Low-temperature electron mobility in a real δ-doped semiconductor

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The low-temperature electron mobility in δ-doped GaAs is calculated by using the Boltzmann equation and the relaxation-time approximation. It is assumed that the electrons are scattered from ionized donors, which are spread uniformly throughout some distance. For donor-ion spreading of 50 to 100 Å the calculated mobilities, although still higher than experimental ones, are for some electron concentrations even 50% lower than those calculated assuming genuine δ doping. The possibility for the observation of such discontinuities which appear in the mobility when the Fermi level passes through the subband bottoms is discussed. [S0163-1829(96)00532-2]

Recently we have calculated the low-temperature two-dimensional electron-gas (2DEG) mobility in δ-doped GaAs assuming that the electrons are scattered from ionized donors localized in a single atomic layer.[1] Our theoretical results were about two times higher than the mobilities deduced from experiments. Temperature-dependent mobilities calculated in Ref. 2 were also higher than the measured ones. Also the theoretical mobilities presented in Ref. 3 for low electron concentrations in δ-doped GaAs exceed the experimental data.

In our case one of the reasons for the discrepancy mentioned above is the enormously high electron mobility in the first excited subband. This is due to the fact that the wave function of the electrons in the first excited subband has a node at the doping plane. Thus, the potential associated with ionized donors experienced by these electrons is weak. Often, in reality the doping profile differs from the intended δ function and is characterized by some smearing of dopants.[4–8] It is evident that a less sharp doping profile will result in a reduction of the mobility of the electrons mentioned above due to nonvanishing overlap of their wave functions with the ionized-donor distribution.

We now calculate the low-temperature 2DEG mobility in δ-Si-doped and in addition weakly p-type GaAs, solving the Boltzmann equation in the relaxation-time approximation using one-, two-, and three-subband models depending on the population of the subbands. In contrast to our previous calculations, where genuine δ doping was considered, we assume now that the electrons are scattered from ionized donors which are spread at uniform density over some distance.

Finally, we discuss the possibility for the observation of discontinuities which are exhibited by the mobility each time the Fermi level coincides with the bottom of a subband. So far, these discontinuities have been studied theoretically as well as experimentally in the case of 2D electron systems in Si/SiO_2 and $Al_xGa_{1-x}As/GaAs$ heterojunctions[9–12] and in multiple-quantum-well structures.[13,14]

The system we deal with is weakly p-type GaAs with a highly doped n^+ layer of finite thickness, with all Si donors being ionized. We model our system assuming a uniform distribution of a positive charge in a thin layer $(-d_0 \leqslant z \leqslant d_0)$.

To find the subband structure of a δ-doped semiconductor we use the envelope-function method as well as the single-particle approximation. To avoid a self-consistency problem when determining the confining potential $V(z)$ we use the Thomas-Fermi (TF) approximation (see Ref. 1 for details). The three-dimensional donor density takes the form $n_D(z)=n_D\vartheta(d_0-|z|)$, where ϑ is the Heaviside step function. Similarly, the density of ionized acceptors is $n_A(z)=n_A\vartheta(d-|z|)$, where d is determined by the condition that for $z=d$, $V(z)$ approaches its bulk value E_c, i.e., the bottom of the conduction band at large z. The potential $V(z)$ is shown schematically in Fig. 1.

The electronic states of 2DEG are described by the following envelope functions and the corresponding eigenvalues $[\boldsymbol{\rho}=(x,y),\ \mathbf{k}=(k_x,k_y)]$:

$$\phi_{n\mathbf{k}}(\mathbf{r})=\frac{1}{2\pi}\exp(i\mathbf{k}\cdot\boldsymbol{\rho})h_n(z), \quad E_{n\mathbf{k}}=E_n+\frac{\hbar^2\mathbf{k}^2}{2m}, \quad (1)$$

where h_n and E_n are solutions of the one-dimensional Schrödinger equation written in the effective-mass approximation with $V=V(z)$. Note that $E_{n\mathbf{k}}$ represents the nth subband whose bottom is E_n. To determine $h_n(z)$ and E_n, we use a variational procedure taking the solutions for the square-well problem as trial functions [Eqs. (7)–(11) in Ref. 1].

We restrict ourselves to the $T=0$ case and calculate the mobility limited by Coulomb scattering. The ionized Si donors are spread out uniformly over a distance $2d_0$, whereas charged acceptors are distributed over a distance $2d$ (see Fig.

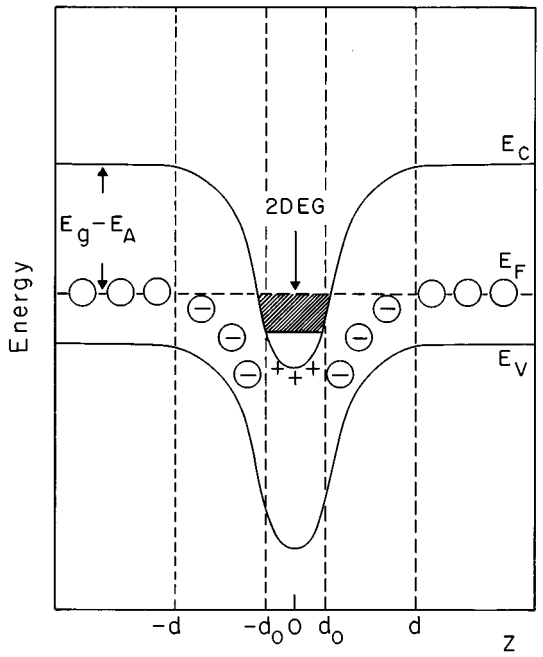

FIG. 1. Schematic sketch of the potential $V(z)$ experienced by electrons in a δ-doped semiconductor with nonvanishing background acceptor density and a finite $(2d_0)$ width of donor distribution.

1). We have checked that for typical $N_D = 2d_0 n_D$ and n_A values, say 10^{12} cm^{-2} (and higher) and 5×10^{15} cm^{-3}, respectively, one can ignore the scattering from the acceptors and take into account the scattering from the donors only.

The low-temperature transport mobility μ and the Hall mobility μ_H are given by

$$\mu = \frac{\Sigma_i n_i \mu_i(E_F)}{\Sigma_j n_j}, \quad \mu_H = \frac{\Sigma_i n_i \mu_i^2(E_F)}{\Sigma_j n_j \mu_j(E_F)}, \tag{2}$$

where μ_i is the mobility in the ith subband, and n_i is the concentration of electrons in this subband. The mobility is related to the relaxation time in the ith subband by

$$\mu_i(E) = \frac{|e|}{m}\tau_i(E). \tag{3}$$

The relaxation times τ_i satisfy coupled linear equations[9,15]

$$P_n(E)\tau_n(E) - \sum_{n' \neq n} P_{nn'}(E)\tau_{n'}(E) = 1, \tag{4}$$

where $P_n(E)$ and $P_{nn'}(E)$ are $(E \geqslant E_n)$

$$P_n(E) = \frac{m}{2\pi\hbar^3}\int_0^{2\pi} d\phi \int dz n_D(z) |V_{\mathrm{eff}_{nn}}(q,z)|^2 (1-\cos\phi)$$
$$+ \frac{m}{2\pi\hbar^3}\sum_{n' \neq n} \vartheta(E-E_{n'})$$
$$\times \int_0^{2\pi} d\phi \int dz n_D(z) |V_{\mathrm{eff}_{nn'}}(q',z)|^2, \tag{5}$$

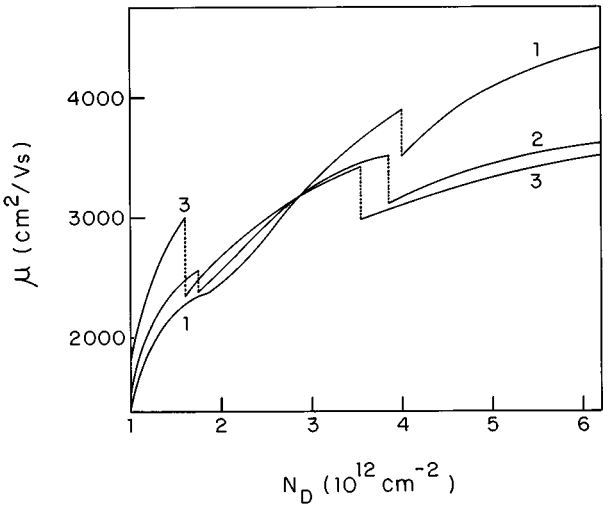

FIG. 2. Calculated transport mobilities of the 2DEG in δ-doped GaAs with background acceptor concentration $n_A = 5\times10^{15}$ cm^{-3} as a function of the areal donor concentration N_D. The width $2d_0$ of the square-shaped donor distribution is 0 (curve 1), 50 Å (curve 2), and 100 Å (curve 3).

$$P_{nn'}(E) = \frac{m}{2\pi\hbar^3}\vartheta(E-E_{n'})\left(\frac{E-E_{n'}}{E-E_n}\right)^{1/2}$$
$$\times \int_0^{2\pi} d\phi \int dz n_D(z) |V_{\mathrm{eff}_{nn'}}(q',z)|^2 \cos\phi. \tag{6}$$

The arguments of the Fourier transforms of the effective potential are $q = \sqrt{2}k(1-\cos\phi)^{1/2}$ and $q' = (k^2 - 2kk'\cos\phi + k'^2)^{1/2}$, where $k = [2m(E-E_n)/\hbar^2]^{1/2}$ and $k' = [2m(E-E_{n'})/\hbar^2]^{1/2}$.

Proceeding along the same lines as in Ref. 1 (see Eqs. (13) and (14) therein) we assume a linear relationship between the matrix elements of the impurity potential and the effective potential experienced by electrons. However, $V_{nn'}(\boldsymbol{\rho})$ and their 2D Fourier transforms $V_{nn'}(\mathbf{q})$ therein should be replaced here by

$$V_{nn'}(\boldsymbol{\rho},z) = \int dz' h_n^*(z') V(\boldsymbol{\rho}, z'-z) h_{n'}(z') \tag{7}$$

and appropriate Fourier transforms with respect to the $\boldsymbol{\rho}$ variable, i.e., $V_{nn'}(\mathbf{q},z)$.

In our numerical calculations we use the dielectric matrix obtained in the random phase approximation (RPA) (Ref. 9; see also Ref. 1 for details).

Low-temperature mobilities limited by the Coulomb scattering are calculated numerically from formulas (3)–(7) and plotted as functions of areal donor concentration N_D in Fig. 2 (transport mobility), Fig. 3 (Hall mobility), and Fig. 4 (subband mobilities) for the doping n^+-layer thickness equal to 0, 50, and 100 Å.

The dependence of transport mobilities on doping n^+-layer thickness is graphically shown in Fig. 5.

The areal electron concentration $n_{2\mathrm{DEG}}$ is less than N_D by about 7×10^{11} cm^{-2} for the considered values of N_D and d_0.

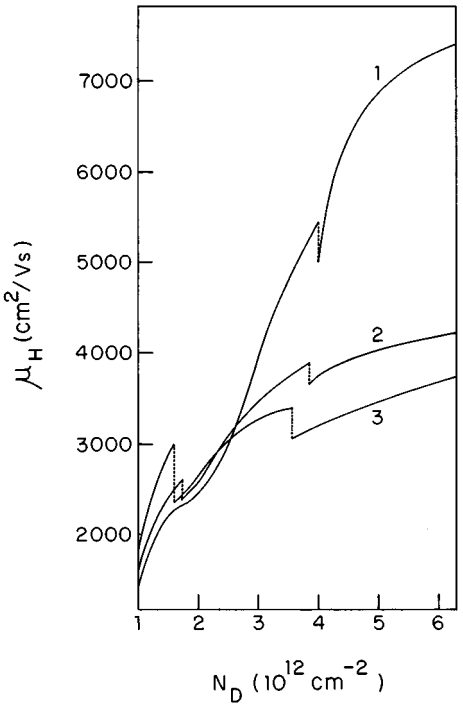

FIG. 3. Calculated Hall mobilities of the 2DEG in δ-doped GaAs for the same cases as in Fig. 2.

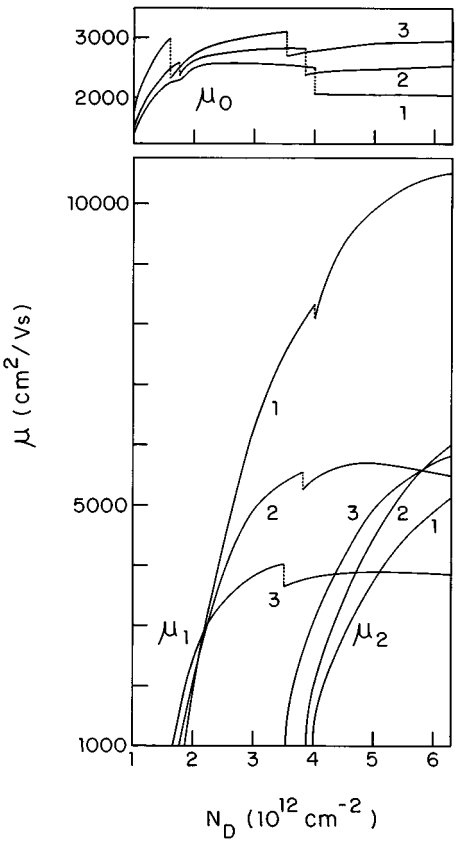

FIG. 4. Calculated subband mobilities μ_i in δ-doped GaAs for the same cases as in Fig. 2.

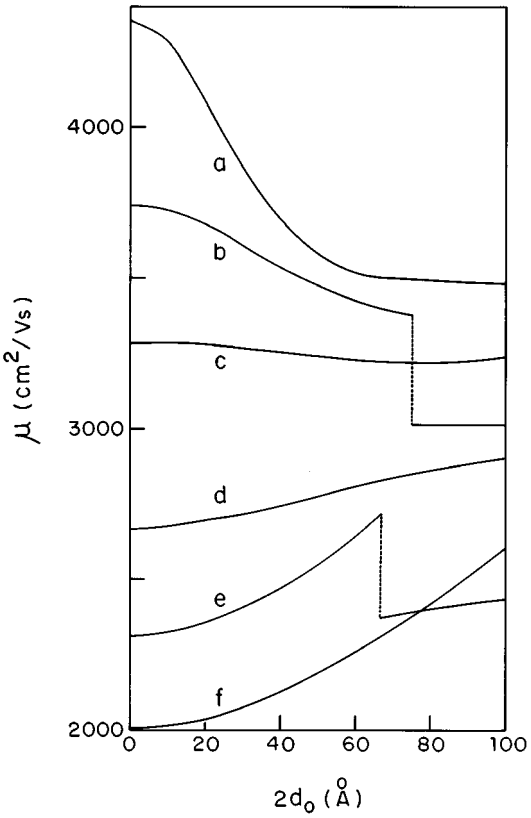

FIG. 5. Calculated transport mobilities of the 2DEG in δ-doped GaAs as a function of the width $2d_0$ of the square-shaped donor distribution. Areal donor concentrations N_D: curve a, 6×10^{12} cm^{-2}; curve b, 3.7×10^{12} cm^{-2}; curve c, 3×10^{12} cm^{-2}; curve d, 2.3×10^{12} cm^{-2}; curve e, 1.7×10^{12} cm^{-2}; and curve f, 1.3×10^{12} cm^{-2}. The background acceptor concentration is $n_A=5\times10^{15}$ cm^{-3}.

The significant scatter among the measured mobilities[2,7,8,16–21] can be attributed to uncertainties in specification of sample parameters. For this reason any comparison with theoretical calculations should be considered to be qualitative rather than quantitative. The results of our previous calculations[1] of the 2DEG mobility in a truly δ-doped semiconductor exceeded the experimental data by a factor of 2. Our present theoretical calculations indicate that introducing broadening into the δ-like doping profiles (real δ-doping semiconductor) would reduce both the transport and the Hall mobilities for some electron concentration by up to 30% and 50%, respectively, when the donor smearing is about 50 to 100 Å. Note that smearing by 50 Å cannot be detected reliably in experiments.[4,7]

By introducing broadening into the doping profiles we are able to explain, at least for higher 2DEG concentrations, the experimentally observed inequality $\mu_2>\mu_1$. For genuine δ doping we have[1] $\mu_1>\mu_2$ (see also the discussion in Ref. 7). One of the ways to broaden the doping profile is annealing. Recently, it was observed that after annealing the mobility in the lowest subband increases by a small amount but the mobilities in the higher subbands decrease strongly.[8,21] The results of our calculations are in accord with these observations: μ_0 and μ_1 behave like that with increasing doping-layer thickness.

Due to structure in the density of states, the low-

temperature 2DEG mobility exhibits discontinuities as a function of electron concentration each time the Fermi level coincides with the bottom of a subband. Theoretically obtained mobility discontinuities are shown in Figs. 2–5. To the best of our knowledge, so far there has been no experimental evidence for these anomalies in μ in δ-doped semiconductors.

We believe that the drops in the mobility are detectable experimentally. This could be achieved by employing annealing, which gives rise to broadening of the doping profile and what follows modifies the position of the Fermi level. Let N_D^{Δ} and N_D^0 be the areal doping concentrations at which the Fermi level coincides with the bottom of a given subband, in the cases of realistic and genuine δ doping, respectively (Δ denotes here the donor spread). The 2DEG mobility in a sample with $N_D^{\Delta}<N_D<N_D^0$ will experience a discontinuity in an otherwise smooth dependence on doping-layer thickness in an interval $[0,\Delta]$. Such a discontinuity will not be present for N_D other than that mentioned above (see Fig. 5). Note that the calculated jumps in mobilities (Fig. 5) are much larger (by a factor of 4) than the error in most experiments.[8,20]

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