Spacer layer thickness fluctuation scattering in a modulation-doped $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum well*

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(Received 10 February 2012; revised manuscript received 19 March 2012)

We theoretically study the influence of spacer layer thickness fluctuation (SLTF) on the mobility of a two-dimensional electron gas (2DEG) in the modulation-doped $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum well. The dependence of the mobility limited by SLTF scattering on spacer layer thickness and donor density are obtained. The results show that SLTF scattering is an important scattering mechanism for the quantum well structure with a thick well layer.

Keywords: spacer layer thickness fluctuation scattering, interface roughness scattering, 2DEG, mobility

PACS: 73.40.Kp, 73.21.Fg **DOI:** 10.1088/1674-1056/21/10/107305

1. Introduction

In the $GaAs/Al_xGa_{1-x}As$ modulation-doped heterostructure (MDH), due to the spacer layer between the channel and doping region, the electrons are confined in the GaAs well and separated from the ionized impurities, reducing the Coulombic scattering rate,[1,2] which is the main scattering mechanism at low temperature. However, the spacer layer thickness fluctuation due to the interface roughness will cause the fluctuation of the two-dimensional electron gas (2DEG) sheet density, which results in a new scattering potential. In the previous work, we have studied spacer layer thickness fluctuation (SLTF) scattering with a triangular potential well in $Al_xGa_{1-x}As/GaAs$ MDHs.[3] We have shown that SLTF scattering is more important than interface roughness scattering when the donor density is high enough. In the present work, we formulate SLTF scattering with a square potential well in the modulation-doped $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum well structure and compare it with interface roughness scattering. At present, many groups have been studying the effects of some scattering mechanisms on group-III nitride semiconductors, for example, Zhang Jinfeng *et al.*[4] have studied the properties of 2DEG mobility in the InAlN/GaN material. Our results from the $GaAs/Al_xGa_{1-x}As$ quantum well can provide a reference point for further study.

2. Theory

A schematic diagram of the structure of the modulation-doped $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum well used in the present study is shown in Fig. 1. In a simple case, only one $Al_xGa_{1-x}As$ barrier layer is modulation-doped, which consists of an undoped region (the spacer layer) with thickness L_s and a doped region. Then, the 2DEG sheet carrier density can be expressed as[5,6]

$$n_s = \sqrt{\frac{2\varepsilon_s\varepsilon_0 N_D v}{e} + N_D^2 \left(L_s + \Delta L_s\right)^2} - N_D L_s, \quad (1)$$

where ε_0 is the vacuum dielectric constant, $\varepsilon_s = 13.18$

*Project supported by the National Natural Science Foundation of China (Grant Nos. 60976008, 61006004, 61076001, and 10979507), the National Basic Research Program of China (Grant No. A000091109-05), and the National High Technology Research and Development Program of China (Grant No. 2011AA03A101).

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is the relative dielectric constant of the $Al_xGa_{1-x}As$ (here we assume that it equals that of the GaAs), e is the free electron charge, N_D is the donor density in the $Al_xGa_{1-x}As$-doped layer, the Al mole fraction in the $Al_xGa_{1-x}As$ barrier is $x = 0.3$, the modified constant ΔL is $\sim$ 80 Å, (1 Å=0.1 nm),[7,8] and v is the band bending, which is determined by the following expression:[5,6]

$$ev = \Delta E_C - \delta - E_F, \tag{2}$$

where the conduction-band discontinuity ΔE_C between $Al_{0.3}Ga_{0.7}As$ and GaAs is 0.248 eV,[9] E_F (0.025 eV at 77 K)[6] is the Fermi level with respect to the GaAs conduction-band-edge energy, and δ (0.025 eV at 77 K)[6] is the energy difference between the conduction band of $Al_{0.3}Ga_{0.7}As$ and E_F.

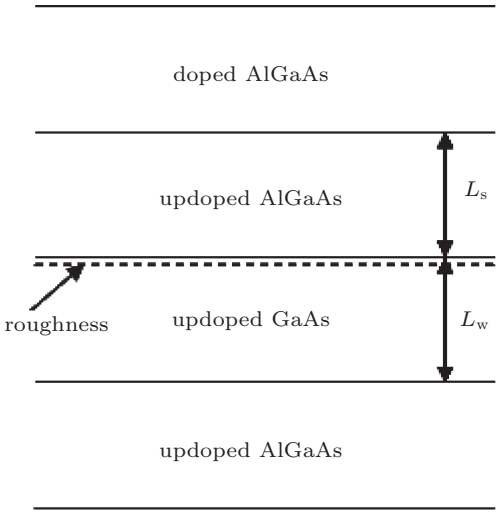


Fig. 1. Schematic diagram of a modulation-doped $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum well.

From Eq. (1), it is easy to find that the 2DEG sheet density n_s is determined by the spacer layer thickness L_s and the donor density N_D. In this work, for simplicity, we assume that the interface between the doped layer and the spacer layer is smooth (as shown in Fig. 1). Then, due to the roughness of the interface between the spacer layer and the well layer, there is a change $\Delta(r)$ in the spacer layer thickness, resulting in the fluctuation of the 2DEG sheet carrier density, which can be expressed as

$$\begin{aligned}\Delta n_s(r) &= \frac{dn_s}{dL_s}\Delta(r) \\ &= \left(\frac{N_D^2 L_s}{\sqrt{2\varepsilon_0\varepsilon_s N_D v/e + N_D^2 (L_s + \Delta L_s)^2}} - N_D\right)\Delta(r). \end{aligned}\tag{3}$$

In this study, we only consider the ground subband. Thus, for this structure, the conduction-band structure can be approximated by a square potential well with an infinitely high potential barrier. In this well, the wave function of electrons in the ground subband is given by[10]

$$\psi(z) = \sqrt{\frac{2}{L_w}}\sin\left(\frac{\pi z}{L_w}\right), \quad 0 < z < L_w, \tag{4}$$

where L_w is the well width (as shown in Fig. 1). Accordingly, from Eqs. (3) and (4) the change of charge density can be obtained as

$$\delta\rho = e\Delta n_s(r)\frac{2}{L_w}\sin^2\left(\frac{\pi}{L_w}z\right). \tag{5}$$

The additional electrostatic potential φ is produced by Poisson's equation[11]

$$-\left(\nabla^2 + \frac{\partial^2}{\partial z^2}\right)\varphi(r,z) = \frac{\rho_{ind} + \delta\rho}{\varepsilon_0\varepsilon_s}, \tag{6}$$

where ρ_{ind} is the induced charge density. It can be obtained by[11,12]

$$\rho_{ind} = -\frac{m^* e^2}{\pi\hbar^2}\psi^2(z)\,\delta\tilde{\phi}(q), \tag{7}$$

where $m^* = 0.067m_e$ (m_e is the free electron mass) is the effective mass and $\delta\tilde{\phi}(q)$ is denoted by $\int_0^{L_w}\delta\phi(q,z)\,\psi^2(z)\,dz$ with $\delta\phi(q,z)$ being the Fourier transform of $\delta\phi(r,z)$ on r. Substituting the above equation into Eq. (6) and performing the Fourier transform on both r and z, we find

$$\begin{aligned}\left(q^2 + k_z^2\right)\delta\phi(q,k_z) = &-\frac{m^* e^2}{\pi\hbar^2\varepsilon_s\varepsilon_0}v(k_z)\,\delta\tilde{\phi}(q) \\ &-\frac{e\Delta n_s v(k_z)}{\varepsilon_s\varepsilon_0},\end{aligned}\tag{8}$$

where $v(k_z) = \int_0^{L_w} e^{ik_z z}\psi^2(z)dz$. It is easy to show that

$$\delta\tilde{\phi}(q) = \int_{-\infty}^{\infty}\frac{dk_z}{2\pi}\delta\phi(q,k_z)\,v^*(k_z). \tag{9}$$

Substituting the above equation into Eq. (8), we obtain

$$\delta\tilde{\phi}(q) = -\frac{\frac{e}{\varepsilon_s\varepsilon_0}\frac{dn_s}{dL_s}I(q)\,\Delta(q)}{1 + \frac{m^* e^2}{\pi\hbar^2\varepsilon_s\varepsilon_0}I(q)}, \tag{10}$$

where

$$I(q) = \int\frac{dk_z}{2\pi}\frac{|v(k_z)|^2}{q^2 + k_z^2}.$$

Equation (10) acts as a scattering potential. Then, the square of the scattering matrix element within the ground subband can be expressed as

$$|M(q)|^2 = \langle|\delta V(q)|\rangle \approx e^2 \left| -\frac{\frac{e}{\varepsilon_s\varepsilon_0}\frac{\mathrm{d}n_s}{\mathrm{d}L_s}I(q)}{1+\frac{m^*e^2}{\pi\hbar^2\varepsilon_s\varepsilon_0}I(q)} \right|^2 S(q), \quad (11)$$

where $S(q) = \pi\Delta^2\Lambda^2\exp(-q^2\Lambda^2/4)$ is the power spectrum of $\Delta(q)$[13] with Δ and Λ being the average height of the spacer layer thickness fluctuation and the lateral size, respectively. From the relationship between the inverse scattering time $1/\tau_s$ and the scattering matrix element $|M(q)|^2$,[14] we have

$$\frac{1}{\tau_s} = \frac{1}{2\pi\hbar}\int \mathrm{d}^2k' |M(q)|^2 (1-\cos\theta)\,\delta(E_k - E'_k), \quad (12)$$

where θ denotes the angle between the initial and final wave vectors k and k'. In this study, for the two-dimensional scattering vector q, we use the relationship of $q = 2k_F\sin(\theta/2)$ with $k_F = \sqrt{2\pi n_s}$.[14] Finally, the mobility of the 2DEG limited by SLTF scattering μ can be obtained from the following equation:

$$\mu = \frac{e\tau_s}{m^*}. \quad (13)$$

3. Results and discussion

From Eqs. (12) and (13), we find that the mobility limited by the SLTF scattering depends on spacer layer thickness L_s and donor density N_D. For the square well with infinite barrier height, $I(q)$ equals $1/(2q)$. Thus, the mobility limited by SLTF scattering is not influenced by well layer thickness L_w. However, for the square well with a finite barrier height, part of the electron wavefunctions will penetrate into the barrier. With well width L_w decreasing, the extent of the wavefunctions penetrating into the barrier increases. Therefore, the 2DEG sheet carrier density n_s in the well decreases, that is, the probability $|\psi(x)|^2$ of the electrons in the well reduces, which leads to a reduction of $I(q)$ where

$$I(q) = \int \frac{\mathrm{d}k_z}{2\pi}\frac{|v(k_z)|^2}{q^2+k_z^2},$$

and

$$v(k_z) = \int_0^{L_w} \mathrm{e}^{\mathrm{i}k_z z}\psi^2(z)\mathrm{d}z,$$

so that the scattering potential drops. Accordingly, the mobility in the square well with the finite barrier height is higher than that in the square well with the infinite barrier height. In this work, we consider that the well layer thickness L_w is large enough, and the finite barrier height can be approximated by the infinite barrier height.

Figure 2 shows the mobilities limited by the SLTF scattering as a function of spacer layer thickness L_s for different values of donor density N_D. Initially, the mobility limited by the SLTF scattering increases slightly with the increase of spacer layer thickness L_s. However, when the spacer layer thickness exceeds a certain value, the mobility rapidly increases. Such a dependence results mainly from the dependence of the square of the matrix element M^2, which is determined by the rate $\mathrm{d}n_s/\mathrm{d}L_s$ for the fixed thickness fluctuation parameter (see Eq. (10)). The rate $\mathrm{d}n_s/\mathrm{d}L_s$ decreases with the increase of spacer thickness L_s. For small L_s, the first term on the right-hand side of Eq. (3) can be neglected, and then the rate $\mathrm{d}n_s/\mathrm{d}L_s$ is affected only by donor density N_D. If the L_s is large enough, the term that may be compared with N_D or even nearly equals N_D cannot be neglected. Thus, the mobility will rapidly increase with L_s further increasing L_s. In the theoretical model used in this study, the spacer layer thickness fluctuation height and lateral size are assumed to be 0.283 nm and 5 nm respectively. The Al mole fraction x in $Al_xGa_{1-x}As$ is assumed to be 0.3.

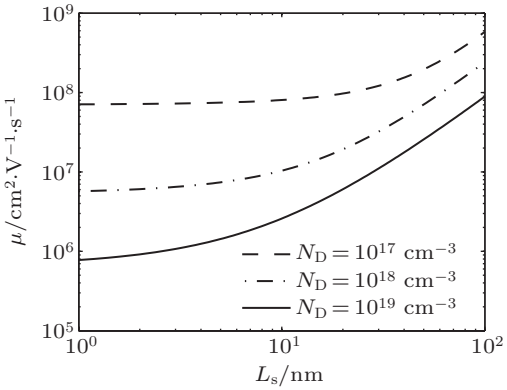


Fig. 2. Calculated mobilities limited by SLTF scattering as a function of spacer layer thickness L_s for different values of donor density N_D. The Al mole fraction x in the $Al_xGa_{1-x}As$ barrier is 0.3. And the parameters of spacer layer thickness fluctuation Δ and Λ are 0.283 nm and 5 nm, respectively.

From Eq. (3), it is also easy to find that the rate $\mathrm{d}n_s/\mathrm{d}L_s$ increases with the increase of donor density N_D. Accordingly, the mobility limited by the SLTF scattering decreases with N_D raising for the

fixed spacer layer thickness L_s. The results are shown in Fig. 3.

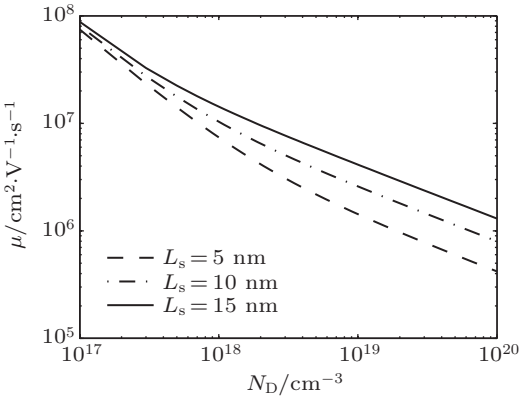


Fig. 3. Calculated mobilities limited by SLTF scattering as a function of donor density N_D for different values of spacer layer thickness L_s. The spacer layer thickness fluctuation parameters and Al mole fraction in the $Al_xGa_{1-x}As$ barrier are the same as those in Fig. 2.

Since experimentally measured Hall mobility has contributions from many other scattering mechanisms, we can gauge only the relative importance of this form of scattering by comparing the interface roughness scattering, which is an important scattering for the 2DEG mobility in the square well. The mobility limited by SLTF scattering (10^6 cm^2/V·s–10^8 cm^2/V·s, as shown in Figs. 2 and 3) is much higher than that limited by the interface roughness scattering for thin quantum wells (10^3 cm^2/V·s–10^5 cm^2/V·s),[9] therefore, the SLTF can be neglected. However for a thick well layer, e.g. 30 nm, due to the fact that it is proportional to L_w^6,[10] the mobility limited by the interface roughness scattering will reach 10^8 cm^2/V·s or even higher. In this case, both the mobility limited by SLTF scattering and that limited by interface roughness scattering are on the same order of magnitude. Accordingly, for high mobility quantum well structure[15] which has a thick well layer, the SLTF scattering cannot be neglected.

4. Conclusion

In the present paper, we calculated the mobility limited by the SLTF scattering in a modulation-doped $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum well. In this work, we considered the well layer thickness L_w to be large enough, the finite barrier height can be approximated by the infinite barrier height. So, for the square well with infinite barrier height, the mobility limited by the SLTF scattering is not influenced by the well layer thickness L_w. In addition, it can be concluded that the SLTF scattering mobility is affected only by donor density N_D for the thin spacer layer L_s, and the mobility limited by the SLTF scattering decreases with N_D rising for the fixed spacer layer thickness L_s. When L_s is large enough, mobility limited by the SLTF scattering will rapidly increase with L_s further increasing L_s. The SLTF scattering is important for a high mobility quantum well structure which has a thick well layer. In such a structure, it can be compared with the interface roughness scattering.

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