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Remote impurity scattering in modulation-doped GaAs/Al$_x$Ga$_{1-x}$As heterojunctions

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We have investigated the time-dependent mobility and density of a modulation-doped GaAs/Al$_x$Ga$_{1-x}$As heterojunction subsequent to the ionization of *DX* centers using the persistent photoconductivity effect. Our results are in excellent agreement with a simple theory of mobility limited by independent charged scattering centers. We show that these scattering centers are fluctuations in the average impurity potential which principally arise due to the presence of both positively and negatively charged impurities, and that the effect of correlation among charged impurities can be treated in terms of the removal of individual potential fluctuations. [S0163-1829(98)05520-9]

I. INTRODUCTION

Much effort has gone into trying to understand the effect of remote ionized impurity scattering on the mobility μ of the two-dimensional electron gas (2DEG) in modulation-doped GaAs/Al$_x$Ga$_{1-x}$As heterostructures.[1–7] Ten years ago, these efforts appeared to be quite successful.[1] Even the simplest approach, which approximated the 2DEG wave function in the growth direction to a δ function, and considered all the remote impurities as independent scattering centers, appeared to work reasonably well.[2] A general tendency for theoretical mobilities to underestimate the experimental values, particularly for large spacer widths, was subsequently attributed to the incorrect assumption that individual donor impurities are independent scattering centers.[3] Because of the separation between the doping layer and the 2DEG in modulation-doped heterostructures, the electrons are unable to distinguish individual impurity atoms, and scatter from fluctuations in the average disorder potential. Invoking this correction led to a considerable increase in the calculated mobilities,[3] such that they then overestimated the low-temperature experimental values.

However, an assumption which all of these studies had in common is that the remote impurities are either neutral or positively charged, as would be expected for shallow donor impurities. A serious difficulty arises with the inclusion of the model of *DX* centers[8] proposed by Chadi and Chang in 1988,[9] in which a neutral Si donor captures an electron from a second Si donor, creating a negatively charged *DX* center, and leaving an unoccupied positively charged shallow donor. Experiments in both GaAs/Al$_x$Ga$_{1-x}$As heterojunctions[10] and bulk Al$_x$Ga$_{1-x}$As samples[11] suggested that, for typical x and doping concentrations of the Al$_x$Ga$_{1-x}$As in heterostructures, the maximum number of Si donors form *DX* centers during cooling, so that prior to illumination there are no neutral donors. Since the total number of Si donors in these structures can be as much as ten times the 2DEG density n_s, this results in a corresponding decrease in the calculated mobility. Attempts to resolve this led to the assertion that the positively and negatively charged impurities correlate their positions to form dipole pairs while the sample is cooled, such that the scattering is reduced.[4] Evidence of such correlations is found in the form of multiple values of μ dependent on the method by which a given n_s is achieved.[5,6] Inclusion of these effects makes the calculation of μ rather complicated, and raises the question of why the earlier theories, which ignored all of the above complications, were in such good agreement with experiment.

In this paper we provide an answer to this question by demonstrating that scattering from remote ionized impurities is consistent with a simple model of an array of independent scatterers, and show that these scatterers are due to fluctuations in the disorder potential. In an earlier work,[7] we used consecutive bursts of illumination from an infrared light-emitting diode (IRLED) to induce the persistent photoconductivity effect, and measured the subsequent changes in n_s and μ of two GaAs/Al$_x$Ga$_{1-x}$As single heterojunctions with different spacer widths. We found that in the narrow (200 Å) spacer sample the rate of increase in n_s dropped exponentially with illumination time. In contrast, the wide (400 Å)

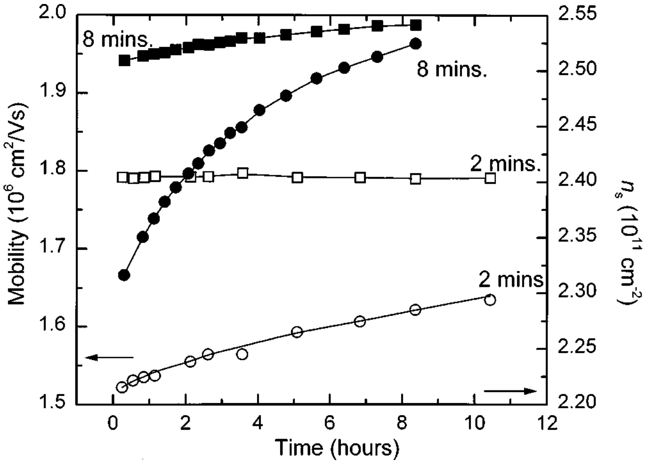

FIG. 1. μ (squares) and n_s (circles) as functions of time after 8 (closed symbols) and 2 (open symbols) min of illumination at 0.3 K. The lines are guides to the eye, and the arrows indicate the dark values.

spacer sample initially showed no change in n_s, but an exponential decrease in the number of independent scattering centers.

For this study we concentrate on the wide spacer sample, but use a slightly different approach, illuminating for a given time, then monitoring the subsequent changes in n_s and μ with no further illumination. In agreement with our earlier work, we find an immediate enhancement of μ (up to 24%). This is followed by a slow increase in n_s which is dependent on a number of experimental parameters, but reproducibly proportional to the change in the number of independent scattering centers. This rather surprising result clearly shows that the scattering due to the remote impurities is indeed from an array of independent scattering centers, as previously assumed.[1,2] We go on to demonstrate that these scattering centers are fluctuations in the average potential,[3] dominated by the effect of having mixed (i.e., positively and negatively) charged impurities. Finally, we show that the effect of impurity charge correlation is equivalent to a reduction in the number of fluctuations.

II. RESULTS AND ANALYSIS

The 400-Å spacer sample was cooled in a ^{3}He cryostat to temperatures between 0.3 and 4.2 K in the dark. Its n_s and μ prior to illumination were reproducibly equal to $(2.21\pm0.02)\times10^{11}$ cm^{-2} and $(1.56\pm0.01)\times10^6$ cm^2/V s, respectively, at 1.3 K and below, with μ dropping to 1.39×10^6 cm^2/V s at 4.2 K. It was then illuminated using an IRLED for a fixed time (2 or 8 min) at a constant current of 1 μA. The subsequent changes in n_s and μ were monitored over a period of up to 10 h at constant temperature using low-field Hall and zero-field resistivity measurements. At the end of this process the sample was warmed up again, and recooled ready for the next measurement. Figure 1 shows μ and n_s as functions of time at 0.3 K after illumination. It can be seen that there is a large immediate increase in μ, 15% in the case of 2-min illumination, and 24% for 8-min illumination. In contrast, the immediate increases in n_s are extremely modest, with no discernible change for 2 min, and a mere 4% increase for 8-min illumination.

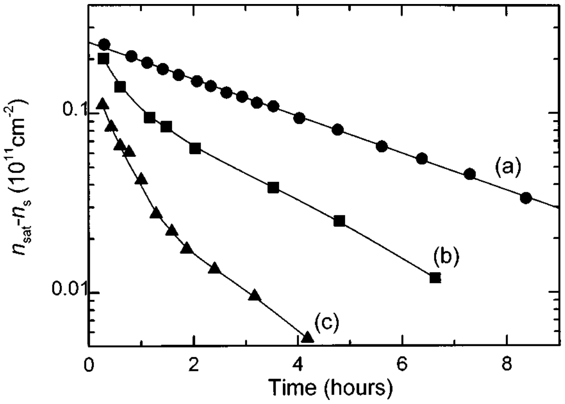

FIG. 2. Time dependence of the change in n_s after 8-min illumination plotted as $n_{\rm sat}$-n_s, where $n_{\rm sat}$ is the apparent asymptotic value of n_s, for (a) 0.3 K, (b) 1.3 K, and (c) 2.3 K. The lines are (a) linear fit, (b) and (c) guides to the eye.

The changes of n_s and μ with time are equally interesting, and it is these on which we now concentrate. As can be seen in Fig. 1, small changes in n_s continue over many hours, with little or no change in μ. For 2-min illumination the rate of change of n_s shows an approximately exponential decrease when monitored for a period of 8 h, with a time constant of about 13 h. In the case of 8-min illumination it is 4 h [Fig. 2(a)]. As the temperature is increased, this behavior is no longer observed, with the increase in n_s slowing faster than an exponential function [Figs. 2(b) and 2(c)]. It is worth noting that the observation of nonexponential behavior at 1.3 and 2.3 K is reliable, since the changes in n_s become very small at higher temperatures on a reasonable time scale. In general, we find that the rate of change in n_s is dependent on the amount of illumination, the time after illumination (nonexponentially), the temperature, and the cooldown. The effects of the last were particularly noticeable for 2-min illumination, so we shall now restrict our discussion to the 8-min case. Despite this wide ranging behavior in n_s and μ as a function of time, we find that there is a consistent relationship between them, independent of time, temperature and cooldown for the same illumination period. Our interpretation goes as follows. First we take the very simplest approximations for calculating μ; a δ function for the 2DEG wave function in the growth direction, and independent scattering from charged impurities. We neglect all other scattering mechanisms. Following Lee *et al.*,[2] we obtain

$$\mu=\frac{An_s^{1.5}}{N+\Delta N}, \qquad (1)$$

where N is the density of scattering centers before illumination, ΔN is the change in the density of scattering centers, and A is a constant which depends on the distance of the wave function from the beginning and end of the doped region of the Al$_x$Ga$_{1-x}$As. In principle, A varies with n_s, but the movement of the 2DEG wave function is rather small compared to the spacer width, so we neglect it and take an average value. In the dark, $n_s=n_{s0}$, $\mu=\mu_0$ and $\Delta N=0$, so we can illuminate N, and rewrite Eq. (1) as

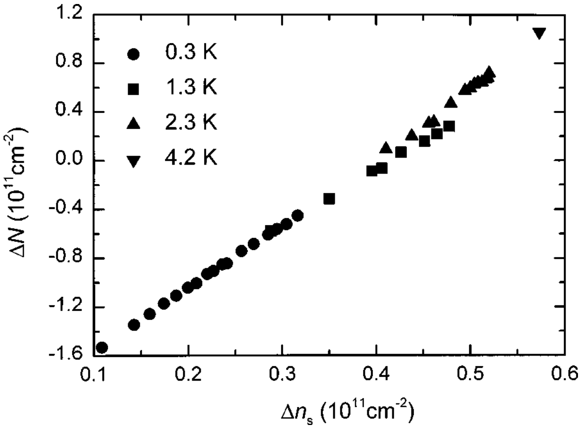

FIG. 3. Change in the areal density of independent scattering centers, ΔN, as a function of the change in n_s for 8-min illumination at 0.3 K (circles), 1.3 K (squares), 2.3 K (up triangles) and 4.2 K (down triangle). The negative values of ΔN correspond to an increase in the mobility.

$$\Delta N = A\left(\frac{n_s^{1.5}}{\mu} - \frac{n_{s0}^{1.5}}{\mu_0}\right). \tag{2}$$

We have not explicitly included the effect of any background impurities in the GaAs in this expression, but since they show the same dependence on n_s as the remote impurities (but with a different value for A), including them simply gives a reduction in ΔN independent of n_s.

The startling result of this simple analysis is shown in Fig. 3, where we plot ΔN as a function of the change in n_s, Δn_s, for all 8-min illumination data. Despite the complex time evolution of n_s and μ, all the data at a given temperature fit on a single straight line. Furthermore, the data at 0.3 and 1.3 K fall on the same straight line. In the case of the 4.2-K data there is only one point because the change in n_s is so fast, but it falls on the same line as the 2.3-K data. The same behavior is also observed for the case of 2-min illumination, but with a larger gradient and more scatter in the data. From these results we can draw two very important conclusions. First, the scattering from remote impurities is entirely consistent with an array of independent charged scattering centers. Second, the change in n_s reproducibly results in a proportionate increase in the density of these scattering centers. Given this, it is tempting to associate the independent scattering centers with individual ionized impurities; however, doing so cannot explain the order of magnitude of μ.

In Fig. 1 we obtain an initial increase of 24% in μ after 8 min of illumination, with a very small change in the density, implying a similar decrease in the number of scattering centers. Figure 3 shows we have removed about 1.5×10^{11} cm^{-2} remote scattering centers, which represents a mere 3% of the Si doping density. The same problem occurs if we calculate μ, taking N to be equal to the number of Si donors. We resolve this by suggesting that the (independent) scattering is caused by fluctuations in the remote impurity potential, and go on to show that the largest fluctuations are caused by the presence of both positively and negatively charged impurities. Figure 4 shows the potential along a line due to a random array of charges. In proceeding with this calculation, we assumed all the parameters of the sample in the dark, i.e., a concentration of 1.33×10^{18} cm^{-3} impurities in a semi-infinite array 380 Å thick placed 400 Å behind the line (see the inset to Fig. 4). For illustrative purposes, we have assumed that the 2.2×10^{11} cm^{-2} electrons in the 2DEG come from impurities closest to the line, i.e., that all the impurities in the depletion region will be positively charged, though it is far from certain that this is the case in practice. The remainder of the impurities in the array have a 50% probability of being either positive or negative. It is immediately obvious from Fig. 4 that the potential due to the random array of both positive and negative charges (dotted line) has considerably larger fluctuations than the array of positive charges in the depletion region (broken line), and that the former fluctuations are reproduced almost exactly in the total potential (solid line). This is true despite the fact that depletion region charges are closer than the array of mixed charges. It is also worth noting that increasing the size of the depletion region does not alter this general picture, it just increases the overall potential without, on average, changing the size of the fluctuations. Given that the fluctuations due to the array of positive charges, which are affected only by the randomness in the impurity position, are considerably smaller than the fluctuations due to mixed charges, which contains contributions from both position and charge, we conclude that the dominant scattering in modulation-doped GaAs/Al$_x$Ga$_{1-x}$As heterojunctions from remote impurities is due to fluctuations in the charge and not the position of impurities.

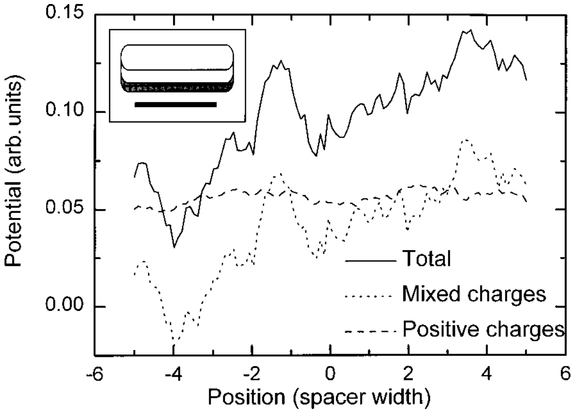

FIG. 4. Potential along a line due to a random array of charged impurities, arranged as shown schematically in the inset. The dark shaded region corresponds to the depletion region (positive charges only), and the light shaded region indicates mixed charges (positive and negative).

III. DISCUSSION

In order to understand the implications of Fig. 4, we may examine a simplified version of the problem by using the fact that the potential is a scalar quantity and considering the potential at the center of a series of concentric rings of positive charges spaced by the average donor impurity separation, a. The number of charges per ring is given by $2\pi r/a$, where r is the radius of the ring, and the potential at the center due to the charges in each ring is therefore the same. Note that the positions of the individual charges on the ring are not important, merely their distance from the center. We now introduce some fluctuations by allowing the positive charges to vary in charge from the average value q. In this case the potential at the center due to the nth ring is given by

$$V_n = \frac{2\pi r q}{a} \frac{1}{r} + V_n^f, \tag{3}$$

where V_n^f is the potential at the center due to the total fluctuation in the charge of the nth ring. The total potential due to N rings is thus

$$V = N \frac{2\pi q}{a} + \sum_n V_n^f. \tag{4}$$

However, since the scattering is from the fluctuations, we subtract the average potential which is equal to the first term, and only the second term in Eq. (4) contributes. We can use this to illustrate several important points. First, the scattering potential from the fluctuations is given by the sum of their individual potentials, i.e., they are independent scattering sources. Second, the scattering potential is dominated by the fluctuations in the closest rings because of their proximity, and because the number of charges increases as we go to larger and larger rings, making it more likely that the fluctuations average out. Finally, we can understand why the largest fluctuations will arise due to variations in the charge, and not the position of the impurities.

In light of the above discussion, we now return to our experimental results, also considering the effect of correlations among the remote impurities. The general argument for such correlations is that while the DX centers are formed during the cooldown process, the Coulomb interaction encourages a uniform, or correlated, distribution of negatively charged DX centers and positively charged ionized donors, reducing the scattering potential. Initially, there may some enhancement of the mobility due to correlation, but it will be reduced or even completely removed by the illumination which randomly selects DX centers to ionize. However, immediately after illumination there are a large number of electrons in the $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ which will distribute themselves among the Si donors, particularly in regions where there is a lack of DX centers. This results in a higher degree of correlation than prior to illumination, and leads to a net enhancement of the mobility. As these electrons slowly diffuse into the 2DEG via the contacts, this correlation will be destroyed, which must, according to our experimental results, be equivalent to increasing the number of scattering centers proportionally with the change in n_s. The diffusion of the electrons in the $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ also results in a net increase in the potential, but this is irrelevant for the scattering. If the distribution of ionized impurities was equally random before and after illumination, one might expect ΔN to return to zero when all the electrons have diffused into the 2DEG. The fact that it does not could be either a result of the illumination destroying the initial correlation of the impurities achieved in the cooldown, or due to the presence of background acceptors in the channel which will shift the data of Fig. 3 upwards. Further evidence for the former explanation is provided by our earlier experiments on another sample,[7] which showed an effectively instantaneous increase in n_s due to the rapid tunnelling rate through the narrow 200-Å spacer. The first burst of illumination resulted in a large increase in n_s with almost no increase in μ, whereas subsequent illumination gave an increase in both, consistent with no change in the number of ionized impurity scatterers. This behavior can be understood as an initial destruction of the correlation, leading to an essentially random distribution by the first illumination, followed by a changing, but equally random, distribution afterwards. This is supported by simulations of random photoionization of DX centers in an array of Si donors of the type of Fig. 4.

Finally we should like to comment on calculations of 2DEG scattering by remote ionized impurities. To our knowledge, the most complete model in the literature was provided by Buks *et al.*,[5] who included the effects of correlations among positively charged donors and negatively charged DX centers as a correction factor to the scattering potential of the individual impurities. However, this leads to the incorrect result that a total lack of correlation results in scattering from the individual ionized impurities. For example, in the case where the impurities are all of one type, this gives the same (maximum) scattering rate, as an uncorrelated distribution of mixed charges, which we have shown is not the case. In some sense our observations should simplify such calculations. We have shown that the fluctuations may be considered as independent scattering centers, and that for a random distribution of charges the scattering potential is unchanged by further random changes in the charge distribution. Furthermore, the results of Fig. 3 show that the effects of correlations among the impurities can simply be treated as a change in the number of independently scattering potential fluctuations.

IV. CONCLUSIONS

We have studied the changes of n_s and μ as the result of the diffusion of electrons from the doped region of the $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ into the 2DEG of a modulation-doped $\mathrm{GaAs/Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ heterojunction. Despite the complicated time evolution of this process, we find that the change in density of independent scattering centers is simply proportional to the change in n_s. We have identified these scattering centers as fluctuations in the average potential due to the presence of oppositely charged impurities, and shown that they are simply related to the effects of charge correlation in the $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$.

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