Effect of high unintentional doping in AlGaAs barriers on scattering times in accumulation layers

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Analyzing possible relaxation mechanisms in two-dimensional electron gas in GaAs-AlGaAs inverted structures we show that the existence of unintentional acceptor doping in the AlGaAs barriers, with concentration as high as 10^{17} cm^{-3}, provides the only explanation for the observed transport and single particle relaxation times.

It is known that unintentional doping in GaAs can put an upper limit on the mobility of electrons in inversion or accumulation layers at low temperatures. Much less is known about unintentional doping in AlGaAs barriers. This doping, usually higher than in GaAs,[1] can limit the mobility of two-dimensional electron gas (2DEG) in GaAs-AlGaAs heterostructures. We demonstrate such situations considering experimental data of two inverted semiconductor-insulator-semiconductor (ISIS) structures, and analyze all possible scattering mechanisms. These structures are favorable for our analysis since the 2DEG is induced via a remote gate and not by doping. We find that the most likely explanation for the experimental data is the unintentional doping in the AlGaAs barrier which can be as high as 6×10^{16} cm^{-3}.

We have used the ratio of the transport time, τ_t, which determines the mobility, to the single particle relaxation time, τ_s, found from the magnetic field dependence of the Shubnikov–de Haas effect (SdH), to select the dominant scattering mechanism. Similarly, Harrang *et al.*[2] could distinguish between Coulomb, surface roughness, and alloy scattering mechanisms, and Mani and Anderson[3] had suggested the mechanism limiting τ_s. Here, by comparing experimentally determined τ_t/τ_s on high-mobility 2DEG with calculated values for different relaxation mechanisms, we show that Coulomb scattering dominates. We also show that charged impurities in the AlGaAs barriers are much more important than impurities in the GaAs and in the GaAs-AlGaAs interface.

The measurements on the first ISIS structure, *A*, were carried out by Smith *et al.*[4] The structure (Fig. 1) was grown on a conducting substrate which acted as a gate. On top of a doped buffer layer an undoped barrier layer (nominally 1850 Å of AlGaAs with an average Al mole fraction of 38%), a channel layer (2000 Å of undoped GaAs), and a cap layer (300 Å of GaAs doped with 2×10^{18} cm^{-3} Si) were grown sequentially. The AlGaAs layer was actually a superlattice of AlAs-GaAs, 14 Å and 23 Å, respectively. Carrier density could be varied with a positive gate voltage relative to the 2DEG in the range 5×10^{10}–8×10^{11} cm^{-2}. We also carried measurements on a second ISIS structure, *B*, with the AlGaAs superlattice 1000 Å wide, the GaAs channel layer 600 Å wide, and a doped AlGaAs cap layer. In both structures the mobility μ and SdH were measured leading to $\tau_t=\mu m/e$, where m and e are the effective mass and the electron charge, and τ_s, via fitting the SdH signal with Ando's exponential behavior in magnetic field.[5] These times are given in the Table I. Notice the large ratio τ_t/τ_s in all cases.

The dependence of the low-temperature mobility on the 2DEG concentration for nearly the same structure was studied previously.[6] Three scattering mechanisms were considered there: scattering from unintentional background impurities in the GaAs, the interface charges, and via interface roughness. We show below that only the third mechanism, roughness scattering, could explain such large ratios of the relaxation times for roughness correlation length long enough. However then, unrealistic large roughness amplitudes are necessary to explain the absolute values of τ_t and τ_s.

A large τ_t/τ_s ratio suggests a dominating of a small angle scattering, resulting usually from long-range scattering potentials. Although the GaAs background impurities and interface charges can give rise to a long-range potential, its range is not long enough to explain the observed times ratios. The most likely mechanism to produce a large τ_t/τ_s is scattering from remote impurities in the AlGaAs barrier layer. These impurities can lead to a rather large τ_t/τ_s even when no spacer layer separates them from the

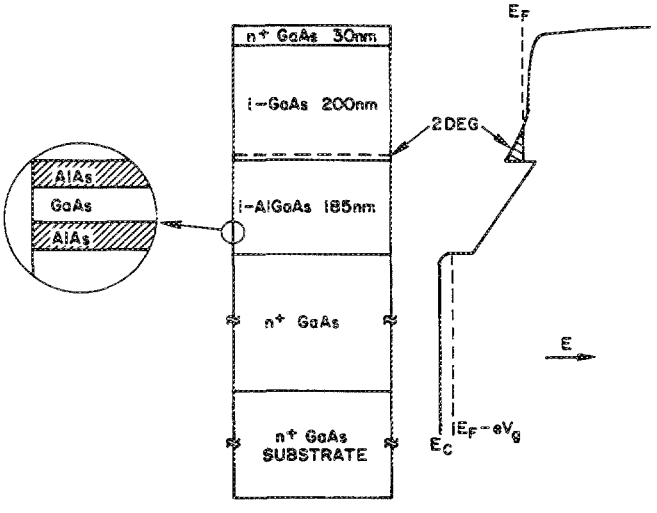

FIG. 1. Description of the ISIS structure used in the experiment (see Ref. 1). Inset shows the superlattice structure of the AlGaAs barrier.

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TABLE I. Relaxation times measured in different structures.

Str.	T (K)	n (10^{11} cm^{-2})	μ (10^5 cm^2/V s)	τ_t (10^{-11} s)	τ (10^{-13} s)	τ_t/τ_s
A	0.75	5.9	6.25	2.4	3.4	71
B	4.2	2.1	4.2	1.7	7.3	23
B	4.2	2.9	5.9	2.3	7	33
B	4.2	3.6	7	2.7	10	27

2DEG.[7,8] To show this we estimate first these scattering times due to Coulomb potentials and subsequently discuss other mechanisms.

The relaxation time for Coulomb scattering can be found from the expression[5]

$$\frac{1}{\tau}=\frac{2\pi e^2 q_s}{\kappa\hbar}\int_0^{\pi}\frac{u[2k_F\sin(\theta/2)]\,f(\theta)\,d\theta}{\{2k_F\sin(\theta/2)+q_s H[2k_F\sin(\theta/2)]\}^2}, \tag{1}$$

where $q_s=2me^2/\kappa\hbar$ is the screening parameter, κ is the dielectric constant, and k_F is the Fermi wave vector. With the z direction normal to the plane of the interface,

$$u(q)=\int N(z)\,dz\left[\int e^{-q|z-z'|}\zeta^2(z')\,dz'\right]^2, \tag{2}$$

$$H(q)=\int e^{-q|z-z'|}\zeta^2(z)\zeta^2(z')\,dz\,dz', \tag{3}$$

where $N(z)$ is the impurity concentration, and $f(\theta)=1$ for τ_s and $f(\theta)=1-\cos\theta$ for τ_t. We use the Fang–Howard variational function $\zeta(z)=(b^3/2)^{1/2}z\exp(-bz/2)$, which is very close to the exact one.[5,9] Here $b=(33\pi me^2 n/2\kappa\hbar^2)^{1/3}$ and n is the electron concentration in the channel. To simplify the calculations we neglect in Eq. (1) screening by the second subband electrons. This screening vanishes for $k_F\sin\theta/2>k_{F1}$, where k_{F1} is the Fermi vector in the second subband, i.e., the long-range potential is screened more effectively than the short-range one. Moreover, the same inequality shows that this screening is weaker than the screening by the first subband electrons. In any case this screening does not affect significantly the ratio τ_t/τ_s, which is important for ascertainment of the main scattering mechanism. We also neglect intersubband scattering. This scattering is much weaker than the intrasubband scattering because of the small spatial overlap between the wave functions of the first and second subbands. Besides, $k_F/k_{F1}\gg 1$ and the intersubband transition is not a small angle scattering event.

For structure *A*, substituting the values $\kappa=13$, $b=3.2\times10^6$ cm^{-1}, $q_s=2.2\times10^6$ cm^{-1}, and $k_F=1.9\times10^6$ cm^{-1} in Eqs. (1)–(3) we obtain $\tau_t/\tau_s=7.1$ due to scattering from impurities in the GaAs [$N(z)=$ const. for $z>0$ and $N(z)=0$ for $z<0$], $\tau_t/\tau_s=61$ due to impurities in the AlGaAs [$N(z)=$ const. for $z<0$ and $N(z)=0$ for $z>0$], and $\tau_t/\tau_s=9.4$ due to interface charge [$N(z)=N_s\delta(z)$]. These numbers are very reasonable: the closer the impurities are to the channel, the smaller is the ratio of the scattering times since the nearby impurities give rise to a comparatively large angle scattering. These results clearly show that, for Coulomb scattering alone, the experimental results can be explained considering only the scattering via ionized impurities in the AlGaAs barrier. Adding contributions of the other Coulomb scattering mechanisms will decrease the ratio of the scattering times. The values of the single particle scattering time and mobility due to scattering from the remote impurities only are

$$\tau_s=\frac{2.2\times10^4}{N}\text{ s},\quad \mu=\frac{3.6\times10^{22}}{N}\text{ cm}^2/\text{V s}. \tag{4}$$

Thus, the experimental data for structure *A* can be explained by an impurity concentration $N\simeq5.8\times10^{16}$ cm^{-3} in the AlGaAs. It was shown before that unintentional charges in AlGaAs, imbedded in *n*-type structures, are negative[1] and might originate from oxidation of AlGaAs.

We discuss now other scattering mechanisms and evaluate their contribution to τ_s and τ_t. As mentioned before, we show that interface roughness is an unlikely mechanism to explain large τ_t/τ_s ratios. For the corresponding relaxation times we use the expression[5,10,11]

$$\frac{1}{\tau}=\frac{2\pi e^2 q_s\Lambda^2\Delta^2}{\kappa\hbar}\times\int_0^{\pi}\frac{\exp[-k^2\Lambda^2(1-\cos\theta)/2]\,f(\theta)\,d\theta}{\{1+q_s H[2k\sin(\theta/2)]/2k\sin(\theta/2)\}^2}, \tag{5}$$

where Λ and Δ are the correlation length and the average step height of the surface roughness, respectively, and Gaussian correlation function for the surface roughness is assumed. All other notations here are the same as in Eq. (1), and the remark about the screening by the second subband electrons concerns Eq. (5) as well. This mechanism can give rise to small angle scattering only if the correlation length is longer than the Fermi wavelength. Then the integral in Eq. (5) can be evaluated analytically leading to $\tau_t/\tau_s\simeq(k\Lambda)^2/3$. Thus the observed ratio of the times can be explained by this mechanism if $\Lambda\simeq730$ Å. Although such a value is bigger than those used in other calculations (see e.g., Refs. 3, 10, and 12) we have not found any experimental evidence against it. However, if we were to accept this value than the observed absolute values of the relaxation times require a roughness height Δ as large as 46 Å or, in other words, about 16 atomic layers. Such a large value for the roughness is very unlikely in usual MBE-grown heterostructures. This value is affected if we choose to use another correlation function, but all our attempts to get a reasonable value for Δ (1–2 monolayers) had failed ruling out this mechanism. Note that the matrix element used in the derivation of Eq. (5) assumes that the insulating AlGaAs layer is an infinite energy barrier. This is justified since the corrections due to the finite height of a thick barrier are not important.[13] We also estimated tunneling across thin AlAs barriers in this superlattice, which have thickness fluctuations, thus giving larger effective roughness. This results only in a small effect which is not affected much by the rather high electric field in the superlattice barrier.

TABLE II. Calculated relaxation times.

n (10^{11} cm^2)	τ_t (10^{-11} s)	τ_s (10^{-13}s)	τ_t/τ_s
2.1	1.6	6.8	23
2.9	2.2	7.8	29
3.6	2.9	8.7	33

Electron-electron and electron-phonon scattering mechanisms depend on temperature and appears to be negligible at 0.75 K. The single particle relaxation time due to electron-electron scattering can be estimated from[14]

$$\frac{1}{\tau_s}=\frac{E_F}{2\pi\hbar}\left(\frac{k_BT}{E_F}\right)^2\ln\frac{E_F}{k_BT}, \tag{6}$$

where E_F is the Fermi energy. For an electron concentration of 5.8×10^{11} cm^{-2} we have $E_F=19$ meV, and thus $\tau_s\simeq3\times10^{-9}$ s, clearly unimportant. Electron-acoustical phonon scattrering is a large angle scattering and thus cannot lead to a large τ_t/τ_s. Moreover, the extrapolation of the mobility limited only by acoustical phonon scattering[15] to a temperature of 0.75 K leads to a value of more than 10^7 cm^2/V s. Alloy scattering, normally present in GaAs-AlGaAs, is absent here because of the absence of an AlGaAs random alloy.

From the above we conclude that the most likely mechanism explaining the experimental data of Ref. 4 is the scattering by ionized impurities (probably acceptors) in the AlGaAs with an average concentration 5.8×10^{16} cm^{-3}, or 1.5×10^{17} cm^{-3} in the AlAs barriers. Such a large unintentional charge will lead to a shift in the threshold voltage $V_{\rm th}$ necessary for accumulating the 2DEG. Using the expression[1,16]

$$V_{\rm th}=(2\pi e/\kappa)Nw^2-E_{Fg}/e\,, \tag{7}$$

where E_{Fg} is the Fermi energy in the gate ($\sim$50 meV in our case) and w is the width of the barrier AlGaAs layer, we find $V_{\rm th}\simeq1.3$ V in close agreement with the experimental value $V_{\rm th}\simeq1.2$ V.

The data taken on structure B were analyzed similarly. Once again it appeared that the high τ_t/τ_s ratios can be explained via the Coulomb scattering from impurities in the AlGaAs barrier. However, an attempt to explain the absolute values of the mobility with the only scattering mechanism which leads to a very high impurity concentration is not consistent with the threshold voltage. This contradiction is lifted if we take into account other scattering mechanisms. Using a concentration of impurities of 2.4×10^{16} cm^{-3} in AlGaAs and 3×10^{13} cm^{-3} in GaAs, and surface roughness parameters $\Lambda=55$ Å, $\Delta=2$ Å (as in Ref. 6) we obtained a reasonable agreement with the experimental data. The results of the calculation are shown in the Table II. The only discrepancy is for $n=3.6\times10^{11}$ cm^{-2} where the experiment shows the decrease of τ_t/τ_s. This unusual behavior may result from intersubband scattering which is effective for a high enough concentration.[4,17–19] Note that even though the choice of the scattering parameters is not unique the chosen values led to the best agreement for the concentration dependence of the mobility, as shown in Fig. 2 . The threshold bias estimated according to Eq. (7) for $N=2.4\times10^{16}$ cm^{-3} is

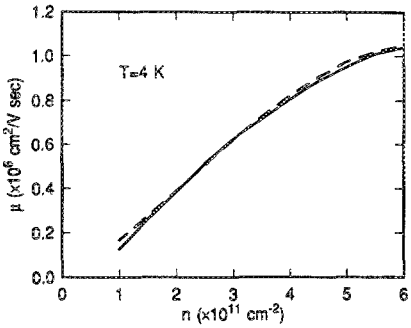

FIG. 2. Concentration dependence of the mobility for the B structure. The solid line is the experiment; the dashed line is calculated from a model invoking Coulomb scattering by charges in AlGaAs and GaAs and surface roughness scattering.

120 meV, close enough to the experimental value of 100 meV.

In conclusion, we have shown that unintentional high doping in MBE-grown insulating AlGaAs layers is the main scattering mechanism in inverted GaAs-AlGaAs structures (not necessarily the case in normal structures). This effect could result from impurity segregation in the AlGaAs toward the GaAs. Since measuring these charges is not easy, our approach, determining them from the ratio of the transport and the single particle scattering times, is a very useful method. This unintentional, relatively high doping, occurring in MBE-grown AlGaAs layers, is routinely neglected, and its importance in determining scatterings is usually overlooked.

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