Ionization energy of magnetodonors in pure bulk GaAs

B. Jouault and A. Raymond
Groupe d'Étude des Semiconducteurs, UMR-CNRS 5650, Université Montpellier II, 34095 Montpellier Cédex, France

W. Zawadzki
Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland
(Received 18 January 2002; published 19 June 2002)

Binding energy of donors in high quality epitaxial GaAs is investigated as a function of the magnetic field between 0 and 12 T. Transverse magnetoresistance and the Hall effect are used as experimental tools. The samples are characterized using temperature dependence of free electron density and mobility, taking consistently into account the Hall scattering factor and the effective conduction depth of the structure. Our analysis of the data at the freeze-out regime of higher magnetic fields allows for the hopping conductivity over donor states. The determined magnetodonor energies are about 1 meV lower than the theoretical ones, which represents a very large improvement in comparison with previous studies.

DOI: 10.1103/PhysRevB.65.245210 PACS number(s): 71.55.Eq, 72.20.My, 73.61.Ey

I. INTRODUCTION

Gallium arsenide has been intensively studied for years because of its interesting fundamental properties, important applications in electronics and optoelectronics, and because it serves as a basis for GaAs/GaAlAs heterostructures and superlattices. Many properties of GaAs are related to impurities, their activation energies, statistics, mutual interactions at higher densities, etc. It has been recognized for a long time that an external magnetic field provides a very effective tool for the understanding of various semiconductor properties and, in particular, of the impurity behavior. More specifically, since the pioneering experiments of Sladek and coworkers[1] and the theoretical work of Yafet, Keyes, and Adams[2] it is known that the magnetic field increases the binding energy of donors. As a result, at low temperatures the electrons can be ''frozen out'' from the conduction band to the donors as the magnetic field B increases. The magnetic freeze-out is caused by the decrease of the magnetic (cyclotron) orbit with increasing B. This brings the electron closer to the donor atom, which makes the Coulomb interaction stronger and enhances the binding energy. A characteristic parameter for the hydrogenic donor in a magnetic field is $\gamma = \hbar\omega_c/2\mathcal{R}$, where $\omega_c = eB/m^*$ is the cyclotron frequency and $\mathcal{R}$ is the effective Rydberg. The latter gives ideally the donor binding energy at $B=0$. In narrow gap semiconductors the parameter γ can reach values of 10^2 at accessible magnetic fields because of the small effective masses and small values of $\mathcal{R}^*$. An interesting property of the magnetodonor problem at high γ values is that it imitates the hydrogen atom in gigantic magnetic fields, not achievable in terrestrial conditions. And so the value of $\gamma=100$ corresponds to the H atom in the field of $B=10^7$ T, available only in the vicinity of neutron stars. This makes the magnetodonor problem of importance not only for the semiconductor physics, but also for the atomic physics and astrophysics (see Ref. 3). GaAs is a medium gap semiconductor, for which the value of $\gamma\approx 3$ can be reached at accessible magnetic fields. The donor activation energy and its behavior in a magnetic field also serves as an indicator of material quality and a degree of impurity compensation. At higher dopings and higher compensations the donor wave functions overlap, which results in a broadening of the donor levels and a decrease of the binding energy (see Ref. 4). At a critical level of doping the activation energy vanishes and the semiconductor undergoes a nonmetal-metal transition. Also this behavior can be strongly influenced by an external magnetic field, as shown by Robert *et al.*[5] for bulk InSb and by Zawadzki *et al.*[6] for the two-dimensional GaAs/GaAlAs system.

Among numerous studies of GaAs there exists to our knowledge only one paper dealing with the binding energy of magnetodonors in this material by means of transport phenomena (see Ref. 7). The activation energies measured in Ref. 7 represented only a fraction of the theoretical values, indicating that the GaAs material was of poor quality. For this reason we undertake here another study of magnetodonor activation energy in GaAs using the material of much higher quality. Also the analysis of the transport data leading to the determination of the binding energy is considerably improved. It is known by now that in order to measure the binding energy with a sufficient precision it is not enough to determine the slope of the free electron density $n(T)$ versus $1/T$, as was done in Ref. 7. Instead, one needs to use the complete electron statistics, taking into account the occupation of both donors and acceptors. In addition, a precision of sample characterization is increased if one describes not only the free electron density $n(T)$, but also the mobility $\overline{\mu}(T)$.[8–10] A serious problem in such an analysis is the fact that using the transport data, i.e., the electric conductivity and the Hall effect, one measures not the real electron density $n(T)$ and the mobility $\overline{\mu}(T)$ but the Hall density $n_H(T)$ and the Hall mobility $\overline{\mu}_H(T)$. A correct sample characterization should take this into account. In our procedure we go beyond the usual approximation that neglects the above differences.[8–10] Another difficulty encountered for modern thin samples grown by epitaxial techniques is the value of the active depth of the sample conducting the current, as opposed to inactive surface and interface depletion layers.

This active depth is not known *a priori*. We deal with this problem as well. At higher magnetic fields, when more and more electrons are frozen out into donor levels, one should allow for a possibility of hopping conduction over the donor states. In our analysis of the experimental data we take into account this effect.

The paper is organized in the following way. In Sec. II we provide a theoretical background for our study. In Sec. III we describe characterization of GaAs samples at low magnetic fields. In Sec. IV we present high field data and determine the donor energies as functions of a magnetic field. Section V contains a discussion of the experimental energies and their comparison with the theory. The paper is concluded by a summary.

II. THEORETICAL BACKGROUND

In order to determine the donor binding energy E_d as a function of magnetic field one has to know the density of donors N_d and that of acceptors N_a in the sample. These quantities can be determined by fitting the temperature dependence of the free electron density $n(T)$ or the electron mobility $\overline{\mu}(T)$, or both. It has been the experience of other workers that fitting the electron density alone is not sufficiently precise,[9] so that one needs a description of mobility as well, especially at lower temperatures where the impurities provide the main scattering mode.

The difficulty in such a procedure is that the measured quantities are not the real density $n(T)$ and the Ohmic mobility $\overline{\mu}$, but the Hall density $n_H(T)$ and the Hall mobility $\overline{\mu}_H$ involving the Hall scattering factor r_H. It has been a common practice to disregard this difficulty by putting $r_H(T)=1$ at all temperatures,[8–10] but we intend to go beyond this simplification. Another problem concerning the sample characterization is related to the effective thickness of the conducting channel in the sample, which directly affects the Hall measurement of $n_H(T)$ since it determines the electron current density. The temperature dependence of the thickness of surface and interface depletion layers for thin samples can lead to a misinterpretation of the transport data (see paper by Lepkowski *et al.*[11] and the review of Look[12]).

In our procedure of sample characterization at low magnetic fields we treat the unknown quantities N_a, N_d, E_d as fitting parameters. Knowing the other material parameters related to electron scattering we compute the Ohmic mobility $\overline{\mu}$ and the Hall factor r_H, which allows us to calculate n_H and $\overline{\mu}_H$. Next we optimize by iteration the values of N_d, N_a, and E_d, by getting the best fit to the measured temperature dependences of $n_H(T)$ and $\overline{\mu}_H(T)$. An additional condition of such an optimization is to obtain a correct value of the sample depth by using known dependences of surface and interface depletion layers on the electron density in GaAs.

The Hall coefficient R_H and the transverse magnetoresistance ρ_{xx} in the classical transport regime are described by the standard relations

$$BR_H=-\frac{\overline{\sigma}_{xy}}{\overline{\sigma}_{xx}^2+\overline{\sigma}_{xy}^2}, \tag{1}$$

$$\rho_{xx}=\frac{\overline{\sigma}_{xx}}{\overline{\sigma}_{xx}^2+\overline{\sigma}_{xy}^2}, \tag{2}$$

where the conductivities are

$$\overline{\sigma}_{xx}=\frac{en}{\langle 1\rangle}\left\langle\frac{\mu}{1+\mu^2B^2}\right\rangle, \tag{3}$$

$$\overline{\sigma}_{xy}=\frac{enB}{\langle 1\rangle}\left\langle\frac{\mu^2}{1+\mu^2B^2}\right\rangle. \tag{4}$$

Here $\mu=e\tau/m^*$ is the mobility, τ is the relaxation time, m^* is the electron effective mass, and B is the magnetic-field intensity. The electron density is

$$n=\frac{1}{3\pi^2}\left(\frac{2m^*k_0T}{\hbar^2}\right)^{3/2}\langle 1\rangle. \tag{5}$$

In the above expressions we use the notation of Zawadzki,[13] simplified for the case of parabolic bands. Thus, in general,

$$\langle A\rangle=\int_0^\infty\left(-\frac{\partial f_0}{\partial z}\right)A(z)z^{3/2}dz \tag{6}$$

describes the integral of the quantity $A(z)$ over the band. Here $f_0(z,\eta)$ is the Fermi-Dirac distribution, $z=\epsilon/k_0T$ and $\eta=\epsilon_F/k_0T$ are the reduced energy and the reduced Fermi energy, respectively. The above average quantities are defined, in general, as

$$\overline{A}=\frac{\langle A\rangle}{\langle 1\rangle}. \tag{7}$$

It can be shown, integrating by parts, that $\langle 1\rangle=(3/2)F_{1/2}$, where $F_{1/2}$ is the Fermi integral. Using the above equations one obtains for $B=0$ the conductivity $\sigma=ne\overline{\mu}$. In the limit of weak magnetic fields ($\mu^2B^2\ll 1$) one has $1/R_He=n/r_H=n_H$ and $R_H/\rho_{xx}=\overline{\mu}\cdot r_H=\overline{\mu}_H$, where the Hall scattering factor is

$$r_H=\frac{\overline{\mu}^2}{\overline{\mu^2}}.$$

As mentioned above, a comparison with the measured values of electron density cannot be directly carried out since experimentally one measures $n_H=1/eR_H$. Thus in order to make the comparison one needs to calculate the mobility and its energy dependence.

In the analysis of the free electron density we use the charge balance equation

$$n+N_a=N_i, \tag{8}$$

where N_i is the density of ionized donors. This density is

$$N_i=N_d\left(1-\frac{1}{1+\frac{1}{2}\exp(-\eta-E_d/k_0T)}\right), \tag{9}$$

where N_d and E_d are the donor density and the donor activation energy mentioned above. Combining Eqs. (5), (8), and (9) one can solve for the Fermi energy $\epsilon_F(T)$ and the free electron density $n(T)$, in which N_a, N_d, and E_d are treated as fitting parameters.

Our analysis of the electron mobility in GaAs follows essentially the procedure of Wolfe, Stillman, and Lindley[8] with some modifications. The ionized impurity (ii) scattering mode is described by the Brooks-Herring formula derived for the screened Coulomb potential. The mobility $\overline{\mu}_{\rm ii}$ for this mode is determined by the densities of ionized impurities N_d, N_a, and the dielectric constant $\kappa_0=12.86$. At low temperatures the electrons are frozen from the conduction band to the donors and the latter become neutral. We describe the neutral impurity (ni) scattering using the formulation of Meyer and Bartoli.[14] At low temperatures, their formula gives a somewhat lower value of the mobility $\overline{\mu}_{\rm ni}$ than that obtained from the early formulation of Erginsoy.[15] The scattering by acoustic phonons (ac) is described within the standard approach of the deformation potential C. The value of the latter is not very well known even for GaAs and it is usually treated as an adjustable parameter, sensitive to the value of the total mobility at its maximum (see below). The value of the longitudinal elastic constant $c_l=(3c_{11}+2c_{12}+4c_{44})/5$ is calculated using $c_{11}=1.221\times10^{11}$ J m^{-3}, $c_{12}=0.566\times10^{11}$ J m^{-3}, $c_{44}=0.599\times10^{11}$ J m^{-3}. The piezoacoustic scattering (pz) is described according to the formulation of Meyer and Polder,[16] using the longitudinal elastic constant given above, the transverse elastic constant $c_t=(c_{11}-c_{12}+3c_{44})/5$, and the piezoelectric constant $h_{14}=0.16$ C/m^2. The scattering of electrons due to the polar interaction with optic phonons (pop) presents some difficulties, since it is basically nonelastic and it may not be described by the relaxation time approximation. In our analysis, we follow Ref. 14 using the Ehrenreich variational approach, which defines an effective temperature-dependent index r. The latter is given in Ref. 17. The polarity is determined by the static dielectric constant given above and the high-frequency dielectric constant $\kappa_\infty=10.9$. The energy of the optical phonon is $\hbar\omega_{op}=k_0\theta$ and we take the Debye temperature $\theta=423$ K. We include the polar scattering for the completeness of the description, but this mode is important at higher temperatures, whereas we are mainly concerned with low temperatures at which the mobility is controlled by impurities. The total scattering rate is given by the Mathiessen relation $1/\mu(\epsilon)=\Sigma_i 1/\mu_i(\epsilon)$. The average mobility for a given temperature is calculated using Eqs (6) and (7).

III. SAMPLE CHARACTERISTICS

We investigated two GaAs samples. Sample S_1 was grown by the liquid phase epitaxy on a semi-insulating GaAs substrate and it had the metallurgical thickness of 15 μm. Sample S_2 was grown by the molecular-beam epitaxy and it had the metallurgical thickness of 10 μm. Both samples had residual donors of unknown origin. Each sample had four Ohmic contacts made of indium. The measurements were made in the range of 4–300 K in magnetic fields up to 12 T.

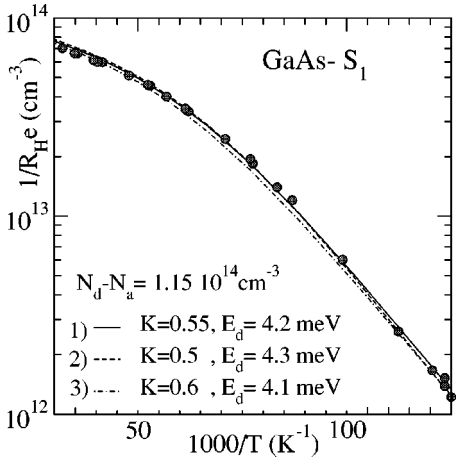

FIG. 1. Hall free electron density in GaAs sample S_1 versus $1000/T$. Full circles represent experimental values measured at the magnetic field $B=0.0097$ T. Solid, dashed, and dashed-dotted lines show the results of theoretical calculation for three impurity parameter sets.

The temperature was carefully measured by two calibrated carbon-glass resistors, which allowed us to have the accuracy of 2% in the whole range.

In order to get initial approximate values of N_d, N_a, and E_d we begin with the so-called exhaustion region of temperatures $E_d<k_0T\ll\epsilon_g$, where ϵ_g is the energy gap. In this region the free electron density is $n=N_d-N_a$, and it is not sensitive to the compensation ratio $K=N_a/N_d$. Thus, assuming in the first approximation $n\approx n_H=1/eR_H$, we determine N_d-N_a and the subsequent fitting of the temperature dependence $n_H(T)$ is reduced to a two-parameter procedure of adjusting K and E_d. The same approximation $n\approx n_H$ allows us to determine the approximate active depth $d_{\rm eff}$ of the sample. The measured Hall resistance R_H is proportional to the inverse of the current density j: $R_H\propto 1/j\propto d_{\rm eff}/I$, where I is the total current. Thus the relation between the measured electron density $n\propto 1/R_H$ and $d_{\rm eff}$ is represented by an hyperbola. On the other hand, as shown by Chandra *et al.*[18] (see also Ref. 12, p. 45–48), there exists a monotonic relation between n and the total depletion layer $d_{\rm depl}$ (a sum of surface and interface depletion layers) for GaAs. Knowing the metallurgical depth d we obtain a second relation between n and $d_{\rm eff}=d-d_{\rm depl}$ for our sample. The hyperbola $n(d_{\rm eff})$ and the latter dependence $n(d_{\rm eff})$ give the values of $d_{\rm eff}$ and n, which are subsequently refined when n_H is no more exactly identified with n.

Figure 1 shows the experimental values of the Hall density $1/eR_H$ measured as a function of temperature at the low magnetic field $B=0.0097$ T. The different curves show three theoretical fits based on Eqs. (1) and (2), accounting for the Hall scattering factor. They are characterized by different adjusted impurity sets of N_d, N_a, E_d. It can be seen that the fit to the electron density alone is not sufficiently precise to decide which of the three sets is the best.

In Fig. 2 we show the experimental Hall mobility $\overline{\mu}_H=\overline{\mu}\cdot r_H$, measured in the same experiment, together with the theoretical Hall mobility calculated using the material pa-

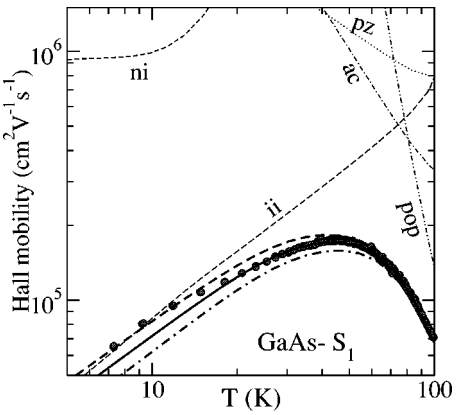

FIG. 2. Hall electron mobility in GaAs sample S_1 versus temperature. Full circles represent experimental values measured at the magnetic field $B=0.0097$ T. Thick solid line shows the total theoretical Hall mobility calculated for the first set of impurity parameters indicated in Fig. 1, thin lines indicate theoretical mobilities for separate scattering modes. The thick dashed line and the dashed-dotted line show the theoretical total Hall mobilities calculated for the second and third parameter sets, respectively.

rameters given above and the first set of impurity parameters indicated in Fig. 1. The deformation potential for the acoustic scattering is adjusted to get correctly the maximum of mobility at $T=48$ K, and we obtain $C=11.5$ eV. The values of C for GaAs, determined by various procedures, range from 7 eV,[8] through 9.3 eV,[19] and 13.5 eV (Ref. 20) to 15.7 eV,[21] to mention just a few papers. The fit to electron mobility in very pure GaAs samples requires C to be between 9 and 10 eV,[22] in reasonable agreement with our estimation. Thin lines show contributions of various modes to the total mobility. The dashed and the dashed-pointed thick curves show the total mobilities calculated using the other two sets of impurity parameters indicated in Fig. 1. It can be seen that neither of the three sets gives a perfect fit to the experimental mobility, the experimental slope at low temperatures being lower than the theoretical ones. The same discrepancy was observed for InP by Anderson and Apsley.[9] We finally take the first set of impurity parameters for the sample S_1.

The same procedure of the sample characterization was carried out for the sample S_2. We obtained similar descriptions of n_H and $\overline{\mu}_H$ as those shown in Figs 1 and 2, the theoretical mobility at high temperatures being slightly higher than the experimental one. This did not affect the precision of the determined impurity parameters, as they were adjusted by the fit at low temperatures. The determined parameters characterizing our two samples are quoted in Table I.

IV. HIGH FIELD DATA

Once the impurity parameters N_d and N_a have been established, one can determine the donor activation energy E_d at higher magnetic fields by measuring and fitting the temperature dependence of the free electron density $n(T)$. This procedure is based on the assumption that at higher fields (for which $B^2\mu^2 \gg 1$) the electric conductivity and the Hall

TABLE I. Parameters of the two unintentionally doped GaAs samples.

Parameter	S_1	S_2
Thickness (μm)	16	10
$\overline{\mu}$ at 77 K ($\mathrm{cm^2\,V^{-1}\,s^{-1}}$)	120 000	94000
$\overline{\mu}_{\mathrm{peak}}$ ($\mathrm{cm^2\,V^{-1}\,s^{-1}}$)	175 000	135 000
N_d-N_a (10^{14} $\mathrm{cm^{-3}}$)	1.15	2.7
$K=N_a/N_d$	0.55	0.40
E_d at $B=0$ T	4.2 meV	4.3 meV
N_d (10^{14} $\mathrm{cm^{-3}}$)	2.55	4.50

effect measure directly n. This point is discussed below.

If the condition $B^2\mu^2=\omega_c^2\tau^2 \gg 1$ is satisfied, the band is quantized into the well-defined Landau level (LL) energies: $\epsilon_{\lambda,k_z}=\hbar\omega_c(\lambda+1/2)+\hbar^2k_z^2/2m^*$. The electron density can be calculated summing over LL's and integrating over k_z. If the Fermi energy ϵ_F is significantly lower than the lowest LL energy $\epsilon_0=\hbar\omega_c/2$ (the freeze-out regime), one has

$$\frac{\hbar\omega_c}{2k_0T}-\eta \gg 1, \tag{10}$$

and the free electron density may be written in the form

$$n=N_c\sum_{\lambda=0}^{\infty}\exp\left(\frac{\epsilon_F-\hbar\omega_c(\lambda+1/2)}{k_0T}\right), \tag{11}$$

where $N_c=eB\sqrt{2\pi m^*k_0T}/(2\pi^2\hbar^2)$. The spin degeneracy of LL's is assumed since in GaAs the electron spin g^* factor is very small. In the presence of magnetic field the density of ionized donors is

$$N_i=N_d\frac{1}{1+2\exp\dfrac{\epsilon_F+E_d-\frac{1}{2}\hbar\omega_c}{k_0T}}. \tag{12}$$

The donor states bound to higher LL's may be neglected because of the inequality (10). For given N_d and N_a the values of η and n can be calculated using Eqs (8), (11), and (12). We have checked *a posteriori* the validity of condition (10). For our range of temperatures ($5\ \mathrm{K}<T<200$ K) and magnetic fields ($1\ \mathrm{T}\leqslant B\leqslant 12$ T) there is $\hbar\omega_c/2k_0T-\eta \geqslant 5$, so that the inequality (10) is satisfied.

The theoretical dependence $n(T)$ should be compared with the experimental one, which poses a problem of how to measure the free electron density at high magnetic fields. The standard answer is $n=1/R_He$. In fact, it can be verified using Eqs. (1) and (2) that in the limit $B^2\mu^2 \gg 1$ the quantity $1/R_He$ approaches n and the scattering factor r_H is not involved. The limit $B^2\mu^2 \gg 1$ means that $\overline{\sigma}_{xx} \ll \overline{\sigma}_{xy}$, which is true when $\overline{\sigma}_{xx}$ and $\overline{\sigma}_{xy}$ are given by Eqs. (3) and (4), respectively, *i.e.*, if the conduction occurs only in the band. In practice, however, as the electrons are being frozen out from the band to the donor states, the latter can conduct by the hopping

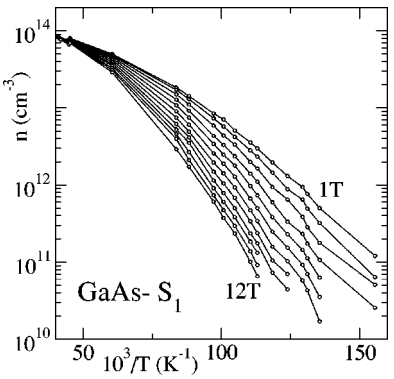

FIG. 3. Experimental free electron density in GaAs sample S_1 versus $1000/T$ in the freeze-out regime for various magnetic fields (from $B=1$ T to $B=12$ T in steps of 1 T). The lines between the points are drawn to guide the eye.

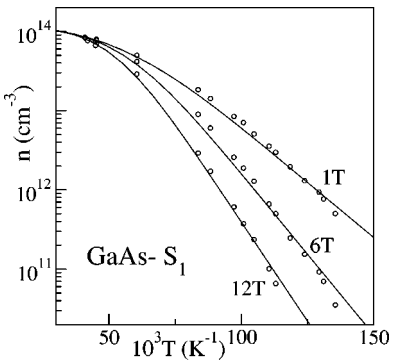

FIG. 4. Free electron density in GaAs sample S_1 in the freeze-out regime versus $1000/T$ for three magnetic fields. The empty circles are experimental points (the same as in Fig. 3), the solid lines represent theoretical fits treating the magnetodonor binding energy $E_d(B)$ as an adjustable parameter.

mechanism. As a result, $\overline{\sigma}_{xx}$ is not strongly suppressed by magnetic field and one may not neglect $\overline{\sigma}_{xx}$ compared to $\overline{\sigma}_{xy}$. In this situation, as proposed by Mansfield[23] for the case of InSb, one can write

$$\overline{\sigma}_{xx}=\overline{\sigma}^b_{xx}+\overline{\sigma}^i_{xx},$$

$$\overline{\sigma}_{xy}=\overline{\sigma}^b_{xy}, \tag{13}$$

where $\overline{\sigma}^b_{xx}$ and $\overline{\sigma}^b_{xy}$ are the band contributions to the conductivity tensor, given, respectively, by Eqs. (3) and (4), while $\overline{\sigma}^i_{xx}$ is the impurity contribution to the conductivity. The component $\overline{\sigma}_{xy}$ is written down without the impurity contribution since the hopping mechanism of conductivity is known to exhibit very small Hall effect. Using Eqs. (1) and (2) one obtains quite generally

$$\overline{\sigma}_{xy}=\frac{BR_H}{\rho^2_{xx}+B^2R^2_H}. \tag{14}$$

Let us now consider the quantity

$$\frac{B^2R_H}{e(\rho^2_{xx}+B^2R^2_H)}=\frac{B}{e}\overline{\sigma}_{xy}=\frac{n}{\langle 1\rangle}\left\langle\frac{B^2\mu^2}{1+B^2\mu^2}\right\rangle, \tag{15}$$

where Eq. (4) has been used. The expression on the right-hand side approaches n in the limit $B^2\mu^2\gg 1$. In the standard procedure one neglects ρ_{xx} compared to $B^2R^2_H$, which we do not do because of the above given reasons. In fact, the experiment shows that at low temperatures ρ_{xx} is not negligible compared to BR_H. Thus, we employ the expression

$$n=\frac{B^2R_H}{e(\rho^2_{xx}+B^2R^2_H)} \tag{16}$$

to measure the free electron density at high magnetic fields (see Robert *et al.*[5] and Raymond *et al.*[24]).

In Fig. 3 we show the measured free electron density in sample S_1 as a function of $10^3/T$ for different magnetic fields between 1 T and 12 T. Figure 4 shows the theoretical fits to experimental curves for three different B values, given as examples.

The fits are based on Eqs. (8), (9), and (11), the values of N_d and N_a were established before (see Table I) and the only fit parameter is the magnetodonor activation energy $E_d(B)$. We performed similar experiments and analysis for the GaAs sample S_2.

V. DONOR BINDING ENERGIES

The determined magnetodonor (MD) binding energies for the two GaAs samples are shown in Fig. 5. The theoretical binding energy of hydrogenic MD is calculated using the variational procedure (see Zawadzki *et al.*[25]). The Schrödinger equation, written in effective atomic units (lengths in the Bohr radius $a^*_B=\kappa\hbar^2/m^*e^2$, energies in the effective Rydberg $\mathcal{R}=m^*e^4/2\kappa^2\hbar^2$) reads in cylindrical coordinates (spin is omitted)

$$\left(-\nabla^2-i\gamma\frac{\partial}{\partial\varphi}+\frac{1}{4}\gamma^2\rho^2-\frac{2}{\sqrt{\rho^2+z^2}}\right)\Psi=E\Psi, \tag{17}$$

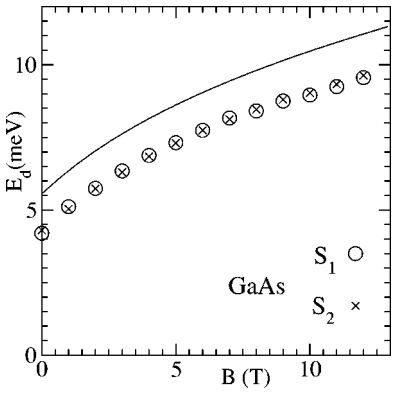

FIG. 5. Binding energies of magnetodonors in GaAs versus magnetic field intensity. Empty circles are experimental energies determined for sample S_1, crosses are those determined for sample S_2. The solid line is a result of variational calculation using the value of $\mathcal{R}=5.52$ meV.

where $\rho^2=x^2+y^2$ and $\gamma=\hbar\omega_c/2\mathcal{R}$. The variational ground MD state is written in the form first proposed by Pokatilov and Rusanov,[26]

$$\Psi = C\exp(-a\rho^2-br), \tag{18}$$

in which $r^2=\rho^2+z^2$, while a and b are the variational parameters. This function gives very good MD binding energies for low and medium γ values, combining the ''atomic'' factor $\exp(-br)$ with the ''magnetic'' factor $\exp(-a\rho^2)$. In our approach we neglect a nonparabolic character of the conduction band in GaAs which becomes of importance at very high magnetic fields (see Miura *et al.*[27]). The calculation is carried out using the effective mass $m^*=0.067m_0$ and the effective Rydberg $\mathcal{R}=5.52$ meV. The result is shown in Fig. 5 by the solid line. The experimental energies are consistently somewhat lower than the theoretical ones. Still, the discrepancy is incomparably smaller than in the case of the GaAs sample investigated by Poehler,[7] indicating that our material is of much higher quality. The experimental MD energies for both our samples are almost the same, except for $B=0$. It is of interest that the value of E_d determined at the low field ($B\approx 0$) is consistent with the estimation at higher fields, although the procedures used in the two cases are somewhat different. This consistency confirms the validity of our assumptions. As to the absolute value of E_d at $B=0$, we determine $E_d\approx 4.2$ meV for the less doped sample S_1 and $E_d\sim 4.3$ meV for the sample S_2. These values are somewhat lower than those determined by Stillman and Wolfe,[28] who found $E_d\approx 5.3$ meV for $N_d=1.7\times10^{14}$ cm^{-3} and $E_d\approx 4.8$ meV for $N_d=3.3\times10^{14}$ cm^{-3}, while Look and Colter[22] obtained similar energies $E_d\approx 4.7$ meV for $N_d=3.1\times10^{14}$ cm^{-3} and $E_d\approx 4.3$ meV for $N_d=3.2\times10^{14}$ cm^{-3}.

It is well known that the donor binding energy decreases with the doping level. The general picture is that, as the doping increases, the donor wave functions begin to overlap and the donor level is broadened. Also, because of the potential fluctuations related to impurities, the conduction band acquires a tail of the density of states on the low energy side. These two features contribute to the decrease of the energy interval between the donor energy and the band.[29] The effect was studied for GaAs by Stillman and Wolfe,[28] for InP by Anderson and Apsley,[9] and recently for 4H-SiC by Pernot *et al.*[10] The influence of magnetic field on the doping-induced semiconductor-metal transition in InSb was investigated by Robert *et al.*[5] and in InP by Kadri *et al.*[30] The residual donors in our GaAs samples can be of different atomic species, which would result in their somewhat different binding energies because of the chemical shift. This would also lead to a broadening of donor level and, in turn, to a decrease of the measured binding energy.

The energy difference between the theoretical and the experimental values shown in Fig. 5 is almost independent of the magnetic field. This is somewhat surprising since as B increases, the donor wave functions shrink (see Zawadzki *et al.*[25]), which should lead to a smaller overlap for neighboring impurities, so that at higher fields the experimental energies should be closer to the theoretical ones. This was indeed the case in experiments of Poehler[7] and Kadri *et al.*[30] for bulk samples and those of Zawadzki *et al.*[6] for GaAs/AlGaAs heterostructures. On the other hand, for a high quality InSb sample, Raymond *et al.*[24] observed the parallel behavior of experimental and theoretical MD binding energies.

In our study we did not attempt to measure directly the Hall scattering factor r_H. This was done for InP at low temperatures[9] and for GaAs at high temperatures.[31] The subject of the Hall factor remains somewhat controversial. The numerical calculations indicate that in GaAs at low temperatures r_H is close to 1,[12] whereas our calculations based on the relaxation time approximation for scattering by ionized impurities give r_H which can reach values of 1.4. Also at higher temperatures the experimental estimation gives smaller values of r_H than those calculated for polar scattering by optic phonons.[31] However, it should be emphasized again that our theoretical fits to the low field data shown in Figs. 1 and 2 include the Hall scattering factor.

It was observed by Look and Colter[22] that GaAs samples of very high quality, having the compensation ratio $K<0.1$, exhibit at low temperatures two maxima of the mobility $\overline{\mu}(T)$. Our samples do not show this feature. Also the fact that the experimental MD energies shown in Fig. 5 do not quite reach the theoretical values indicates that there is still room for an improvement as far as the sample quality is concerned.

VI. SUMMARY

We investigated two GaAs bulk epitaxial samples of high quality with the use of transport experiments in order to determine the donor binding energy and its dependence on magnetic-field intensity up to 12 T. Both free electron density and electron mobility were modeled theoretically to characterize the samples, taking carefully into account the Hall scattering factor as well as the surface and the interface depletion layers of the investigated structures. Our analysis allowed for the existence of hopping conduction over the donor states in the freeze-out regime of higher magnetic fields. The theoretical donor energies were calculated using a two-parameter variation procedure. At all magnetic fields the experimental binding energies were only about 1 meV lower than the theoretical ones. This represents a very substantial improvement in comparison with the previous studies of GaAs and confirms the high quality of the material used.

[1] R.W. Keyes and R.J. Sladek, J. Phys. Chem. Solids **1**, 143 (1956); R.J. Sladek, *ibid.* **5**, 157 (1958); **8**, 515 (1958).

[2] Y. Yafet, R.W. Keyes, and E.N. Adams, J. Phys. Chem. Solids **1**, 137 (1956).

[3] C.L. Littler, W. Zawadzki, M.R. Loloee, X.N. Song, and D.G. Seiler, Phys. Rev. Lett. **63**, 2845 (1989).

[4] M.I. Dyakonov, A.L. Efros, and D.L. Mitchell, Phys. Rev. **180**, 813 (1969).

[5] J.L. Robert, A. Raymond, R.L. Aulombard, and C. Bousquet, Philos. Mag. B **42**, 1003 (1980).

[6] W. Zawadzki, M. Kubisa, A. Raymond, J.L. Robert, and J.P. Andre, Phys. Rev. B **36**, 9297 (1987).
[7] T.O. Poehler, Phys. Rev. B **4**, 1223 (1971).
[8] C.M. Wolfe, G.E. Stillman, and W.T. Lindley, J. Appl. Phys. **41**, 3088 (1970).
[9] D.A. Anderson and N. Apsley, Supercond. Sci. Technol. **1**, 187 (1986).
[10] J. Pernot, W. Zawadzki, S. Contreras, J.L. Robert, E. Neyret, and L. Di Cioccio, J. Appl. Phys. **90**, 1869 (2001).
[11] T.R. Lepkowski, R.Y. DeJule, N.C. Tien, M.H. Kim, and G.E. Stillman, J. Appl. Phys. **61**, 4808 (1987).
[12] D. C. Look, *Electrical Characterization of GaAs Material and Devices* (Wiley, New York, 1989).
[13] W. Zawadzki, Adv. Phys. **23**, 435 (1974).
[14] J.R. Meyer and F.J. Bartoli, Phys. Rev. B **24**, 2089 (1981).
[15] C. Erginsoy, Phys. Rev. **79**, 1013 (1950).
[16] H.G.J. Meijer and D. Polder, Physica (Amsterdam) **19**, 255 (1953).
[17] H. Ehrenreich, J. Appl. Phys. **32**, 2155 (1961).
[18] A. Chandra, C.E.C. Wood, D.W. Woodard, and L.F. Eastman, Solid-State Electron. **22**, 645 (1979).
[19] D.D. Nolte, W. Walukiewicz, and E.E. Haller, Phys. Rev. Lett. **59**, 501 (1987).
[20] E.E. Mendez, P.J. Price, and M. Heiblum, Appl. Phys. Lett. **45**, 294 (1984).
[21] P. Pfeffer, I. Gorczyca, and W. Zawadzki, Solid State Commun. **51**, 179 (1984).
[22] D.C. Look and P.C. Colter, Phys. Rev. B **28**, 1151 (1983).
[23] R. Mansfield, J. Phys. C **4**, 2084 (1971).
[24] A. Raymond, J.L. Robert, W. Zawadzki, and J. Wlasak, J. Phys. C **17**, 2381 (1984).
[25] W. Zawadzki, P. Pfeffer, S.P. Najda, H. Yokoi, S. Takeyama, and N. Miura, Phys. Rev. B **49**, 1705 (1994).
[26] E.M. Pokatilov and M.M. Rusanov, Fiz. Tverd. Tela (Leningrad) **10**, 3117 (1968) [Sov. Phys. Solid State **10**, 2458 (1968)].
[27] N. Miura, H. Nojiri, P. Pfeffer, and W. Zawadzki, Phys. Rev. B **55**, 13 598 (1997).
[28] G.E. Stillman and C.M. Wolfe, Thin Solid Films **31**, 69 (1976).
[29] B. I. Shklovskii and A. L. Efros, *Electronic Properties of Doped Semiconductors* (Springer-Verlag, Berlin, 1984).
[30] A. Kadri, K. Zitouni, L. Konczewicz, and R.L. Aulombard, Phys. Rev. B **35**, 6260 (1987).
[31] G.E. Stillman, C.M. Wolfe, and J.O. Dimmock, J. Phys. Chem. Solids **31**, 1199 (1970).