Influence of DX centers in the $Al_xGa_{1-x}As$ barrier on the low-temperature density and mobility of the two-dimensional electron gas in GaAs/AlGaAs modulation-doped heterostructure

Bin Yang, Zhan-guo Wang, Yong-hai Cheng, Ji-ben Liang, Lan-ying Lin, Zhan-ping Zhu, Bo Xu, and Wei Li

Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, People's Republic of China

(Received 7 November 1994; accepted for publication 2 January 1995)

In GaAs/AlGaAs modulation-doped heterostructure, adopting triangular quantum well approximation and including the seven major scattering mechanisms, we considered the existence of the DX centers in the $Al_xGa_{1-x}As$ barrier and calculated the dependence of low-temperature two-dimensional electron gas (2DEG) density and mobility on spacer layer thickness, Al composition and Si-doping concentration of the $Al_xGa_{1-x}As$ barrier. The calculated results explained the experimental results that cannot be explained by the previous studies. Our calculations demonstrate that DX centers in the $Al_xGa_{1-x}As$ barrier play an important role in determining low-temperature 2DEG density and mobility. © *1995 American Institute of Physics.*

It is well known that extremely high low-temperature electron mobility can be achieved in GaAs/AlGaAs modulation-doped heterostructures (MDH).[1,2] Such superior low-temperature transport properties attracted great attention in the fields of both fundamental physical studies[3] and high-speed device implementations.[4] To approach maximum mobility in GaAs/AlGaAs MDH, besides making extensive experimental studies, people have expended great efforts to theoretically calculate the dependence of low-temperature two-dimensional electron gas (2DEG) density and mobility on spacer-layer thickness (d),[5,6] Al composition (x),[6] Si-doping concentration (N_D),[7] and doping profile,[8] etc. But up to this date, the experimental dependence of low-temperature 2DEG density on Al composition and Si-doping concentration has not yet been successfully explained by the calculated results.[6,7,9] As for the optimum Al composition for maximum mobility, several authors[1,2,10] published their experimental results, but the mechanism is not clear so far.

Our recent study discovered that the large discrepancies between calculation and experiment in the previous studies[6,7] mainly resulted from one thing: the authors had not taken into account the existence of the DX centers in the $Al_xGa_{1-x}As$ barrier and their influence on low-temperature 2DEG density and mobility. Because these deep centers[11] hardly ionize at low temperature in the dark, neglecting their existence and their influence on 2DEG density will result in large discrepancies. In this letter, we took into account the existence of these DX centers. Adopting a triangular quantum well approximation and including the seven major scattering mechanisms in GaAs/AlGaAs MDH, we systematically calculated the dependence of low-temperature 2DEG density and mobility on Al composition (x), Si doping concentration (N_D), and spacer layer thickness. Our calculated results successfully explained the experimental results[1,2,10] that cannot be explained by the previously calculated results.[6,7]

Through experiments, Schubert and Ploog[11] concluded that when Si is doped into $Al_xGa_{1-x}As$, in the range of $0<x\leqslant 0.2$, only a shallow donor level is introduced ($E_D\approx 6$ meV); but when $0.2<x\leqslant 0.4$, a deep donor level (the level of the DX centers) is also introduced ($E_{dd}=140\pm 10$ meV), i.e., the shallow donors and the DX centers coexist in $Al_xGa_{1-x}As$ in this case. Because these deep donors result in persistent photoconductivity (PPC) effect in both GaAs/AlGaAs MDH and Si-doped $Al_xGa_{1-x}As$ epilayer ($x>0.2$),[1,11,12] so we think that in GaAs/AlGaAs MDH, the DX centers play an important role in determining low-temperature 2DEG density. We also noticed that Schubert[8] observed the influence of DX centers on the low-temperature 2DEG density in GaAs/AlGaAs MDH in his experiment. So in this letter, we use N_1 and N_d to denote the shallow donor and the deep donor concentration, respectively, then $N_D=N_l+N_d$, N_D is the total Si-doping concentration in the $Al_xGa_{1-x}As$ barrier.

Approximately, we use the following equation to calculate the shallow donor and the deep donor concentration in the Si-doped $Al_xGa_{1-x}As$ barrier according to the experimental results reported in Ref. 11:

$$\frac{N_l}{N_D}=1-4.75(x-0.2), \quad 0.2\leqslant x\leqslant 0.4. \tag{1}$$

In this letter, the low-temperature ($T=5$ K) 2DEG density and mobility are discussed. Because at 5 K in the dark, the shallow donors do not freeze out, but the deep donors hardly ionize,[11] approximately, we suppose only shallow donors contribute to 2DEG density. Let E_F denote the Fermi energy level of the GaAs/AlGaAs 2DEG system: in our calculation, when $T=5$ K in the dark, we suppose E_F is pinned at the shallow donor level ($E_D=6$ meV); N_r denotes the remote ionized impurity concentration, then $N_r\leqslant N_1$.

Adopting a triangular quantum well approximation, Fig. 1 shows the energy band diagram of the GaAs/AlGaAs MDH. Let V_b and x denote the barrier height and Al composition, respectively, then

$$V_b=\frac{70}{100}\times 1.247x=872.9x. \tag{2}$$

 0003-6951/95/66(11)/1406/3/$6.00

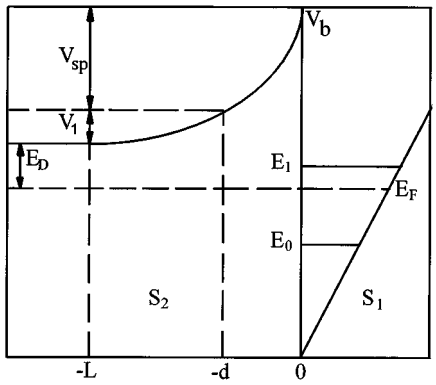

FIG. 1. Energy band diagram of GaAs/AlGaAs MDH. S_1 is GaAs layer, S_2 is $Al_xGa_{1-x}As$ layer, E_0, E_1, and E_F are the ground state subband energy level, first excited state subband energy level, and the Fermi energy level, respectively.

The potential energy drop on the spacer layer (d) is denoted as V_{sp},

$$V_{sp}=\frac{e^2 d(N_s+N_{depl})}{\epsilon_0\epsilon_2}, \tag{3}$$

where ϵ_2 is the dielectric constant of $Al_xGa_{1-x}As$ ($\epsilon_2=12.1$), N_s is 2DEG density, N_{depl} is the fixed space charge in the GaAs layer, and e is electron charge. Let $N_{depl}=5\times10^{10}$ cm^{-2} in our calculation.[13] The potential energy drop within the Si-doped $Al_xGa_{1-x}As$ layer is denoted as V_1,

$$V_1=\frac{e^2(N_s+N_{depl})^2}{2\epsilon_0\epsilon_2 N_r}. \tag{4}$$

When the 2DEG system is in equilibrium with the donors in the $Al_xGa_{1-x}As$ layer, we have the equation:

$$V_b=E_0+\frac{\pi\hbar^2 N_s}{m}+E_D+V_1+V_{sp}, \tag{5}$$

where E_0 (Ref. 14) is the 2DEG ground state subband energy level calculated by the triangular quantum well approximation, m is the electron effective mass, $m=0.067m_0$, E_D is the binding energy of the shallow donors measured from the bottom of the $Al_xGa_{1-x}As$ conduction band. From Eqs. (1)–(5) and E_0,[14] we have the relation of x, d, N_s, N_r, and N_D, thus the dependence of 2DEG density and mobility on d, x, N_s, and N_D can be calculated.[13] When only the ground state subband is occupied by electrons, 2DEG mobility[5,13] is limited by deformation potential, piezoelectric acoustic, polar optical, remote ionized impurity, background ionized impurity, alloy disorder, and interface roughness scattering.[6,12] Including these seven major scattering mechanisms, both our calculated temperature and 2DEG density dependence of 2DEG mobility[12,13] are in good agreement with our experimental data. In order to eliminate any ambiguities, AlGaAs/GaAs interface roughness is supposed to be the same, $\Delta=2.83$ Å, $\Lambda=6$ Å, in this letter. Influence of interface roughness scattering on 2DEG mobility is reported in another paper.[12]

Figure 2 shows the calculated dependence of 2DEG density on spacer layer thickness for $0.2\leqslant x\leqslant 0.4$. Obviously,

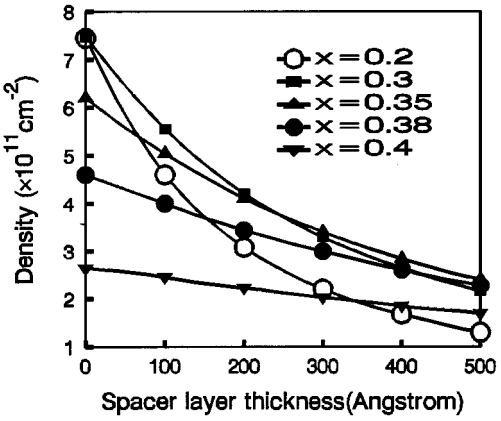

FIG. 2. Calculated dependence of 2DEG density on spacer layer thickness, parameters used in our calculation are background ionized impurity concentration $N_b=2.5\times10^{14}$ cm^{-3}, $N_D=5\times10^{17}$ cm^{-3}, $T=5$ K.

2DEG density decreases with increasing spacer layer thickness. When $x=0.4$, N_s has the smallest value. This is because when $x=0.4$, most of the Si atoms become deep donors, only the small amount of shallow donors contribute to low-temperature 2DEG density. For larger spacer layer thickness ($d>200$ Å), when $x\sim0.35$, 2DEG density is higher than the others. We grew GaAs/AlGaAs MDH by MBE, with $N_D=5\times10^{17}$ cm^{-3}, $x=0.3$; when $d=150$ Å and $d=250$ Å, respectively, the measured 2DEG densities at 5 K are 5×10^{11} cm^{-2} and 3.4×10^{11} cm^{-2}, respectively. Obviously, our calculated results for $x=0.3$ are in agreement with these experimental data. The results in Fig. 2 are also in agreement with Hiyamizu's experimental results.[15] The previous authors did not consider the existence of DX centers. They roughly supposed that the Fermi level was pinned at the donor level whose binding energy was estimated to be 50 meV (Ref. 6) or 100 meV,[16] thus resulting in large discrepancies. At room temperature or when 2DEG density is saturated with illumination at low temperatures, we suppose E_F is pinned at the deep donor level ($E_{dd}\approx140$ meV). Then we obtained approximately the same results reported in Ref. 9.

The calculated dependence of 2DEG mobility on spacer layer thickness for $0.2\leqslant x\leqslant 0.4$ is shown in Fig. 3. Obviously,

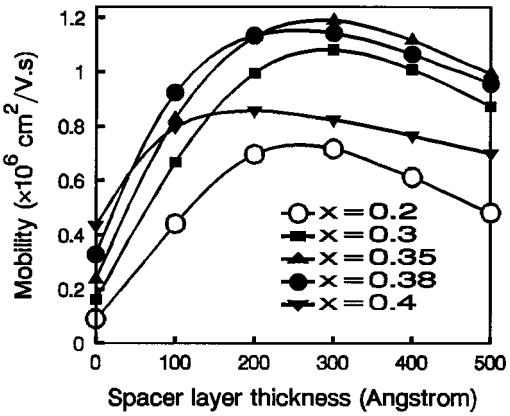

FIG. 3. Calculated dependence of 2DEG mobility on spacer layer thickness. Parameters used in our calculation are background ionized impurity concentration $N_b=2.5\times10^{14}$ cm^{-3}, $N_D=5\times10^{17}$ cm^{-3}, $T=5$ K.

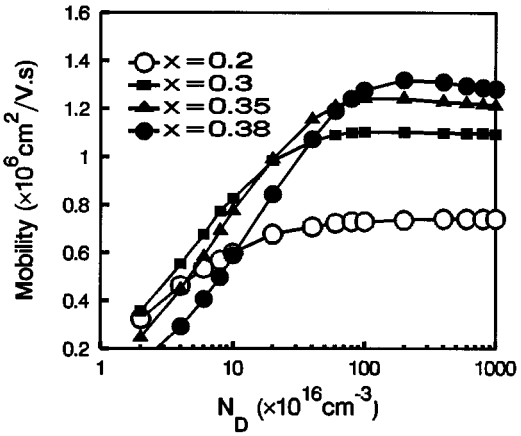

FIG. 4. Calculated dependence of 2DEG mobility on Si-doping concentration in $Al_xGa_{1-x}As$ barrier. Parameters used in our calculation are background ionized impurity concentration $N_b=2.5\times10^{14}$ cm^{-3}, $d=300$ Å, $T=5$ K.

for $d<200$ Å, when $x\sim0.38$, 2DEG mobility is larger than the others; this result is in agreement with the experimental results by Drummond *et al.*[10] Drummond *et al.* fabricated a series of GaAs/AlGaAs MDH by MBE. The spacer layer thickness of their samples was 75 Å. Their results demonstrated that when $x=0.38$, the maximum 2DEG mobility was obtained. Figure 3 also shows that for $d>200$ Å, when $x\sim0.35$, 2DEG mobility is larger than the others. This result is in agreement with experimental results of Pfeifier[1] and Saku.[2] In Fig. 3, when $x=0.2$ or $x=0.4$, 2DEG mobility is much smaller. This is because when $x=0.2$, the barrier height is smaller ($V_b\approx200$ meV) which results in strong alloy disorder scattering;[12] 2DEG mobility is small. When $x=0.4$, because of the influence of the DX centers, 2DEG density is much smaller (Fig. 2), which results in very strong ionized impurity scattering, and 2DEG mobility is also small. So Al composition (x) is a very important parameter in GaAs/AlGaAs MDH. In the range of $0.2\leqslant x\leqslant0.4$, larger values of x enhance the barrier height, which is good for obtaining higher low-temperature 2DEG density and mobility; but larger values of x also enhance the amount of DX centers, which are unfavorable for obtaining high low-temperature 2DEG density and mobility. Both these two factors should be considered in choosing the proper value of x. The previous authors did not consider the existence of the DX centers in their calculation, so their calculated results cannot explain the experimental results.

It is known from Fig. 4 that for $0.2\leqslant x\leqslant0.38$, when 1×10^{16} cm$^{-3}<N_D<1\times10^{18}$ cm^{-3}, 2DEG mobility increases steeply with increasing N_D. But when $N_D>1\times10^{18}$ cm^{-3}, 2DEG mobility levels off with increasing N_D. These results show the same dependence of 2DEG mobility on Si-doping concentration as Saku's experimental results.[2] Our calculation demonstrated that when 1×10^{16} cm$^{-3}<N_D<1\times10^{18}$ cm^{-3}, 2DEG density increases steeply with increasing N_D,[13] so the screening effect of 2DEG to ionized impurity scattering increases with increasing N_D, which results in increasing 2DEG mobility. But when $N_D>1\times10^{18}$ cm^{-3}, 2DEG density is high enough ($N_s>3.5\times10^{11}$ cm^{-2}) to make interface roughness scattering and alloy disorder scattering begin to effectively scatter the 2DEG,[6,12] which limits the further increase in 2DEG mobility. It was reported[2] when $N_D>1\times10^{18}$ cm^{-3}, parallel conduction becomes noticeable, so we should choose $N_D\leqslant1\times10^{18}$ cm^{-3}.

In conclusion, the influence of the DX centers on low-temperature 2DEG density and mobility is studied and the dependence of low-temperature 2DEG density and mobility on 2DEG structure parameters is calculated in this letter. Our calculated results are in good agreement with experimental results and demonstrate that the deep donors in the AlGaAs barrier play an important role in determining the low-temperature 2DEG density and mobility in GaAs/AlGaAs MDH.

[1] L. Pfeiffer, K. W. West, H. L. Stormer, and K. W. Baldwin, Mater. Res. Soc. Symp. Proc. **45**, 3 (1989).
[2] T. Saku, Y. Hirayama, and Y. Horikoshi, Jpn. J. Appl. Phys. **30**, 902 (1991).
[3] D. C. Tsui and H. L. Stormer, IEEE J. Quantum Electron. **QE-22**, 1711 (1989).
[4] T. Minura, Surf. Sci. **113**, 454 (1982).
[5] W. Walukiewicz, H. E. Ruda, J. Lagowski, and H. C. Gatos, Phys. Rev. B **30**, 4571 (1984).
[6] T. Ando, J. Phys. Soc. Jpn. **51**, 3900 (1982).
[7] K. Lee, M. Shur, T. J. Drummond, and H. Morkoc, J. Appl. Phys. **54**, 2093 (1983).
[8] E. F. Schubert, L. Pfeiffer, K. W. West, and A. Izabelle, Appl. Phys. Lett. **54**, 1350 (1989).
[9] E. F. Schubert, *Doping in III–V Semiconductors* (Cambridge University Press, New York, 1993), p. 398.
[10] T. J. Drummond, W. Kopp, R. Fischer, and H. Morkoc, J. Appl. Phys. **52**, 1028 (1982).
[11] E. F. Schubert and K. Ploog, Phys. Rev. B **30**, 7021 (1984).
[12] B. Yang, Y.-h. Cheng, Z.-g. Wang, J.-b. Liang, Q.-w. Liao, L.-y. Lin, Z.-p. Zhu, B. Xu, W. Li, Appl. Phys. Lett. **65** 3329 (1994).
[13] B. Yang, Y.-h. Cheng, Z.-g. Wang, J.-b. Liang, Q.-w. Liao, L.-y. Lin (unpublished).
[14] T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[15] S. Hiyamizu, J. Saito, K. Nanbu, and T. Ishikawa, Jpn. J. Appl. Phys. **22**, L609 (1983).
[16] F. Stern, Appl. Phys. Lett. **43**, 974 (1983).