# Ionized-Impurity Scattering of Quasi-Two-Dimensional Quantum-Confined Carriers

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Hall-effect measurements of electron mobility in anti-modulation-doped GaAs/AlGaAs quantum wells indicate that the ionized-impurity scattering of a quasi-two-dimensional electron gas immersed in the identical concentration of ionized impurities is greater than that of a bulk electron gas of the same density. This enhancement results from an increase of the overlap of the electronic wave function with the impurities, a decrease in screening, and an increase in large-angle scattering. The enhanced scattering rate may be further increased by confining the dopant ions to a deltalike doping profile in the center of the well.

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This Letter reports the first detailed study of ionized-impurity scattering of electrons in a quasi-two-dimensional system in which the electrons and ionized impurities occupy the same quasi-two-dimensional region. There have been many studies of the interaction of ionized-impurity scattering on a two-dimensional electron gas (2DEG) over the years. These are primarily concerned with ionized-impurity scattering of electrons in accumulation or inversion layers when the electron density is much greater than the ionized-impurity density or when they are spatially separated. The calculations of Stern and Howard[1] already indicated in 1967 that by increasing the 2DEG concentration without increasing the ionized impurities, the mobility could be significantly increased. The concept is most remarkably demonstrated in the AlGaAs/GaAs modulation-doped heterojunction system. By doping only the higher-band-gap AlGaAs away from the interface, the ionized-impurity scattering of the 2DEG can become extremely small. When simultaneously the background impurities in the GaAs are reduced and the interfaces are optimized, the mobilities may exceed $10^7$ cm$^2$/V s.[2]

The introduction of small concentrations of impurities into the region of the 2DEG dramatically degrades the mobility.[3-5] This is expected because when the added impurity concentration is small compared to the 2DEG concentration, the electron screening is essentially unaffected, but the effective number of scattering centers is increased. A more fundamental question is *how the dimensionality itself affects the ionized-impurity scattering in a semiconductor.* In the case of a bulk semiconductor, the total wave function of the electrons overlaps with the ionized impurities which are the same in number as the electron density. If such a uniformly doped bulk semiconductor is confined in one dimension —that is to say, confined to be quasi-two-dimensional —the overlap of the electronic wave function with the ionized impurities (an effective impurity concentration) will be altered because the electronic wave function will be peaked in the center, but vanishing at the edges of the resulting quantum well. Furthermore, the electronic screening in two dimensions is entirely different than in three dimensions, being both shorter ranged and weaker at short range.[6]

This study offers the first experimental evidence that, in fact, the ionized-impurity scattering in uniformly doped quantum wells is greater than in a similarly doped bulk semiconductor. It further explains this result through a detailed calculation of the ionized-impurity scattering rates in a quasi-two-dimensional system.

The GaAs/$Al_xGa_{1-x}As$ heterojunction system was chosen to study ionized-impurity scattering in a quasi-two-dimensional system. Because the mobility of electrons in GaAs (without impurities) is high and because the interface between GaAs and $Al_xGa_{1-x}As$ is single crystalline, this system is well suited for considering only the scattering due to ionized impurities.

To compare ionized-impurity scattering in three dimensions to that in two dimensions, we compare Si-doped bulk GaAs to uniformly doped GaAs quantum wells with AlGaAs barriers. All samples were grown by molecular-beam epitaxy (MBE) under identical conditions on (100)-oriented undoped GaAs substrates. All sources were solid and a low substrate temperature of about 560 °C was used. The bulk GaAs was 0.25 $\mu$m thick and doped with Si to a level of $6\times10^{17}$ cm$^{-3}$. The quantum wells, which were in multiple-quantum-well samples with 25 to 50 periods, were 100 Å wide with 34-Å-wide barriers of $Al_{0.4}Ga_{0.6}As$. These barriers are narrow enough to ensure that the two-dimensional concentration of traps in the AlGaAs is small compared to the two-dimensional electron and dopant concentrations, yet are thick enough to contain the wave function in the GaAs quite well. All quantum wells are also doped to an average three-dimensional concentration of $6\times10^{17}$ cm$^{-3}$. The quantum wells were prepared with progressively narrower doping profiles, maintaining the same average doping concentration. The widest doping profile comprised 84% of the well width; the entire well was not doped in order to prevent *D-X* center formation near the interfaces. The narrow-profile limits of these sample series includes samples delta doped[7,8] with sheet densities of $5\times10^{11}$ cm$^{-2}$ in the 100-Å wells. (In delta-doped samples, the sheet density of donor atoms is grown on one atomic plane; the final profile is determined by diffusion, but is still quite narrow.) Wells 100 Å wide

TABLE I. Samples used in this study grown by MBE.

| Sample | Well width | Dopant width | $N_{3D}$ ($cm^{-3}$) | $N_{2D}$ (per well) ($cm^{-2}$) |
|---|---|---|---|---|
| S1 | Bulk | ··· | $6\times10^{17}$ | ··· |
| S2 | 100 Å | 84 Å | $7\times10^{17}$ | $6\times10^{11}$ |
| S4 | 100 Å | 40 Å | $1.5\times10^{18}$ | $6\times10^{11}$ |
| S5 | 100 Å | 20 Å | $3\times10^{18}$ | $6\times10^{11}$ |
| S6 | 100 Å | $\delta$ | ··· | $5\times10^{11}$ |
| S7 | 100 Å | $\delta$ (off center) | ··· | $6\times10^{11}$ |
| S8 | Bulk | $\delta$ every 100 Å | $6.4\times10^{17}$ (average) | $6.4\times10^{11}$ (per $\delta$) |

were also delta doped off center with a similar sheet density of $6\times10^{11}$ $cm^{-2}$. The various samples are summarized in Table I.

Van der Pauw–Hall measurements were made on the samples between 10 and 300 K using low electric and magnetic fields. In heavily doped semiconductors, such as the samples studied here, the Hall factor is very close to unity, regardless of scattering mechanism. The solid curves of Fig. 1 show the temperature dependence of the mobilities of three uniformly doped samples: S1 and S2. S1 is bulk GaAs and S2 has 100-Å wells. The mobility of the bulk sample is what is typically measured at this doping level and is well understood theoretically.[9] Mobilities for the doped quantum wells are significantly lower than that observed in bulk GaAs for all temperatures. Previous data[10,11] indicate that interface-roughness scattering of a 2DEG in 100-Å-wide wells is quite small and can, in these samples, be safely ignored.

The confinement of the electronic wave function affects the ionized-impurity scattering in two ways:

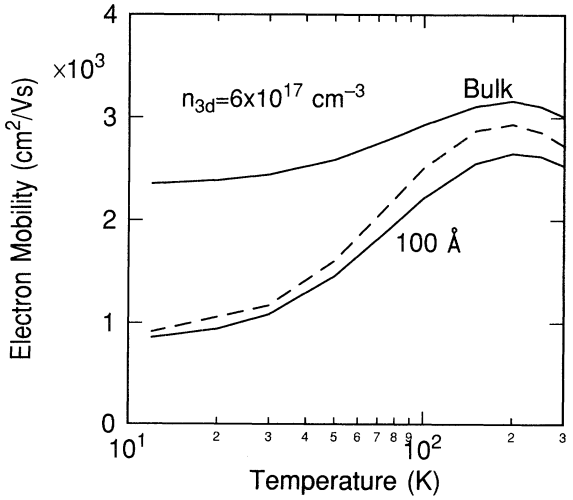


FIG. 1. Measured Hall mobilities as functions of temperature for bulk GaAs and 100-Å-wide quantum wells. Both samples have average doping concentrations of $6\times10^{17}$ $cm^{-3}$. The solid curves are measured data; the dashed curve is adjusted as described in the text in order to make an appropriate comparison with bulk.

First, it changes the way the wave function overlaps with the impurities, and second, it changes the electron screening term in the dielectric function. Following Ando,[12] the relaxation time for electrons in one-subband scattering from ionized impurities is given by

$$\frac{\hbar}{\tau_c(k)} = 2\pi \int dz\, N(z) \sum_q \left[\frac{2\pi e^2}{q\varepsilon(q)}\right]^2 |F(q,z)|^2 \times (1-\cos\theta)\delta(\mathcal{E}_{\mathbf{k}}-\mathcal{E}_{\mathbf{k}-\mathbf{q}}), \quad (1)$$

where $N(z)$ is the doping profile, $q=2k\sin(\theta/2)$, and $\mathcal{E}_{\mathbf{k}}=\hbar^2k^2/2m$, with $\mathbf{k}$ is the wave vector and $\theta$ the scattering angle. The static dielectric function is given by

$$q\varepsilon(q) = q + (2\pi e^2/\kappa)(2m/2\pi\hbar^2)F(q), \quad (2)$$

where $\kappa$ is the dielectric constant and $m$ is the electron effective mass. Here we use the $T=0$ formula for the polarization term which introduces only small errors away from $T=0$ in the case of these degenerate samples. In two-dimensional systems, degenerate statistics result in no explicit $n_{2D}$ dependence of the polarization. The form factor appearing in Eq. (1), $F(q,z)$, is a measure of the overlap of the electron density with charge centers at location $z$ and is given by

$$F(q,z) = \int dz' |\zeta(z')|^2 \exp(-q|z-z'|), \quad (3)$$

where $\zeta(z)$ is the $z$ component of the total electronic envelope wave function $\Psi(\mathbf{r},z)=\zeta(z)\exp(i\mathbf{k}\cdot\mathbf{r})$. The other form factor $F(q)$ which appears in Eq. (2) may be thought of as the "screening of the screening"[13] and is given by

$$F(q) = \int dz \int dz' |\zeta(z)|^2 |\zeta(z')|^2 \exp(-q|z-z'|); \quad (4)$$

because it never exceeds unity, it only decreases the screening. The sum over $q$ in Eq. (1) may be replaced by an integral over $\theta$ so that Eq. (1) is written

$$\frac{\hbar}{\tau_c(k)} = \frac{4\pi m e^4}{\hbar^2} \int_0^\pi d\theta (1-\cos\theta) \frac{1}{[q\varepsilon(q)]^2} \times \int dz |F(q,z)|^2 N(z). \quad (5)$$

The mobility is finally given by

$$\mu(T) = e\langle\tau_c\rangle/m. \quad (6)$$

The temperature dependence of $\mu(T)$ enters in the averaging of $\tau_c(k)$ over $k$. We choose a simple wave function,

$$\zeta(z) = \sqrt{2/W}\cos(\pi z/W),$$

where $W$ is the width of the quantum well. This wave function along with the one-subband approximation is justified by noting that even with such narrow barriers, especially in the 100-Å case, the wave function squared is close to zero at the interface and that the second subband is nearly unpopulated. A self-consistent solution of Schrödinger's and Poisson's equations[14] shows that compared to the conduction-band offset, the band bending with these doping levels is small. The doping profile

$N(z)$ for symmetrically doped samples is given by

$$N(z)=\begin{cases}(1/uW)n_{2D}, & |z|<uW/2,\\ 0, & |z|>uW/2,\end{cases}$$

where $u$ is the fraction of the well which is doped. In the case of the delta-doped wells,

$$N(z)=n_{2D}\delta(z-z_\delta),$$

where $z_\delta$ is the position of the delta-doping spike. It is then straightforward to evaluate the integrals of Eqs. (3) and (4) analytically and of Eqs. (5) and (6) numerically to obtain the theoretical mobilities as functions of dopant distribution, temperature, and well width. We ignore certain corrections which have been incorporated into more detailed calculations of ionized-impurity scattering in the bulk semiconductors,[15] such as multiple scattering, as well as the effect of well-to-well screening which we expect to be small.

The data displayed by the solid curves of Fig. 1 do not really provide a definitive comparison of ionized-impurity scattering in two dimensions to ionized-impurity scattering in three dimensions because although the bulk sample is uniformly doped, the wells are doped in the center 84% which will result in lower mobility than if they were uniformly doped. (Uniform doping over 100% of the wells was avoided to prevent $D$-$X$ center formation at the interfaces.) The quantum-well mobilities may be corrected, however, by using Matthiessen's rule to subtract the extra scattering rate resulting from the slightly more concentrated dopant profile. The dashed curve of Fig. 1 depicts the measured mobilities of the 100-Å well corrected as described. These data are slightly different from the raw data of the solid curve and demonstrate unambiguously that quasi-two-dimensional confinement results in a decrease of mobility and therefore an increase in ionized-impurity scattering over a broad temperature range. This effect may be compared with an analogous enhancement of scattering processes for 2D excitons over those for 3D excitons.[16] We have also examined samples with well widths of 50, 200, and 400 Å and find that progressively wider wells lead to progressively higher mobilities, apparently asymptotically approaching that for bulk GaAs.

Conceptually, one is tempted to make a connection to three-dimensional scattering by associating the three-dimensional case with a quantum-well system, but with $\zeta(z)$ constant. If one makes this assumption, mobilities are, indeed, calculated to be higher than in the quasi-two-dimensional case described. This connection is not justified, however, because in three dimensions the screening is different, as well as the density of states. To truly go continuously from two to three dimensions in this way, one would need to consider an infinite number of subbands in the calculation. More realistically, the dimensionality-enhanced scattering of electrons by ionized impurities results, in part, from the details of the screening and overlap with the impurities. The overlap with impurities can be thought of as an effective doping concentration $N_{\rm eff}$, where

$$N_{\rm eff}(q)=\frac{1}{W}\int|F(q,z)|^2N(z)dz.$$

We easily see that

$$\lim_{q\to 0}N_{\rm eff}(q)=n_{2D}/W$$

and that $N_{\rm eff}\geq N_{2D}/W$ for all $q$. In three dimensions, $N_{2D}/W$ is replaced by $N_{3D}$, with $N_{\rm eff}\geq N_{3D}$.

The screening term is also completely different in two dimensions than it is in three dimensions. For large $q$, the three-dimensional scattering is smaller ($\sim q^{-2}$) than it is in two dimensions ($\sim q^{-1}$). In the opposite limit of large $r$, the three-dimensional system is much more effectively screened, with the scattering matrix element going as $e^{-qr}$ compared to the two-dimensional system in which it goes as $r^{-3}$.[6] Additionally, we see that the most effective scattering events are those of backscattering, where $\theta=\pi$. In a three-dimensional system, the total fraction of solid angle with $\theta=\pi\pm\Delta\theta/2$ is $\Delta\theta^2/16$. In a two-dimensional system, the total fraction of angle with $\theta=\pi\pm\Delta\theta/2$ is $\Delta\theta/2\pi$. Thus, backscattering is relatively easier in a two-dimensional system, since $\Delta\theta$ enters only linearly.

From Fig. 1 it is clear that uniformly doped quantum wells have a lower mobility than identically doped bulk GaAs and, of course, studies of modulation-doped quantum wells show that when the dopants are largely moved out of the quantum well, the mobility is higher. Figure 2 shows the effect of concentrating the dopants into the center of the well. In each case, the areal concentration is about $6\times10^{11}$ cm$^{-2}$, but the distributions vary. When the fraction of the well which is doped reaches zero, the well is delta doped in the center; when the fraction is 1.0, it is uniformly doped. The solid curves of Fig. 2 are cal-

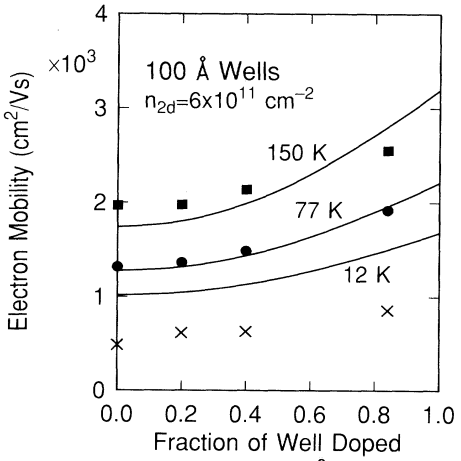


FIG. 2. Electron mobility for 100-Å quantum wells as a function of temperature and fraction of the well which is doped. The curves are calculated as described in the text and the symbols are experimental data taken at 150 K (■), 77 K (●), and 12 K (×).

culated as described above with no corrections or adjustable parameters. (Phonon scattering is not included in the calculations.) The symbols are experimental data. We see that the doping profile has a significant impact on the ionized-impurity mobility and that the model described above describes the physics adequately, except at low temperatures. The reason for the discrepancy at lower temperatures is unknown. At higher temperatures (and especially for larger fractions of the well which is doped), phonon scattering becomes important. A structure was also prepared which was otherwise identical to the delta-doped quantum-well sample (S6) except that it contains no AlGaAs barriers. Sample S8 consists of deltalike spikes of $6\times10^{11}$ cm$^{-2}$ located every 100 Å. The mobility $\mu(T)$ for this sample is nearly identical to that of the bulk GaAs of identical doping for all temperatures.

From Fig. 2 we see that the lowest mobility is observed in the wells with delta doping in the center. This effect results from all of the ionized impurities being localized where the electronic wave function is maximum (i.e., maximizing $N_{\text{eff}}$). By moving the delta doping away from the center, we can increase the mobility. Figure 3 shows the mobility versus temperature for three samples. The solid curves are experimental. The one labeled "Uniform" is uniformly doped in the center 84% of the well. The lowest curve is for the center-delta-doped wells. The third curve is from sample S7, which is also delta doped, but with the doping midway between the center and the edge of the well. From Fig. 3, we see that the mobility is higher than when the dopants are all at the center of the well. The dashed curves of Fig. 3 are calculated mobilities (with only ionized-impurity scattering included) for the same cases. If the dopants were moved farther from the center, the mobility would be even higher; by moving them entirely out of the wells, we are back to the modulation-doped example.

In conclusion, this study demonstrates unambiguously that ionized-impurity scattering of electrons in GaAs/$Al_xGa_{1-x}As$ quantum wells is more effective than in identically doped bulk GaAs. This can be understood through the details of the overlap of the ionized impurities with the wave function and the screening along with the greater probability in the two-dimensional system to experience backward scattering. Detailed calculations of ionized-impurity scattering in a quantum well have been described for the first time; these calculations indicate that wells of about 100 Å will experience the greatest enhancement of ionized-impurity scattering. Both the experimental and theoretical data further show that the ionized-impurity scattering in quasi-two-dimensional systems increases with decreasing temperature. Although there is some discrepancy between the measured and calculated data at very low temperatures, the present theoretical results agree well with the measured data of the effect of dopant distribution on mobility. This effect is observed both by changing the concentration of the dopant profile as well as by changing the position.

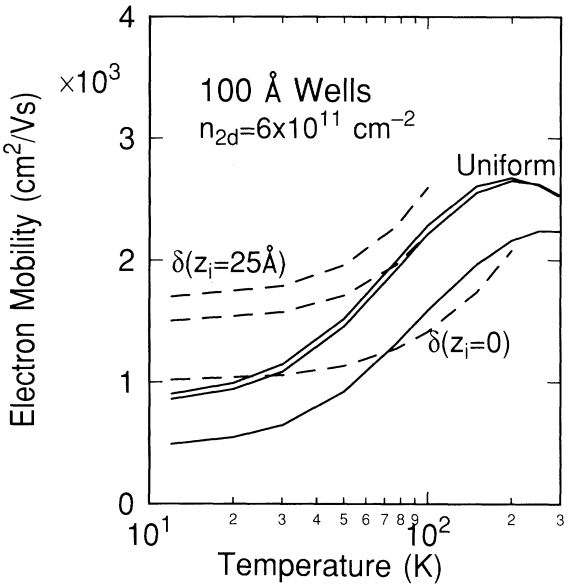


FIG. 3. Electron mobilities for 100-Å quantum wells as functions of temperature for wells uniformly doped in the center 84% of the well, delta doped in the center of the well, and delta doped midway between the center and edge of the well. The solid curves are experimental and the dashed curves theoretical.

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