonide doped with suitable impurities is a highly promising material for the experimental study of impurity states. This is due, on the one hand, to the process of a reliably established set of parameters that describe adequately the dispersion law of the Γ electrons[2-5] (Fig. 1), and on the other hand by the distinguishing features of the band spectrum of GaSb, namely the low energy gap $\varepsilon_{\Gamma L}$ between the Γ and L conduction bands ($\varepsilon_{\Gamma L}$ 80–90 meV, Refs. 3–5) and the high rate of its change under pressure $\alpha=\left|\partial\varepsilon_{\Gamma L}/\partial p\right|$ 10 meV/kbar.[4]

This results in the following: 1) The donor states split-off from the L minima are resonant and cross the conduction Γ band quite close to the bottom of the latter, so that the Γ electrons can be used as a reference of sort for the study of the impurity donor states. 2) The high baric rate α of the approach of the Γ and L terms makes it possible to vary, with the aid of pressure, the relative position of the Γ band and of the impurity level located near the L band. This in turn induces a transfer of the Γ electrons to this level. In this situation, the number of electrons transferred to the impurity band can be determined from the degree of filling, at various pressures, of the Γ extremum characterized by the Fermi energy $\varepsilon_{F\Gamma}$ of the Γ electrons, using the charge-conservation condition, and determine in final analysis the behavior of the state density in the impurity band.

The procedure for determining the baric dependences of the Fermi energy $\varepsilon_{F\Gamma}(p)$ of the Γ electrons from oscillation measurements is quite simple and was described in our preceding papers.[6,7]

The aim of our present paper was to investigate in detail the impurity donor states and the character of the restructuring of the energy spectrum of GaSb:Te at a pressure p up to 15 kbar in a wide range of tellurium densities (2×10^{17}–2.2×10^{18} cm^{-3}) by studying the oscillatory and galvanomagnetic effects in a magnetic field up to 50 kOe and in the temperature interval 4.2–300 K.

EXPERIMENTAL RESULTS

Single-crystal ingots of gallium antimonide doped with tellurium were kindly furnished by R.V. Parfen'ev (A.F. Ioffe Physicotechnical Institute, Leningrad, samples 1–3 and 6) and D.G. Andrianov and G.P. Kolchina (Rare Metals Institute, Moscow, samples 4, 5, and 7). Table I lists some of the characteristics of these samples. The method of mounting the samples in the high-pressure

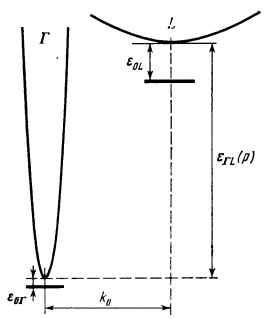

FIG. 1. Structure of conduction band of donor-doped gallium antimonide.

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TABLE I.

Sample number	Sample code	n_{ac}*, 10^{17} cm^{-3}	ρ_{300}, 10^{-3} Ω·cm	$\rho_{4.2}$, 10^{-3} Ω·cm	μ, 10^3, cm^2/V·sec	n_Γ*, 10^{17} cm^{-3}
1	GS-1	1.9	17	10	3.25	2.0
2	GS-41	3.4	10	5.1	3.6	2.8
3	GS-44	5.5	12	3.2	3.6	4.2
4	152	4.4	14	2.1	6.8	5.5
5	94-1	12.3	3.2	0.52	9.8	11.4
6	GS-40-1	7.7	4.05	0.115	7.1	12.3
7	46	11.0	2.5	0.4	14.9	13.5

* $T=4.2$ K.

chamber and the procedure used in the galvanomagnetic and oscillation measurements under pressure are described in detail in Ref. 6.

For each fixed value of the pressure we recorded at liquid helium temperature the Shubnikov–de Haas quantum oscillations (SdHO) of the longitudinal magnetoresistance (Fig. 2). The period of these monochromatic oscillations, which correspond to the extremal section S_Γ of the spherical Fermi surface of the Γ electrons, determines the Γ-band filling, which is characterized by the Fermi energy $\varepsilon_{F\Gamma}$. Since hydrostatic compression causes the direct gap in Γ to increase linearly[5]:

$$\varepsilon_{g\Gamma}(p)=(811.3+14.5\cdot p\ \text{(kbar)})\ \text{MeV}, \tag{1}$$

the mass m_Γ at the bottom of the Γ band, which enters in the Kane dispersion law, also changes: $m_\Gamma=m_\Gamma(p)$. Assuming that the Kane matrix element and the spin-orbit interaction are independent of pressure, we can write

$$m_\Gamma(p)=m_\Gamma(0)\,\varepsilon_{g\Gamma}(p)/\varepsilon_{g\Gamma}(0). \tag{2}$$

Here $m_\Gamma(0)=0.043m_0$.[3,6] Thus, using the dispersion law

$$\varepsilon_{F\Gamma}(p)\left(1+\frac{\varepsilon_{F\Gamma}(p)}{\varepsilon_{g\Gamma}(p)}\right)=\frac{p_{F\Gamma}^2}{2m_\Gamma(p)}=\frac{S_\Gamma(p)}{2\pi m_\Gamma(p)}, \tag{3}$$

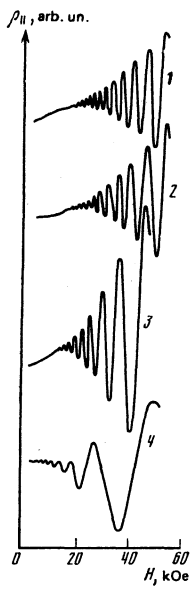

FIG. 2. Quantum oscillations of longitudinal magnetoresistivity ($\rho_{\parallel}$) of sample No. 7 at various pressures (kbar): 1) 1.0; 2) 3.4; 3) 5.6; 4) 8.3.

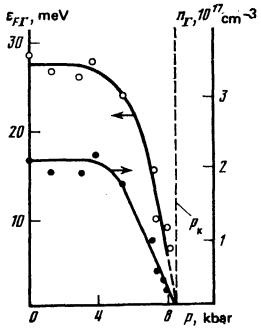

FIG. 3. Baric dependences of the density n_Γ and of the Fermi energy $\varepsilon_{F\Gamma}$ of the Γ electrons of sample No. 1.

it is easy to determine from the experimental value of $S_\Gamma(p)$ the Fermi energy $\varepsilon_{F\Gamma}(p)$ of the Γ electrons as a function of pressure, by substituting $m_\Gamma(p)$ (2) and $\varepsilon_{g\Gamma}(p)$ (1) in (3).

Baric plots of n_Γ and $\varepsilon_{F\Gamma}$ which are typical of samples with $N_d\lesssim 5\times10^{17}$ cm^{-3} are shown in Fig. 3. These plots are characterized by the presence of a pressure region in which the indicated values remain constant, and by the presence of a certain critical pressure p_{cr} at which they vanish (see Fig. 3).

The amplitude $\Delta\rho/\rho$ of the SdHo in a fixed magnetic field depends strongly on the pressure (Fig. 4). For example, for sample 2 in the pressure interval 1.5 kbar $\lesssim p\lesssim$ 7.3 kbar it increases by 700 times, and for sample 2 when p is changed from 4.8 to 9 kbar it increases by 350 times. The pressure dependences of the Hall coefficient R and of the Hall mobility μ, calculated from the Hall emf in a weak magnetic field ($\mu H\ll 1$) and from the resistivity at $T=4.2$ K are shown for sample number 1 in Fig. 5.

In the pressure region $p\lesssim 5$ kbar, the Hall coefficient is constant, and the mobility increases slightly. The shapes of the $R(p)$ and $\mu(p)$ curves at higher pressures also point to the existence of a certain critical pressure, which coincides with p_{cr}, at which the extremal section S_Γ vanishes. Passage through the pressure p_{cr} in weakly doped samples ($N_d\lesssim 5\times10^{17}$ cm^{-3}) is accompanied by

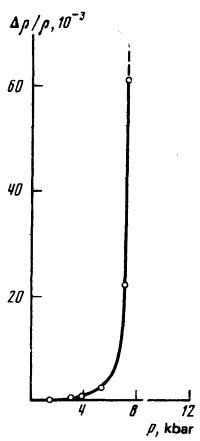

FIG. 4. Dependence of the amplitude $A=\Delta\rho/\rho$ of the SdHO in a fixed magnetic field $H_0=30$ kOe on the pressure p for sample No. 1.

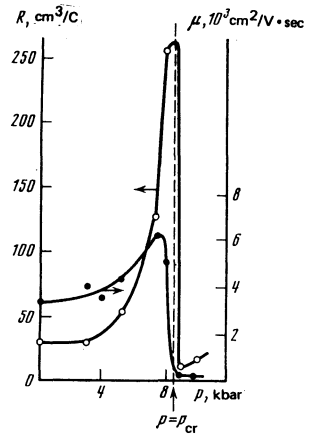

FIG. 5. Baric dependences of the Hall coefficient R and of the mobility μ at $T = 4.2$ for sample No. 1.

a jumplike decrease of the Hall coefficient R and of the mobility μ, by factors ~20 and 150–300, respectively. In samples with large tellurium contents, this transition takes place with a smaller change of R and μ.

It should also be noted that for single crystals with $N_d \gtrsim 10^{18}$ cm^{-3} the baric dependence of the Fermi energy $\varepsilon_F(p)$ of the Γ electrons is characterized by the absence of a plateau in the region $p \leq 6$ kbar, and by the presence of longer sections with linear decrease of $\varepsilon_{F\Gamma}$ with pressure than in the case of samples with $N_d \lesssim 5\times10^{17}$ cm^{-3}. These sections terminate at $p = p_{cr}$, where $\varepsilon_{F\Gamma}$ vanishes (Fig. 6, samples number 5 and number 7).

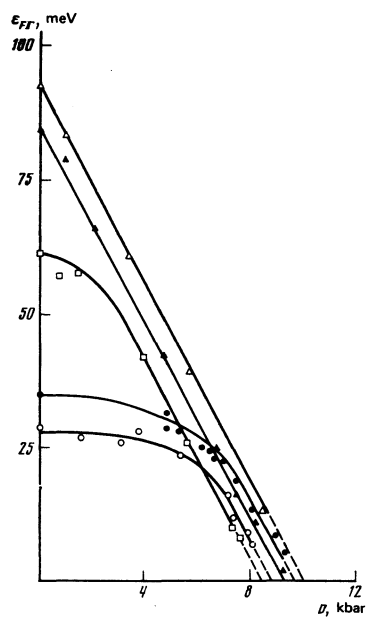

FIG. 6. Baric dependences of the Fermi energy $\varepsilon_{F\Gamma}$ of the Γ electrons for samples No. 1 (○), 2 (●), 4 (□), 5 (▲), and 7 (△). Solid lines—computer calculation by formula (25) with the following parameters: No. 2) $N_0 = 2.82\times10^{17}$ cm^{-3}, $N_d = 2.9\times10^{17}$ cm^{-3}, $\gamma = 7$ meV; No. 7) $N_0 = 2.05\times10^{17}$ cm^{-3}, $N_d = 2.0\times10^{17}$ cm^{-3}, $\gamma = 14$ meV. The data for samples 1 and 5 are given in Table III. The same values $\varepsilon_{\Gamma L} = 93$ meV and $\alpha = 10.1$ meV/kbar were used for all samples.

TABLE II.

Parameters*	Γ	L
m/m_0	0.043	0.3
a_B, Å	190	20
ε_0, meV	2.4	21
$N_d^0 = 1/a_B^3$, cm^{-3}	$1.4\cdot10^{17}$	$1.0\cdot10^{20}$

*$\varkappa = 13.8$,[3] $a = 6.096$ Å,[2] $k_0 = 0.893\cdot10^8$ cm^{-1}.[2]

In all the investigated samples, the transition through $p = p_{cr}$ is accompanied also by a qualitative change of the character of the dependence of the resistivity ρ on the temperature: in the region $p \lesssim p_{cr}$ the resistivity decreases monotonically with decreasing temperature, whereas at $p \gtrsim p_{cr}$ distinct linear sections appear on the $\ln\rho = f(1/T)$ curves and attest to the presence of a certain activation energy $\varepsilon_{i\text{-}L}$.

RESTRUCTURING OF ENERGY SPECTRUM OF GaSb: Te UNDER PRESSURE

1. Impurity donor states near the Γ and L extrema

A distinguishing feature of the behavior of donor impurities in gallium anitmonide, which has in the conduction band closely lying Γ and L minima characterized by essentially different effective masses [$m_\Gamma = 0.043m_0$ (Ref. 8), $m_L = (0.2\text{–}0.6)\,m_0$ (Refs. 3 and 9)] is the presence of two different donor impurity states whose parameters are determined by the masses m_Γ and m_L and by the dielectric constant $\varkappa$. Table II lists the values, calculated by the effective-mass method, which is valid at $a_B \gg a$ (a is the lattice parameter), of the Bohr radius (a_B) and of the impurity-state energy (ε_0) for the Γ and L extrema (k_0 is the distance between them).

The impurity states near the Γ band have a larger Bohr radius, $a_B^\Gamma \gg a_B^L$, and when the tellurium density N_d in the GaSb : Te is increased, the strong-doping condition $a_B{}^3 N_d \gg 1$ is first satisfied for these very states. As a result, the donor electrons are no longer connected with definite centers and can move freely in the crystal, filling the free states in the Γ band.

Under stong-doping conditions, the impurity level loses its individuality, and the presence of a random impurity potential manifests itself only in a distortion of the bottom of the Γ conduction band. The total density of the carriers in the system (Γ electrons + electrons at the impurity centers) is given by[1]

$$g_{i+\Gamma}(\varepsilon) = \frac{\sqrt{2}\, m_\Gamma^{3/2}\gamma^{1/2}}{\pi^2\hbar^3} G_0\left(\frac{\varepsilon}{\gamma}\right), \tag{4}$$

where

$$G_0(x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{x} e^{-y^2}(x-y)^{1/2}\, dy, \tag{5}$$

$$\gamma^2 = 4\pi e^4 N_d r_D/\varkappa^2. \tag{6}$$

In the last relation, r_D is the Debye screening radius[1]:

$$r_D = \left(\frac{\pi}{3}\right)^{1/6} \frac{a_B}{2} \frac{1}{(N_d a_B^3)^{1/6}}. \tag{7}$$

At energies $\varepsilon > \gamma$ (in our case, $\varepsilon \gtrsim 12$ meV) the func-

tion $g_{i\to\Gamma}$ is close in the positive region ($\varepsilon > 0$) to the state density in the undistorted Γ band, while in the negative region ($\varepsilon < 0$) the value of $g_{i\to\Gamma}$ decreases exponentially towards the interior of the forbidden band.

Thus, the strong-doping condition is satisfied for GaSb : Te in the entire investigated range of tellurium densities $2.0\times10^{17} \lesssim N_d \lesssim 2.2\times10^{18}$ cm^{-3} for the impurity states near the Γ band, and consequently there is only a small number of electrons outside this band, on the tail of the state density. On the other hand, for impurity states that are split-off from the L band we have $N_d^0 \approx 1.0\times10^{20}$ cm^{-3}, and the weak-doping condition $N_d \ll N_d^0$ is satisfied in the entire tellurium-density range.

In the case of weak doping, in the absence of correlation in the distribution of the impurities and at extremely low compensation, the following equation is valid for the state-density function $g_{iL}(\varepsilon)$ (Ref. 1)

$$g_{iL}(\varepsilon) = \frac{N_d}{\gamma\sqrt{\pi}} \exp\left\{-\frac{\varepsilon^2}{\gamma^2}\right\}. \qquad (8)$$

The energy ε is reckoned here from the center of impurity band, and the parameter γ characterizes its width. An increase of the degree of compensation leads to a slower decrease of the state density with increasing distance from the center of the impurity band, but even in this case $g_{iL}(\varepsilon)$ decreases more rapidly than in proportion to $1/\varepsilon^2$.

2. Structure of energy spectrum at $p = 0$ and baric rates of band displacements

The presence of the experimentally observed critical pressure p_{cr} corresponding to complete depletion of the Γ band (Fig. 3) and to a jumplike decrease of the Hall coefficient (Fig. 5) allows us to draw certain conclusions concerning the structure of the GaSb : Te spectrum at $p = 0$ and concerning the character of its restructuring under pressure.

The linear sections of the plots of the Fermi energy of the Γ electrons $\varepsilon_{F\Gamma}(p)$ point to a pressure-induced upward shift of the Γ band and to a transfer of the Γ electrons to another energy state with a substantially higher density $g(\varepsilon)$ and with a lower mobility. Since the Γ and L terms come closer together under pressure, this state could correspond to the L band (as was in fact assumed, e.g., by Filipchenko *et al.*[10]), were it not for the existence of a split-off impurity level,[11-13,6,7] located closer to the bottom of the Γ band and therefore becoming filled earlier (Fig. 1). In this situation, the critical pressure p_{cr} corresponds to the passage of the bottom of the Γ band through the impurity-band filling boundary.

The initial transfer of the Γ electrons under pressure to an impurity level[11-13,6,7] rather than to the L band[10] is confirmed also by the decrease of the carrier mobility at $p \gtrsim p_{cr}$ (Fig. 5). The ratio of the band mobilities $\mu_\Gamma/\mu_L \sim m_L/m_\Gamma$, even for the heaviest masses m_L cited in the literature,[9] does not exceed 14, whereas experiment yields a change of mobility by 150–300 times on going through the critical pressure p_{cr}. Consequently, after complete depletion of the Γ band, conduction in the impurity band sets in, with a mobility $\mu_i \ll \mu_\Gamma$. Practically the same mobility ratio ($\mu_\Gamma/\mu_i \approx 150$) was obtained earlier by Becker.[12]

The transfer of band electrons to an impurity level leads to deionization of the donors and by the same token to an increase in the mean free path of the electrons. In experiment, this process manifests itself in increase of the amplitudes A of the SdHO (Fig. 4). However, a contribution to the increase of the amplitude is made also by the pressure-induced decrease of the number of Landau levels in a fixed magnetic field, owing to the decrease of the extremal section, S_Γ, so that the resultant increase of A is quite large (Fig. 4).

We note that actually the decrease of the Γ-electron density n_Γ under pressure (Fig. 3) can cause in principle, besides donor-center deionization that leads to a lowering of the Dingle temperature T_D, also an increase of this temperature, since the decrease of n_Γ manifests itself also in an increase of the Debye screening radius r_D (7). However, by virtue of the weak dependence of r_D on n_Γ, the first tendency in the change of T_D prevails over the second, so that the temperature T_D decreases as $p \to p_{cr}$, and the amplitude A increases rapidly (Fig. 4).

In samples with tellurium density $N_d \lesssim 7\times10^{17}$ cm^{-3}, the Fermi level $\varepsilon_{F\Gamma}$ in the initial state at $p = 0$ is located below the impurity level, therefore the plots of $\varepsilon_{F\Gamma}(p)$ (Fig. 6) first show a plateau whose length decreases with increasing filling of the Γ band, and vanishes completely in single crystals with $N_d \gtrsim 7\times10^{17}$ cm^{-3} (see Fig. 6, samples No. 5 and No. 7). This means that in alloys with $N_d \gtrsim 7\times10^{17}$ cm^{-3} the Fermi level $\varepsilon_{F\Gamma}$ crosses the impurity band even at zero pressure.

The fact that the linear decrease of $\varepsilon_{F\Gamma}(p)$ has the same slope for all curves (Fig. 6) shows that the baric rate

$$\partial\varepsilon_{\Gamma-i}/\partial p \approx \partial\varepsilon_{F\Gamma}/\partial p$$

of approach of the Γ band to the impurity level is independent of the density N_d of the tellurium. Taking into account the small change of the mass of the state density m_L of the L band an of the dielectric constant $\varkappa$ at a pressure $p \lesssim 15$ kbar,[14] the energy gap ε_{i-L} between the impurity level and the bottom of the Γ band can be regarded as constant, i.e., $\partial\varepsilon_{i-L}/\partial p \approx 0$.

In this case the baric rate $\partial\varepsilon_{F\Gamma}/\partial p$ determined from the slope of the linear sections of the $\varepsilon_{F\Gamma}(p)$ curves (Fig. 6) makes it possible to determine also the rate of approach $\partial\varepsilon_{\Gamma L}/\partial p$ of the Γ and L bands:

$$\frac{\partial\varepsilon_{\Gamma L}}{\partial p} \approx \frac{\partial\varepsilon_{\Gamma-i}}{\partial p} + \frac{\partial\varepsilon_{i-L}}{\partial p} \approx \frac{\partial\varepsilon_{F\Gamma}}{\partial p}. \qquad (9)$$

The mean value of $\partial\varepsilon_{F\Gamma}/\partial p$ for all the investigated samples is (10.1 ± 0.2) meV/kbar in the tellurium-density interval $2\times10^{17} \lesssim N_d \lesssim 2.2\times10^{18}$ cm^{-3}. The obtained baric rate agrees with the estimates of Kosicki *et al.*[15]:

$$\partial\varepsilon_{\Gamma L}/\partial p\,(T = 300\ \text{K}) \approx 9.5\ \text{meV/kbar},$$

who investigated at room temperature the dependence of the resistivity on the pressure in GaSb:S, GaSb:Se, and GaSb:Te, as well as with the data of Ref. 5, which cites the value

$$\partial\varepsilon_{\Gamma L}/\partial p=(9.5-11)\ \text{meV/kbar}.$$

Extrapolation of the linear sections of the $\varepsilon_{F\Gamma}(p)$ curves to zero pressure makes it possible to determine, at $p=0$, the distance $\varepsilon_{\Gamma-i}$ from the bottom of the Γ band to the center of the impurity band. Adding $\varepsilon_{\Gamma-i}$ to the activation energy calculated at $p>p_{cr}$ from the slope of the lines $\ln\rho=f(1/T)$ corresponding to the thermal transfer of the electrons from the impurity level to the L band, we obtain the energy gap $\varepsilon_{\Gamma L}$ at $p=0$:

$$\varepsilon_{\Gamma L}=(93\pm4)\ \text{meV}.$$

This value does not depend on the density of the tellurium, in contrast to the data of Ref. 16, which points to a strong density dependence of the energy $\varepsilon_{\Gamma L}$. The obtained value of the gap $\varepsilon_{\Gamma L}$ is practically equal to that given by Noack,[4] who determined this parameter from luminescence measurements under uniaxial compression.

DETERMINATION OF THE STATE DENSITY IN THE IMPURITY BAND SPLIT-OFF FROM THE L EXTREMUM

1. Splitting of impurity band

In gallium antimonide, the L conduction band corresponds to four equivalent extrema; consequently, the associated impurity band, characterized by the state density $g_{iL}(\varepsilon)$, is also fourfold degenerate in the effective-mass method, and its total capacity is equal to

$$\int_{-\infty}^{\infty} g_{iL}(\varepsilon)\,d\varepsilon=4N_d. \tag{10}$$

This degeneracy should actually be lifted if account is taken of the small value of the Bohr radius $a_B^L\approx20$ Å. At distances of this order, the Coulomb potential can no longer approximate correctly the real potential of the donor center. This makes it necessary to consider an additional short-range potential whose matrix elements do not increase as rapidly at large distances in K space, and therefore connect wave functions belonging to different extrema of L_i $(i=1,\ldots,4)$. In final analysis this leads to a lifting of the degeneracy of the impurity states.[1]

By way of an analog of the impurity level split off from the L band in GaSb, we can consider the impurity level in germanium, in which the impurity state also lies near the L extremum. It is known[1] that the impurity ground state in germanium is split into a singlet (wave function of s-type) and a triplet (wave function of p-type), with the singlet state lower in energy.[1]

Consequently, in analogy with germanium, one can expect the lower impurity energy level in GaSb:Te to be likewise not degenerate:

$$\int_{-\infty}^{\infty} g_{iL}(\varepsilon)\,d\varepsilon=N_d. \tag{11}$$

Since the number of Γ electrons does not exceed the density $n_\Gamma\lesssim N_d$ of the introduced tellurium (undoped GaSb single crystals are always of p-type during their growth), the previously observed[6] filling of the L band as a result of the transfer effect is possible when account is taken of (11) only if the state-density function of the singlet level overlaps strongly enough the L extrema. If there is no overlap, then it is impossible to fill the L band either by doping GaSb with donors, or by inversion of the Γ and L extrema under pressure, since in either case the filling boundary is located in such a case in the impurity band.

2. Width of impurity singlet band

When determing the form of the function $g_{iL}(\varepsilon)$ (11), account must be taken of the broadening of the hydrogenlike impurity level split off from the L extremum, both on account of transition of electrons from the level into the continuous spectrum (into the Γ band) and on account of the overlap of the wave functions of the donor centers.

Bassani *et al.*[17] have shown that for the first of these mechanisms the width γ_Γ of the impurity level is proportional to the state density in the Γ band and to the square of the matrix element $u(k)$:

$$\gamma_\Gamma=\pi|u(k)|^2 g_\Gamma(\varepsilon), \tag{12}$$

and $u(k)$ can be estimated as follows:

$$u(k)\approx\frac{4\pi e^2}{\varkappa k_0^2}4\pi\int_0^\infty\frac{2}{(2\pi)^3}\Phi_0(k)k^2dk=8\pi^{1/2}\frac{e^2}{\varkappa k_0^2 a_B^3}(N_d a_B^3)^{1/2}. \tag{13}$$

Here $\Phi_0(k)$ is the wave function in k space, normalized to the volume $V_0=1/N_d$, for an isolated donor center[1]:

$$\Phi_0(k)=\frac{8\pi^{1/2}}{V_0^{1/2}}\frac{a_B^{3/2}}{((ka_B)^2+1)^2}. \tag{14}$$

In gallium antimonide, this equation can be used to describe impurity states split-off from the L band, since in the investigated density range the mean distance between impurities is $\bar r\approx N_d^{-1/3}\approx10^{-5}-10^{-6}$ cm and satisfies the condition $\bar r\gg a_B^L>a$. Substituting $a_B=a_B^L$, $\varkappa$, and k_0 from Table III in (13), we find that

$$u(k)\approx1.8N_d^{1/2}(a_B^L)^{3/2}\ \text{meV}. \tag{15}$$

In the approximation with a quadratic isotropic Γ-electron dispersion law

$$g_\Gamma(\varepsilon)=\frac{3}{2}\frac{n_\Gamma(\varepsilon)}{N_d}\frac{1}{\varepsilon} \tag{16}$$

TABLE III.

Sample № 1			Sample № 5		
p, kbar	$\varepsilon_{F\Gamma}^{exp}$, meV	$\varepsilon_{F\Gamma}^{theor}$, meV	p, kbar	$\varepsilon_{F\Gamma}^{exp}$, meV	$\varepsilon_{F\Gamma}^{theor}$, meV
0	26.36	26.35	0	84.5	84.6
1.5	25.3	26.36	0.9	80.9	76.92
3.8	26.8	26.35	2.2	66.82	65.65
5.3	23.83	25.84	4.7	48.55	42.74
7.15	15.78	14.19	6.55	24.18	25.93
7.3	10.14	10.36	7.4	17.5	18.52
7.85	8.7	7.37	8.2	10.9	10.85
8	6.43	6 83	9.2	1.09	1.18
$\varepsilon_{\Gamma L}=93$ meV, $\alpha=10.1$ meV/kbar $N_0=1.95\cdot10^{17}$ cm^{-3}, $N_d=2\cdot10^{17}$ cm^{-3}, $\varepsilon_{i-L}=9$ meV, $\gamma=5$ meV			$\varepsilon_{\Gamma L}=93$ meV, $\alpha=10.1$ meV/kbar. $N_0=1.2\cdot10^{18}$ cm^{-3}, $N_d=1.2\cdot10^{18}$ cm^{-3}, $\varepsilon_{i-L}=4$meV, $\gamma=3.75$ meV		

we obtain

$$\gamma_\Gamma \leqslant 1.1 N_d (a_B^L)^3 \text{ meV}. \quad (17)$$

Putting $N_d \sim 5\times10^{18}$ cm^{-3} (which is even more than the maximum investigated density N_d), we obtain the maximum broadening γ_Γ due to the transitions to the continuous spectrum

$$\gamma_\Gamma \leqslant 5\cdot10^{-2} \text{ meV}. \quad (18)$$

A similar result was obtained in the estimate of the width of the resonance level in CdTe by means of a simplified model,[18] where it was shown that the width γ is smaller by two orders of magnitude than the activation energy ε_0. (An estimate of γ_Γ for GaSb in this model yields $\gamma_\Gamma \lesssim 0.2$ meV.) We note that under pressure γ_Γ should decrease even more, since the state density in the Γ band decreases because of its upward shift relative to the impurity level.

We estimate now the broadening γ_i due to the interaction of the nearest impurity atoms. According to Mott[19]

$$\gamma_i \approx 2zI. \quad (19)$$

Here z is the coordination number and I is the overlap integral. For wave functions of the type (14) this integral is given by[19]

$$I=\left[\frac{3}{2}\left(1+\frac{\bar r}{a_B}\right)+\frac{1}{6}\left(\frac{\bar r}{a_B}\right)^2\right]\frac{e^2}{\varkappa a_B}\exp\left\{-\frac{\bar r}{a_B}\right\}. \quad (20)$$

In particular, at $a_B = a_B^L$, $N_d \approx 2\times10^{17}$ cm^{-3}, and $z=4$, we have $\gamma_{iL} \approx 5$ meV, which exceeds by two orders the parameter γ_Γ corresponding to transitions from the level to the continuous spectrum.

Under hydrostatic compression, the distance $\bar r$ between the impurity centers decreases, i.e., the overlap integral and the width γ_{iL} proportional to it should increase. In the interval $p \lesssim 15$ kbar, however, the change of I due to this mechanism is small enough to be disregarded.

Thus, in all the investigated samples, in the interval $2\times10^{17} \lesssim N_d \lesssim 2.2\times10^{18}$ cm^{-3}, the broadening of the impurity level split-off from the L extremum and due to transitions into the continuous spectrum is negligibly small compared with the broadening due to the interaction of the impurity atoms. Therefore an approximation of the state density $g_{iL}(\varepsilon)$ of the impurity band by a Lorentz function[6,7]

$$g(\varepsilon)=\frac{N_d}{\pi\gamma}\frac{1}{(\varepsilon/\gamma)^2+1}, \quad (21)$$

is generally speaking incorrect.

3. Determination of the function $g_{iL}(\varepsilon)$

The pressure-induced upward shift of the Γ extremum leads to a transfer of the Γ electrons to the impurity band. By determining from oscillation measurements the number of transferred electrons $N_d - N_a - n_\Gamma$ and the position of the Fermi level $\varepsilon_{F\Gamma}(p)$ relative to the center of the impurity band ($\varepsilon'=0$, see Fig. 1)

$$\varepsilon' \equiv \varepsilon_{F\Gamma}(p) - [\varepsilon_{\Gamma L}(p) - \varepsilon_{i-L}]$$
$$= \varepsilon_{F\Gamma}(p) - \left[\varepsilon_{\Gamma L}(0) - \frac{\partial \varepsilon_{\Gamma L}}{\partial p} p - \varepsilon_{i-L}\right], \quad (22)$$

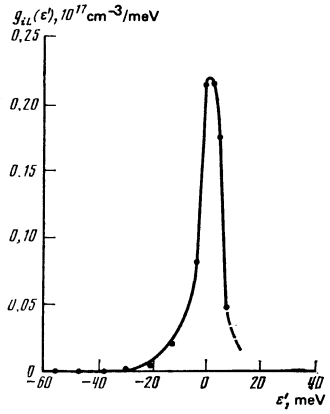

FIG. 7. Plot of state density in the impurity band (sample 2).

we can reconstruct the variation of the state density $g_{iL}(\varepsilon')$, inasmuch as in the equation

$$N_d - N_a - n_\Gamma = n_i(\varepsilon') = \int_{-\infty}^{\varepsilon'} g_{iL}(\varepsilon)\,d\varepsilon \quad (23)$$

we know (accurate to $N_a = \text{const}$) the left-hand side and the integration limit ε', which is determined from (22) using the previously known parameters $\varepsilon_{F\Gamma}(p)$, $\varepsilon_{\Gamma L}(0)$, $\partial\varepsilon_{\Gamma L}/\partial p$, and ε_{i-L}.

Thus, by plotting first the density $n_i(\varepsilon')$ against ε', we can obtain the sought function $g_{iL}(\varepsilon')$ (Fig. 7) by differentiating the dependence of n_i on ε':

$$g_{iL}(\varepsilon') = \partial n_i(\varepsilon')/\partial\varepsilon'. \quad (24)$$

The most suitable for the determination of the function $g_{iL}(\varepsilon)$ are GaSb : Te samples with density $N_d \approx (2-3)\times10^{17}$ cm^{-3}, although their Fermi level at $p=0$ is relatively far from the impurity level (Fig. 1). Under pressure, therefore, it is possible to fill gradually the completely empty impurity band, and in the ideal case $n_a = 0$, the total capacity of the N_d level (11) is exactly equal to the initial number $n_\Gamma(0) = N_d$ of Γ electrons, owing to the lifting of the degeneracy. That is to say, the impurity band can be filled to the top. In this case

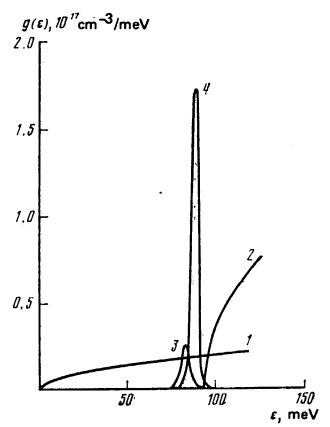

FIG. 8. State density in the impurity band of GaSb:Te: 1) Γ band, 2) L band (for one extremum), 3) impurity band, sample 1, 4) impurity band, sample 5.

one can determine the entire function $g_{iL}(\varepsilon)$, including the tails of the state density. In samples with $N_d \gtrsim 10^{18}$ cm^{-3}, there is no such possibility, for even at $p=0$ the impurity band itself is partially filled.

Figure 7 shows the function $g_{iL}(\varepsilon')$ for a GaSb : Te crystal with $N_d = 2.0\times10^{17}$ cm^{-3}. The presence of an extended plateau on the $n_\Gamma(p)$ dependence (Fig. 3) points to a rapid damping of $g_{iL}(\varepsilon')$ with increasing distance from the center of the impurity band. As $\varepsilon' \to 0$, the function $g_{iL}(\varepsilon')$ increases rapidly, and has a bell-shaped maximum near $\varepsilon' \approx 0$. The obtained $g_{iL}(\varepsilon')$ curve is quite close in shape (Fig. 7) to the exponential dependence (8).

Unfortunately, in the described method of directly determining the state density in the impurity band it is difficult to obtain a very detailed pressure dependence of the baric functions $\varepsilon_{F\Gamma}(p)$, owing to the use of high-pressure chambers with kerosene–oil mixture.[20] In the calculations for the remaining samples we therefore used the function (8) for the state density in the impurity band without additional modification.

Knowing the form of the function $g_{iL}(\varepsilon)$ and solving with a computer the electroneutrality equation with respect to $\varepsilon_{F\Gamma}$,

$$N_d = N_a + n_\Gamma(p) + n_i(p) + n_L(p), \qquad (25)$$

we can determine how adequately the computed function $\varepsilon_{F\Gamma}(p)$ describes the experimental curves at the chosen form (8) of the state-density function. The electron densities in the Γ and L bands were determined in the usual manner in terms of the corresponding state-density masses, and Eq. (23) was used to determine $n_i(p)$.

The computer calculations have shown that the theoretical curve is highly sensitive to the values of the parameters γ and $N_d - N_a = N_0$, and varies very little when m_L is in the range $(0.3-0.6)m_0$. By varying the parameters in (25) we succeeded in describing well all the experimental baric dependences of the Fermi energy (Fig. 6).

The characteristic parameters of the samples together with the theoretical and experimental $\varepsilon_{F\Gamma}(p)$ dependences are given in Table III (see also the caption of Fig. 6). These parameters confirm above all that the impurity band is not degenerate and that its capacity is equal to the number N_d of donors. The width of the impurity band γ depends both on the density N_d and on the degree of compensation, and lies in the interval 3–14 meV, in good agreement with the theoretical estimates ($\gamma_i \sim 5$ meV) based on the overlap integral.

The state density in the conduction band of GaSb : Te, determined using the parameters obtained in the present paper and listed in Table III, is shown in Fig. 8.

We note finally that the attempt to describe the experimental $\varepsilon_{F\Gamma}(p)$ relations for samples with $N_d \approx (2-3)\times10^{17}$ cm^{-3} by solving Eq. (25) with a Lorentz function (21) were unsuccessful in view of the impossibility of obtaining in this case extended plateaus on the $\varepsilon_{F\Gamma}^{theor}(p)$ curve (Figs. 3 and 6), although a satisfactory agreement between $\varepsilon_{F\Gamma}^{theor}(p)$ and $\varepsilon_{F\Gamma}^{exp}(p)$ was obtained earlier[6] for samples with $N_d \approx 10^{18}$ cm^{-3}. The last result is the consequence of the fact that at $N_d \sim 10^{18}$ cm^{-3} the section with a weak variation of $\varepsilon_{F\Gamma}$ is not realized, and the shape of the $\varepsilon_{F\Gamma}^{theor}(p)$ curve is not very sensitive to the shape of the state-density tail.

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