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# Maximum low-temperature mobility of two-dimensional electrons in heterojunctions with a thick spacer layer

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The calculation of the mobility of the two-dimensional electron gas limited by the remote ion scattering is presented which takes into account the correlation in the spatial distribution of the charged impurities caused by the Coulomb interaction. The correlation function of the charge is characterized by the freezing temperature $T_0$. The low-temperature distribution of the charge is supposed to be a snapshot of the equilibrium distribution corresponding to this temperature. At low enough $T_0$ this distribution corresponds to the ground state of the system consisting of the charged and neutral impurities. The effect of the correlation is shown to be very essential at low $T_0$ and at large spacer thickness. The numerical calculations are performed for modulation-doped $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As/GaAs}$ heterostructures. Input parameters are as follows: spacer width ($s$), temperature ($T_0$), density of the channel electrons ($N_s$), and density of the charge in the depletion layer ($N_{\mathrm{depl}}$).

## I. INTRODUCTION

The low-temperature mobility of the two-dimensional electron gas (2D EG) is determined mainly by ionized impurity scattering. It can be either remote impurity scattering, which comes from the ionized impurities, separated by the spacer layer from the 2D EG, or the residual ion scattering by ions located within undoped regions on both sides of the 2D EG. In what follows, the heterostructures $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As/GaAs}$ are discussed. In this case the first scattering mechanism usually prevails if the thickness of the spacer layer ($s$) is less than approximately 40 nm.

Modern technology tends to decrease the residual ion concentration (which is usually not less than $10^{14}\ \mathrm{cm}^{-3}$), while the remote ion density cannot be decreased essentially at a given concentration of the 2D EG because the remote impurities are the main source of the electrons in the channel. That is why it is interesting to estimate the mobility which is only limited by scattering by remote ions. This is the maximum mobility which can be reached at a given concentration of the 2D EG and at a given $s$.

It is supposed in the course of the usual mobility calculations that there is no correlation in the distribution of the charged impurities.[1] It is known, however, that the correlation can strongly effect the mobility both in three-dimensional[2,3] and two-dimensional[4] cases. It has been shown in Refs. 5 and 6 that in the case of the heterostructures the correlation has to appear due to the Coulomb interaction between the charged impurities if not all of them are ionized. It occurs because at high enough temperatures the electrons can move from one impurity to the other to establish the equilibrium distribution at a given temperature. Due to this mechanism the spatial distribution of the charged impurities becomes correlated even if the total impurity distribution obeys Poisson's law.

Two different models of the correlation have been developed in Refs. 5 and 6. The first model assumes that the thermodynamic equilibrium in the system of electrons localized at the impurities exists only in the temperature range $T > T_0$, where $T_0$ is a freezing temperature. Below $T_0$, electron transitions between the impurities do not lead to the equilibrium in a reasonable experimental time. Therefore, the low-temperature spatial distribution of the charged impurities represent a snapshot of the distribution at $T = T_0$. We call this model nonequilibrium. One can think that $T_0$ is of the order of the critical temperature for the persistent photoconductivity, i.e., $T_0$ should be about 100–150 K.

The second model supposes that the equilibrium exists even at helium temperatures. Then the interaction energy is much larger than the temperature, and the space distribution of the charge corresponds to the ground state of the interacting system. We call this model equilibrium. It is assumed in the both models that donors in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ are either positively charged with a single charge or neutral.

It is difficult at present to choose between these models. We think that the experimental confirmation of the nonequilibrium model would be the dependence of the low-temperature mobility on the cooling regime. The most important in this case must be the cooling rate within the temperature interval near $T_0$.

## II. NONEQUILIBRIUM MODEL

In the framework of the nonequilibrium model one can calculate the fluctuations of the charge analytically.[5,6] Let $c(\mathbf{r})$ be the deviation of the area concentration of the charged impurities from its average value. For the scattering-time calculations one should know the correlation function $D(\mathbf{r})$ of the charges:

$$D(\mathbf{r}-\mathbf{r}')=\langle c(\mathbf{r})c(\mathbf{r}')\rangle\ , \tag{1}$$

where $\mathbf{r}$ and $\mathbf{r}'$ are the vectors in the plane parallel to the 2D EG.

For Poisson distribution of charged impurities one has

$$D(q)=c\ , \tag{2}$$

where $c$ is the average area concentration of the charged impurities, and

$$D(\mathbf{q})=\int D(\mathbf{r})\exp(i\mathbf{q}\cdot\mathbf{r})d^2r\ . \tag{3}$$

It has been shown[5,6] that the correlation function $D(q)$, corresponding to the snapshot of the distribution at $T=T_0$, looks like in the nonideal plasma:

$$D(q)=\frac{cq}{q+q_0[1-\exp(-2qs)]}\ , \tag{4}$$

where $q_0=2\pi ce^2/\kappa T_0$ is the reciprocal screening length of the nondegenerate plasma at temperature $T_0$ and $\kappa$ is the dielectric constant. The case $q \ll q_0$ is of interest. At $qs \gg 1$, one gets

$$D(q)=q\kappa T_0/2\pi e^2\ . \tag{5}$$

At $q \ll q_0$ the fluctuations are much smaller than it follows from Eq. (2). At $qs \ll 1$, one obtains equation

$$D(q)=\kappa T_0/4\pi e^2 s \tag{6}$$

with the same $q$ dependence as in Eq. (2), but with a small effective concentration $\kappa T_0/4\pi e^2 s$.

The interpretation of Eqs. (4)–(6) is very simple. If $D(q)=c_{\text{eff}}$, then the mean-square fluctuation of charge $\langle Q^2\rangle$ in a square $R\times R$ is

$$\langle Q^2\rangle=e^2 c_{\text{eff}} R^2 \tag{7}$$

because each charged impurity has a charge $e$. In the nonideal plasma the charge $\langle Q^2\rangle$ should be estimated from the condition that the interaction energy of the fluctuations in the neighboring squares $\langle Q^2\rangle/\kappa R$ is of the order of $T_0$. It gives that $\langle Q^2\rangle$ is of order of $\kappa R T_0$. One can get the same estimate from Eqs. (5) and (7) using $c_{\text{eff}}$ as obtained from Eq. (5) at $q=R^{-1}$. However, the above expression for interaction energy is valid only if $R \ll s$, otherwise one should take into account the screening of the electric field by the plane with 2D EG, which works like a metallic film. The interaction energy at $R \gg s$ is of the order of energy of the plane condenser with the area $R^2$ and distance $s$ between plates. This is $\langle Q^2\rangle s/\kappa R^2$ (here we neglect numerical factors which cannot be taken into account exactly in this estimate). Then $\langle Q^2\rangle$ is of the order of $T_0\kappa R^2/s$. This is the same result, as follows from Eqs. (6) and (7).

Here it is supposed that all the charged impurities are in one plane. It is the case for the δ doping. For the thick doped layer, one should take into account the fluctuations of the positions of the charged impurities in the direction perpendicular to the 2D EG. It can be shown, however,[6] that in the nonequilibrium model this fluctuations give a small contribution to the random potential as compared with the fluctuations of the charge given by Eq. (4).

## III. EQUILIBRIUM MODEL

In the equilibrium model, the spatial distribution of charged impurities corresponds to the ground state of the system, i.e., to the minimum of electrostatic energy of the random electric field created by all charges. We suppose that the total distribution of impurities obeys Poisson's law. If a very small part of impurities is ionized, so that the distance between charges is much larger than the distance between points, where these charges can be located, the ground-state distribution of ions looks like the Wigner crystal (but without long-range order[7]). We consider a more realistic case when these distances are comparable, and the aim is to calculate the spatial fluctuations of the charge in the ground state.

This problem has been solved by computer simulation in Ref. 6. In that simulation, however, the screening of the Coulomb interaction of the charged impurities by the 2D EG has not been taken into account. Therefore, the simulation results of Ref. 6 cannot be used directly for the mobility calculations.

In this paper we use an analytical approach to this problem which has also been proposed in Ref. 6 to describe the fluctuations of area density of charge. This approach does take into account the screening by the 2D EG, but ignores the fluctuations of the impurity coordinates in the direction perpendicular to the 2D EG. Therefore, it is valid for δ-doped layers with a thickness of order of the mean distance between impurities or smaller. It has been shown in Ref. 6 that for thick layers the perpendicular fluctuations give the same or even larger contribution to the random potential as the fluctuations of the area density.

The main idea of this approach is to connect the function $D(q)$ with the mezoscopic fluctuations of chemical potential $E_F$ in the finite sample. Suppose that the plane with impurities is divided into squares $R\times R$, where $R$ is larger than the distance between impurities. Assume that we have found the distribution of charged impurities in each square, minimizing the total electrostatic energy at an additional condition that each square is neutral. The neutrality in this system is provided by the negative homogeneous background charge, which is equal to the average charge of impurities. So the additional condition assumes that the total number of charged impurities in each square is fixed and equal to the average number. The above distribution does not correspond to the ground state of the system because the energy can be reduced due to the exchange of charges between the squares. That is why chemical potentials of the different squares are different.

Let $E_F(\mathbf{r})$ be the smooth random function which is the chemical potential averaged over many squares in the vicinity of point $\mathbf{r}$. This is a work function of a random two-dimensional system. Potential $\phi(\mathbf{r})$, which appears in the ground state due to the transfer of electrons between the squares can be obtained from the following condition:

$$E_F(\mathbf{r})+e\phi(\mathbf{r})=E_F(N_d,c)\ , \tag{8}$$

where $E_F(N_d,c)$ is the equilibrium chemical potential of the infinite system. It depends both on the total impurity concentration $N_d$ and on the concentration of charged impurities $c$.

The function $\delta E_F=E_F(\mathbf{r})-E_F(N_d,c)$ must be related to the fluctuations of impurity concentration. Following Ref. 6, we assume that this relation is local. Then,

$$\delta E_F=(dE_F/dN_d)_c(N_d(\mathbf{r})-N_d)\ . \tag{9}$$

For Gaussian fluctuations one has

$$\langle [N_d(\mathbf{r})-N_d][N_d(\mathbf{r}')-N_d]\rangle=N_d\delta(\mathbf{r}-\mathbf{r}')\ . \tag{10}$$

The mean-square fluctuation of the chemical potential in a finite sample with area $s$, as obtained from Eqs. (9) and (10), is

$$\langle \delta E_F^2\rangle=\left[\frac{dE_F}{dN_d}\right]_c^2\frac{N_d}{s}\ . \tag{11}$$

The correlation function of the potential, obtained from Eqs. (8)–(10) is given by

$$e^2\langle\phi(\mathbf{r})\phi(\mathbf{r}')\rangle=[(dE_F/dN_d)_c]^2N_d\delta(\mathbf{r}-\mathbf{r}')\ . \tag{12}$$

The potential $\phi(\mathbf{r})$ is related to the excess charge $ec(\mathbf{r})$ by the following equation:

$$\phi(\mathbf{r})=e\int c(\mathbf{r}')\left[\frac{1}{|\mathbf{r}-\mathbf{r}'|}-\frac{1}{[(\mathbf{r}-\mathbf{r}')^2+4s^2]^{1/2}}\right]d^2r'\ . \tag{13}$$

The screening of the Coulomb interaction be the 2D EG is taken into account by the second term of Eq. (13). Using Eqs. (1), (12), and (13) one obtains

$$D(q)=\frac{1}{(2\pi)^2}\frac{\kappa^2q^2}{e^4}\left[\frac{dE_F}{dN_d}\right]_c^2\frac{N_d}{[1-\exp(-2qs)]^2}\ . \tag{14}$$

One gets from Eqs. (11) and (14) at $q=2\pi/R$

$$D\left[\frac{2\pi}{R}\right]=\frac{\kappa^2}{e^4}\langle\delta E_F^2\rangle\left[1-\exp\left[-\frac{4\pi s}{R}\right]\right]^{-2}\ . \tag{15}$$

Equation (15) relates the correlation function of the charge to the mezoscopic fluctuations of the chemical potential. This relation has been checked up by the computer simulation in Ref. 6. [See also discussion of the validity of the local approximation used in Eq. (9).] Equation (14) relates $D(q)$ to the thermodynamic function $(dE_F/dN_d)_c$. To calculate $E_F(N_d,c)$ one should find the spatial distribution of the ionized impurities in the ground state of the system. This problem has been solved by computer simulation.

## IV. CALCULATIONS OF THE MOBILITY

In this paper we present calculations of the mobility limited by remote impurity scattering, taking into account the correlation in the distribution of the charged impurities. Both nonequilibrium and equilibrium models are considered. In the first case, the correlator Eq. (4) is used, and the results are valid for both thick and thin doped layers. For the second model, we used the correlator Eq. (14), with the function $(dE_F/dN_d)_c$ as obtained by the special computer simulation. These results are valid for δ-doped layers only. To estimate the effect of the correlation we have also performed the mobility calculations without the correlation. In this case $D(q)=c$ for all $q$.

Calculations of the mobility are performed using the standard procedure:[1]

$$\mu^{-1}=\frac{2\pi m^2e^3}{\kappa^2\hbar^3}\int_0^{2\pi}\frac{\exp(-2qs)}{(q+q_s)^2}D(q)F^2(q)(1-\cos\theta)d\theta\ , \tag{16}$$

where $F(q)$ is the form factor

$$F(q)=\left[\frac{b}{b+q}\right]^3\ . \tag{17}$$

Here $b$ is the characteristic size of the wave function of the 2D EG in the perpendicular direction:

$$b=\left[\frac{48\pi me^2(N_{\text{depl}}+\frac{11}{32}N_s)}{\kappa\hbar^2}\right]^{1/3}\ ,$$
$$q=2k_F\sin(\theta/2)\ , \tag{18}$$

$k_F=(2\pi N_s)^{1/2}$ is the Fermi wave vector and $m=0.07m_0$ is the effective mass of the electrons. $N_s$ is the concentration of the 2D EG and $N_{\text{depl}}$ is the area concentration of charges in the depletion layer. $q_s=2me^2/\kappa\hbar^2$ is the inverse screening radius of the 2D EG. We do not distinguish between the dielectric constants of GaAS and GaAlAs and put $\kappa=12.55$.

Our results are good at large enough $s$ because in this case the small values of $q$ give the main contribution to the integral Eq. (16), and the expressions Eqs. (4) and (14) for $D(q)$ are valid. Therefore, the deviation of the form factor $F(q)$ from the unity is not important for our calculations and that is why we ignore the $q$ dependence of the dielectric constant.

The thickness of the spacer layer $s$ can be related to the other parameters in the following way:[8]

$$s=\frac{\kappa(V_b-E_{Db}-E_0-\pi\hbar^2N_s/m)}{4\pi e^2(N_{\text{depl}}+N_s)}\ , \tag{19}$$

where $V_b$ is the barrier height and $E_{Db}$ is the donor binding energy in the barrier. It is assumed here that each donor in the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ alloy gives rise to a deep level. Stern[9] has argued that this is the case at $x>0.2$, where $x$ is the concentration of aluminum in the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ alloy.

Following Ref. 10 we use the equations

$$V_b = 600(1.425x - 0.9x^2 - 1.1x^3)\ \text{meV}\ , \tag{20}$$

$$E_{Db} = 707x - 146\ \text{meV}\ , \tag{21}$$

where $E_0$ is the energy of the lowest subband of the channel electrons:

$$E_0 = \left[\frac{3}{2}\right]^{5/3}\left[\frac{4\pi e^2\hbar}{m^{1/2}\kappa}\right]^{2/3}\frac{N_{\text{depl}} + \frac{55}{96}N_s}{(N_{\text{depl}} + \frac{11}{32}N_s)^{1/3}}\ . \tag{22}$$

Note that the area concentration of the charged impurities $c$ can be found from the equation

$$c = N_{\text{depl}} + N_s\ . \tag{23}$$

The mobility calculations discussed in the next section use Eqs. (16)–(23).

## V. RESULTS AND DISCUSSION

### A. Nonequilibrium model

In this case Eqs. (4) and (23) are used for $D(q)$. The results of the mobility calculations at the different values of $T_0$, $s$, $N_s$, and $N_{\text{depl}}$ are shown in Figs. 1 and 2. In Figs. 1(a) and 1(b) the reciprocal mobility is plotted against $N_s$ at five different values of $s$, at $T_0 = 100$ and 150 K, and two different values of $N_{\text{depl}}$. The thickness of the spacer layer and the electron density $N_s$ are considered here as independent variables. That is why $\mu^{-1}$ decreases with the increasing density. The dotted lines show the reciprocal mobility calculated without taking into account the correlation. One can see that the effect of the correlation is very strong, especially for large $s$ and $N_s$. In this case the correlation enhances the mobility approximately 25 times. The effect of the correlation increases with decreasing temperature $T_0$.

The physical interpretation of these results is as follows. At large $s$ the harmonics of the random potential with $q$ of the order of $s^{-1}$ give the main contribution to the scattering. Indeed, the short-range harmonics are small as $\exp(-2qs)$ at a distance $s$ from the plane with impurities [see Eq. (16)], and long-range harmonics give a small contribution to the transport cross section. At such values of $q$ the function $D(q)$ is given by Eq. (6). It is independent of the concentration of charged impurities $c$, it increases with $T_0$ and decreases as $s$ increases. The influence of the density of depletion charges is essential at small $N_s$ only as it follows from Eq. (23).

In Fig. 2 the reciprocal mobility is plotted against $N_s$ for three different values of the aluminum concentration $x$, taking into account that $N_s$ and $s$ are connected by Eq. (19). In this case $\mu^{-1}$ increases with $N_s$ because $s$ decreases with increasing $N_s$.

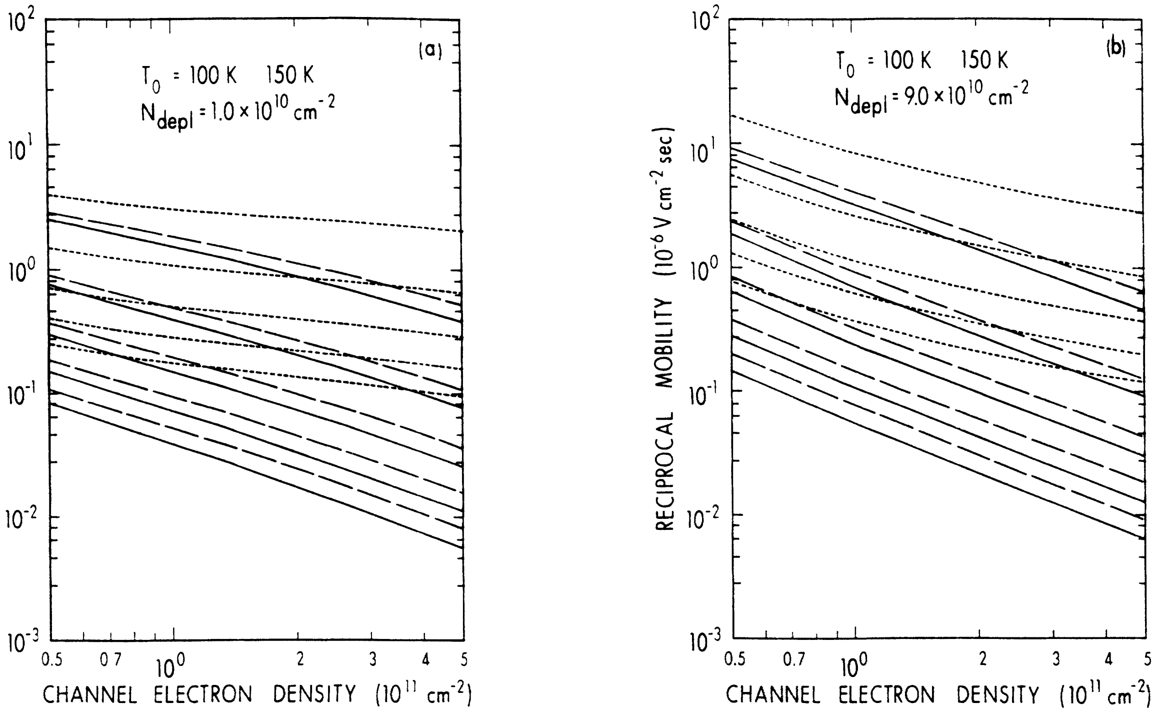

FIG. 1. Calculated low-temperature reciprocal mobility vs channel electron density $N_s$ for a $\text{Al}_x\text{Ga}_{1-x}\text{As/GaAs}$ heterostructure. The dotted lines show the results of the calculations without correlation. The dashed lines and the solid lines show the reciprocal mobility calculated with the correlation in the nonequilibrium model at $T_0 = 150$ and 100 K, respectively. Each series consists of the five lines with the following values of $s$: 10, 20, 30, 40, and 50 nm. One can distinguish between them because in each series the reciprocal mobility monotonically decreases with $s$. Densities of the depletion charges are as follows: $N_{\text{depl}} = 1.0 \times 10^{10}\ \text{cm}^{-2}$, and $9.0 \times 10^{10}\ \text{cm}^{-2}$ for (a) and (b) respectively.

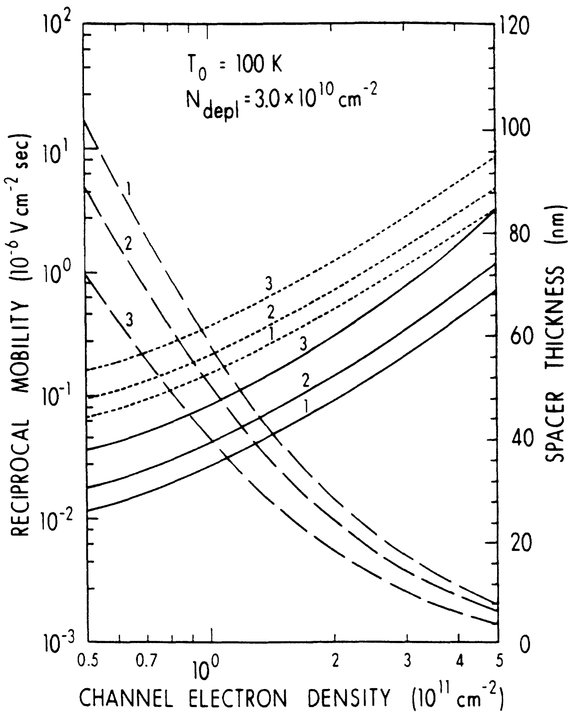

FIG. 2. Calculated low-temperature reciprocal mobility and spacer thickness vs channel electron density $N_s$ for a $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}/\mathrm{GaAs}$ heterostructure at the following values of $x$: 1, $x=0.25$; 2, $x=0.30$; and 3, $x=0.35$. The results of the calculations without correlation are shown by the dotted lines. The reciprocal mobility (left scale) calculated with the correlation in the framework of the nonequilibrium model at $T_0=100$ K is shown by the solid lines. The spacer layer thickness $s$ (right scale) as determined from Eq. (19) for each value of $N_s$, is shown by the dashed lines. $N_{\mathrm{depl}}=3.0\times10^{10}\ \mathrm{cm}^{-2}$.

### B. Equilibrium model

To use the function $D(q)$ given by Eq. (14), one should know the derivative $(dE_F/dN_d)_c$. The function $E_F(N_d,c)$ can be written in a general form as follows:

$$E_F=\frac{e^2N_d^{1/2}}{\kappa}g(K)\ . \tag{24}$$

Here $g(K)$ is a function of the relative concentration $K$, where $K=c/N_d$ is the fraction of the charged impurities. Therefore,

$$\left[\frac{dE_F}{dN_d}\right]_c=\frac{e^2}{N_d^{1/2}\kappa}\left[\frac{g}{2}-Kg'\right]\ . \tag{25}$$

The function $g(K)$ has been calculated by computer simulation by Bello *et al.*[7] However, the accuracy of their calculations is not enough to get the derivative in Eq. (25). Therefore, we have to repeat the calculations, using basically the same algorithm. The simulation has been performed with approximately 400 different arrays consisting of 500 impurities for 80 different values of $K$ within the interval $0\le K\le 0.8$. Our results are shown in Fig. 3. One can see that the expression in the large parentheses of the right-hand side of Eq. (25) increases with $K$ very strongly. We have used these results and Eq. (14) for the mobility calculations in the equilibrium model.

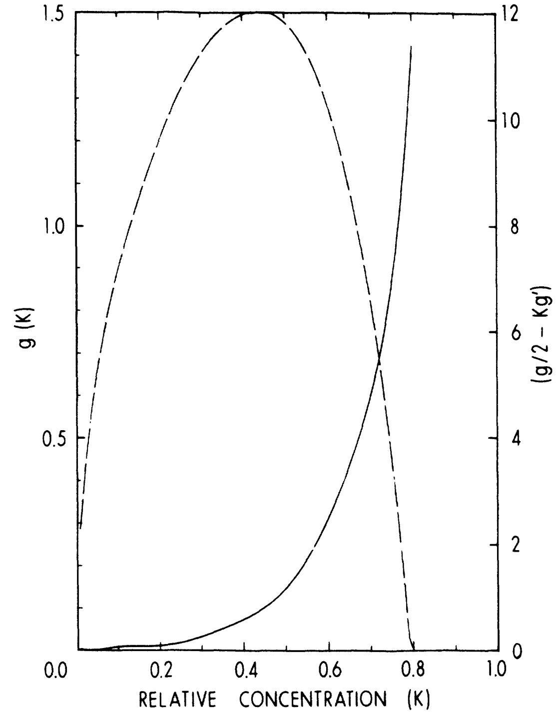

FIG. 3. The dimensionless chemical potential (dashed line, left scale) and the dimensionless derivative $(dE_F/dN_d)_c$ (solid line, right scale) plotted against relative concentration $K$ as obtained by the computer simulation.

It should be noted that Eq. (14) is valid only at small enough values of $q$, while at large $q$ the correlation is absent,[6] and $D(q)=c$. We have taken this into account by putting $D(q)=c$ for such values of $q$ for which Eq. (14) gives $D(q)>c$.

The results of the mobility calculations are given in Figs. 4(a)–4(c) for five different values of $s$ and three values of $N_{\mathrm{depl}}$. The effect of the correlation is very strong (a few orders of magnitude) at small compensation degrees $K=c/N_d$. The reason is that in this case the number of charged impurities is very small as compared with the number of neutral ones, and due to the Coulomb repulsion the distribution of charge becomes very homogeneous on a large scale. The effect is more pronounced for the thick spacer layers because, as it has been mentioned before, the harmonics with $q=s^{-1}$ give the main contributions to the scattering. But it follows from Eq. (14) that at fixed $qs$ the function $D(q)$ is proportional to $q^2$.

The sharp concentration dependence of the mobility is determined mainly by the concentration dependence of the function $(dE_F/dN_d)_c$. These results are, however, valid only for δ-doped layers. In the case of the thick doped layers the fluctuations of the coordinates of impurities in the perpendicular direction to the 2D EG should essentially decrease the mobility.

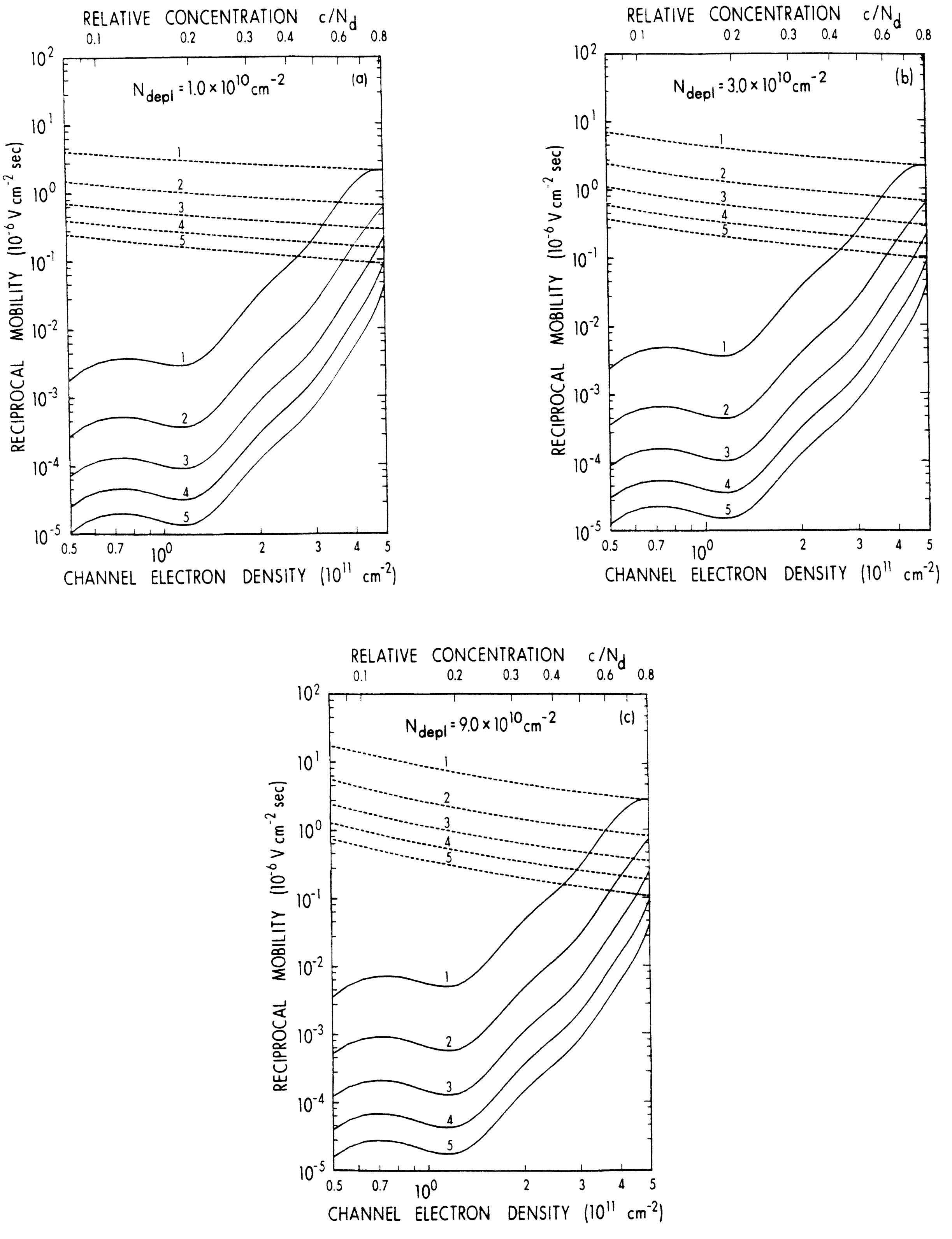

FIG. 4. Calculated low-temperature reciprocal mobility vs channel electron density $N_s$ for a $Al_xGa_{1-x}As$/GaAs heterostructure. The corresponding relative concentration $K = c/N_d$ is given in the upper scale. The results of the calculations without correlation are shown by the dotted lines. The reciprocal mobility calculated with the correlation in the framework of the equilibrium model is shown by the solid lines. The values of $s$ are as follows: 1, 10 nm; 2, 20 nm; 3, 30 nm; 4, 40 nm; and 5, 50 nm. $N_{depl} = 1.0 \times 10^{10}$ cm$^{-2}$, $3.0 \times 10^{10}$ cm$^{-2}$, and $9.0 \times 10^{10}$ cm$^{-2}$, for (a), (b), and (c), respectively.

Our main conclusion is that the correlation in the distribution of the charged impurities caused by the impurities' Coulomb interaction essentially increases the calculated values of the mobility of the channel electrons limited by the remote ion scattering. This correlation necessarily occurs if the impurities in the doped layer of a heterostructure are partly ionized and partly neutral. The effect of the correlation increases as the freezing temperature $T_0$ decreases and as the spacer thickness $s$ increases. In the equilibrium model, at small relative concentrations $c/N_d$, the correlation increases the mobility by a few orders of magnitude.

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