Dislocation core effect scattering in a quasitriangle potential well

Xiaoqing Xu, Xianglin Liu,[a] Shaoyan Yang, Jianming Liu, Hongyuan Wei, Qinsheng Zhu,[b] and Zhanguo Wang

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

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A theory of scattering by charged dislocation lines in a quasitriangle potential well of $Al_xGa_{1-x}N/GaN$ heterostructures is developed. The dependence of mobility on carrier sheet density and dislocation density is obtained. The results are compared with those obtained from a perfect two-dimensional electron gas and the reason for discrepancy is given. © *2009 American Institute of Physics*. [DOI: 10.1063/1.3098356]

The promising possibilities of large gap semiconductors, such as GaN, AlN, and AlGaN alloys, together with their heterostructures, for advanced photonic and electronic device applications have recently raised some attention for the experimental and theoretical studies of their transport properties.[1,2] $Al_xGa_{1-x}N/GaN$ heterostructures have been an area of active research, owing to the demonstration of high power microwave high electron mobility transistors. In practice, the layers are mainly grown by epitaxial methods such as metal-organic vapor-phase epitaxy and molecular beam epitaxy on highly lattice-mismatched sapphire substrates.[3,4] Transmission electron microscopy observation reveals, GaN is generally characterized by very large dislocation densities (typically in the range of 10^8-10^{10} cm^{-2}). Dislocation scattering in three-dimensional bulk GaN has been analyzed with great efforts,[5–7] however, it was not so much considered in $Al_xGa_{1-x}N/GaN$ two-dimensional electron gas (2DEG). Jena *et al.*[8] developed a typical theory of dislocation scattering in a perfect 2DEG. He elicited the screened potential of a charged dislocation from the scattering potential of a point charge, and gave the dependence of mobility on 2DEG sheet density and dislocation density. However, a real $Al_xGa_{1-x}N/GaN$ heterostructure has a quasitriangle potential well determined by solving the Poisson and Schrödinger equations self-consistently. Ando *et al.*[9] and Stern and Howard[10] have made efforts to bring forward the Fourier transferred screened potential of a point charge in both cases of zero and nonzero thickness for the charge distribution of electrons. In this paper, we deduce the Fourier transferred screened potential of a dislocation based on a more realistic case of a quasitriangle potential well approximation, and calculate the electron mobility in $Al_xGa_{1-x}N/GaN$ heterostructures. Afterward, we take a comparison of our results with those obtained by Jena *et al.*[8] from a perfect 2DEG, and attempt to give reasons for the discrepancy.

A schematic diagram of the conduction-band structure of a $Al_xGa_{1-x}N/GaN$ heterostructure near the interface is shown in Fig. 1. In a simple case, the GaN layer (at $z \geq 0$) and the $Al_xGa_{1-x}N$ layer (at $z \leq 0$) are both nominally undoped with all the electrons originating from surface states. Suppose the $Al_xGa_{1-x}N$ barrier is grown pseudomorphically on a relaxed GaN layer, a polarization field will be present at the $Al_xGa_{1-x}N/GaN$ interface. Thus, the electrons are confined to the trianglelike well at the interface, leading to a quantization of the energy-band structure into subbands. In this paper, only the ground subband is taken into consideration and the areal (2D) electron concentration is labeled as N_s. The simplest approximation for the wave function $\chi(z)$ and the charge distribution of electrons $g(z)$ is the one made for inversion layers by Fang and Howard[11]

$$g(z) = |\chi(z)|^2 = \frac{b^3}{2} z^2 e^{-bz}, \tag{1}$$

where b is the variational parameter.[3]

The dielectric constants $\varepsilon_0\varepsilon_b$ for GaN and AlN are close so we treat them uniformly in this paper. The additional electrostatic potential ϕ produced by an external source is related to the charge density by Poisson's equation. Using the charge distribution of $g(z)$, the relation can be expressed as[9]

$$\nabla^2\phi - 2q_s\phi(r)g(z) = -\frac{4\pi\rho_{\text{ext}}}{\varepsilon_0\varepsilon_b}. \tag{2}$$

Here ρ_{ext} is the external charge density, r is the in-plane vector, and $q_s = 2/a_B^*$ is the 2D Thomas Fermi wave vector, with a_B^* being the effective Bohr radius in the material. To find the screened Coulomb potential for our 2D system, we use a conventional Fourier–Bessel expansion for the potential $\phi(r,z) = \int_0^\infty qA_q(z)J_0(qr)dq$, where J_0 is the zero-order

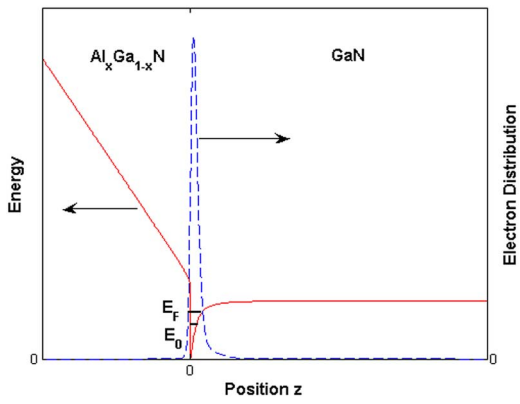

FIG. 1. (Color online) Schematic diagram of the energy-band structure in a $Al_xGa_{1-x}N/GaN$ heterostructure, showing the ground subband (E_0), Fermi energy (E_F), and the charge distribution of electrons (blue curve) in the quasitriangle well.

[a]Electronic mail: xlliu@red.semi.ac.cn.
[b]Electronic mail: qszhu@semi.ac.cn.

Bessel function, $A_q(z)$ is the Fourier–Bessel coefficient, and q is the in-plane wave vector. The average potential felt by the electrons is

$$\bar{\phi}(r) = \int_0^\infty g(z)\phi(r,z)dz, \tag{3}$$

whose Fourier–Bessel transform is labeled as $\bar{A}_q$. As in the case of a point charge located at $z=z_0$, $\bar{A}_q$ can be divided into $\bar{A}_{ql}$ (for $z_0 \leq 0$) and $\bar{A}_{qr}$ (for $z_0 \geq 0$),

$$\bar{A}_{ql} = \frac{e^2}{2\varepsilon_0\varepsilon_b}\frac{P_0 e^{qz_0}}{q+q_sP_{av}}, \tag{4}$$

$$\bar{A}_{qr} = \frac{e^2}{2\varepsilon_0\varepsilon_b}\frac{P(z_0)}{q+q_sP_{av}}. \tag{5}$$

The parameters P_0, P_{av}, and $P(z_0)$ are all functions of q and b, and the detailed expressions for them can be referred to Ando *et al.*[9]

As a dislocation can be modeled by a line of charge, we deduce the screened dislocation potential by integrate over the dislocation line with charge density ρ_L,

$$\bar{A}(q) = \int_{-\infty}^0 \bar{A}_{ql}dz_0 + \int_0^\infty \bar{A}_{qr}dz_0 = \frac{e\rho_L}{2\varepsilon_0\varepsilon_b}\frac{P_0}{(q+q_sP_{av})q} + \begin{cases} \dfrac{e\rho_L}{2\varepsilon_0\varepsilon_b}\dfrac{1}{(q+q_sP_{av})}\dfrac{b^3}{(b-q)^3}\left[\dfrac{1}{q}-\dfrac{a_0}{b}-\dfrac{a_1}{b^2}-\dfrac{2a_2}{b^3}\right] & \text{for(b} \neq \text{q)} \\ \dfrac{e\rho_L}{2\varepsilon_0\varepsilon_b}\dfrac{1}{(q+q_sP_{av})}\dfrac{15}{8b} & \text{for(b = q).} \end{cases} \tag{6}$$

ρ_L is given to a good approximation by ef/c_0, where c_0 is the lattice spacing in the (0001) direction of wurtzite GaN, and f is the fraction of filled states. Then, according to Xu *et al.*,[12] the differential cross-section $\sigma(\theta)$ can be obtained.

$$\sigma(\theta) = \frac{2\pi m^*}{\hbar^3 v}\left|\int_0^\infty \bar{\phi}(r)J_0(qr)rdr\right|^2,$$

$$= \frac{m^*}{2\pi\hbar^3 v}|\bar{A}(q)|^2, \tag{7}$$

where θ is the deflection angle of the particles from their original direction of motion, ν is the electron velocity, and m^* is the effective electron mass. Since there are N_{dis} dislocation lines piercing the 2DEG per unit area, using the screened potential given by Eq. (6), the scattering rate for a degenerate 2DEG is given by

$$\frac{1}{\tau_{\text{dis}}^{2D}} = N_{\text{dis}} \cdot \frac{m^*}{2\pi\hbar^3} \cdot 2\int_0^\pi |\bar{A}(q)|^2(1-\cos\theta)d\theta. \tag{8}$$

The formula for scattering rate we have obtained in Eq. (8) is essentially the same as what is used by Jena *et al.*,[8]

$$\frac{1}{\tau_{\text{dis}}^{2D}} = N_{\text{dis}} \cdot \frac{m^*}{2\pi\hbar^3 k_F^3} \cdot \int_0^{2k_F} |\bar{A}(q)|^2 \frac{q^2 dq}{\sqrt{1-(q/2k_F)^2}}. \tag{9}$$

In fact, Eqs. (8) and (9) are the same by transforming the integral variable q in Eq. (9) into θ, using the relation of $q = 2k_F \sin(\theta/2)$ with $k_F = \sqrt{2\pi N_s}$ (Ref. 9), and N_s being 2DEG density. Therefore, the difference in the scattering rate can only originate from the different expressions for the potential $\bar{A}(q)$ in the two equations. Based on $g(z)$, the function for charge distribution, we obtain

$$\lim_{b\to\infty} g(z) = \lim_{b\to\infty}\frac{b^3}{2}z^2e^{-bz} = \begin{cases} \infty & \text{for(z = 0),} \\ 0 & \text{for(z} \neq \text{0),} \end{cases} \tag{10}$$

and

$$\int_0^\infty g(z)dz = \int_0^\infty \frac{b^3}{2}z^2e^{-bz}dz = 1, \tag{11}$$

for any value of b, and then for any value of N_s,[3] which means that the charge distribution function used for a quasitriangle well can be converted to $\delta(z)$ for a perfect 2DEG. Thus, using the limiting qualification $b\to\infty$, the parameters P_0, P_{av}, and $P(z_0)$ in Eqs. (4) and (5) can be transformed as

$$P_0 \to 1, \quad P_{av} \to 1, \quad P(z_0) \to e^{-qz_0},$$

so that $\bar{A}(q)$ in Eq. (6) can be simplified as

$$\bar{A}(q) = \frac{e\rho_L}{2\varepsilon_0\varepsilon_b}\frac{2}{(q+q_s)q}, \tag{12}$$

which is just the screened potential for dislocation scattering in the ideal 2DEG. As discussed above, the effect of dislocation scattering on transport in a quasitriangle well can be reverted to the same as the case of a perfect 2DEG, of which the typical result has been deduced by Jena *et al.*[8] Therefore, our theory developed for dislocation core effect scattering in a quasitriangle well should be more reasonable for general cases.

The 2DEG mobilities inhibited by dislocation scattering with different carrier densities and different dislocation densities are plotted in Fig. 2, where the result of Jena *et al.*[8] on perfect 2DEG is also presented for a comparison. It can be seen that the result of Jena *et al.*[8] presented here is not totally the same as in his paper. That is because Jena *et al.*[8] used an approximation of $\tau_{\text{dis}}^{2D} \propto k_F^4/(1.84k_F/q_s - 0.25)$, while in our study, we treat it in its original form without any approximation. It is clear that our mobilities are lower than those obtained by Jena *et al.*[8] The reason is that 2DEG in a quantum well with nonzero thickness experiences weaker screening than that of the ideal 2DEG. Without regard to screening effect, as for a point charge located at $z_0 < 0$, the potential felt by the electrons in a quantum well with nonzero thickness is weaker than the case of an ideal 2DEG, due to a

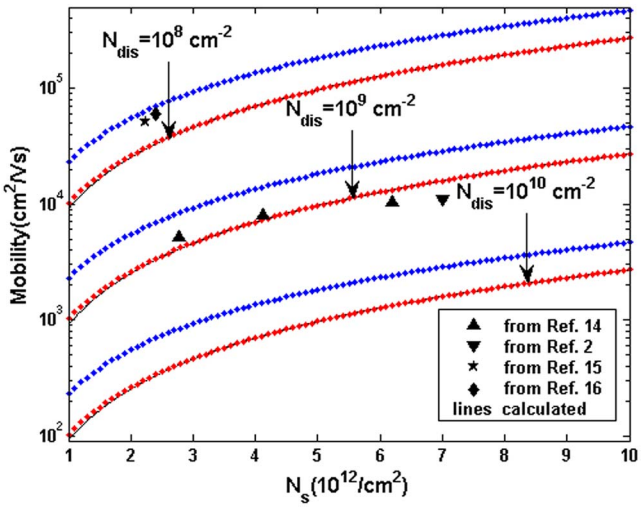

FIG. 2. (Color online) Dislocation scattering inhibited 2DEG mobility. Calculated mobilities for three different dislocation densities have been shown (red curves), and the result of Jena *et al.* (Ref. 9) on perfect 2DEG is presented for comparison (blue curves). Our result predicts an approximate $N_s^{1.4734}/N_{\mathrm{dis}}$ dependence of mobility in the typical carrier density range of $10^{12}-10^{13}$ cm^{-2}, and the fitting curves are also plotted (black). Experimental data are plotted with different symbols, and the references for the data are listed in the figure.

larger distance between the point charge in a dislocation line and the free electrons in the quantum well, while it is stronger for $z_0>0$, with a smaller distance. In the case of a dislocation piercing through the 2DEG in $x-y$ plane, the total scattering potential is uniform in both cases of electron distribution. This conclusion can also be elicited from the unscreened potential equation

$$U(q)=\frac{e\rho_L}{\varepsilon_0\varepsilon_b q^2}, \tag{13}$$

where $U(q)$ is the bare potential energy, which is obtained by integrating the unscreened point charge scattering potential[13] $V(q)=e^2/2\varepsilon_0\varepsilon_b\cdot e^{-q|z-z_0|}/q$ over z with charge density ρ_L. It is clear from Eq. (13) that such potential is independent of the electron distribution; therefore, the unscreened dislocation scattering potential should be the same in both cases of electron distribution. Thus, the lowering of mobilities in our result as compared with those of Jena *et al.*[8] should be attributed to the weakening of screening effect. Numerical imitation using the method of least-squares reveals an approximate $N_s^{1.4734}$ dependence of the mobility in the typical carrier density range of $1\times10^{12}-1\times10^{13}$ cm^{-2}, and the fitting curves are also plotted in Fig. 2. Experimental data from different references[2,14–16] are included in Fig. 2 for a comparison with our theoretical results. Theoretically, for dislocation density of 10^{10} cm^{-2} and in the typical carrier density range we discussed, maximum electron mobility will be in the range of 10^2-10^3 cm^2/V s, which means that dislocation scattering will be one of the dominant scattering mechanisms when dislocation density is in the order of 10^{10} cm^{-2}. A reduction in the dislocation density to 10^8 cm^{-2} or less will effectively improve the electron mobility. Smorchkova *et al.*[15] obtained a mobility of 51 700 cm^2/V s at 13 K in a $Al_{0.09}Ga_{0.91}N/GaN$ heterostructure grown on sapphire with a sheet carrier density of 2.23×10^{12} cm^{-2} (symbol ★ in Fig. 2). It should have a dislocation density lower than 10^8 cm^{-2} based on Fig. 2. Moreover, Frayssinet *et al.*[16] succeeded in obtaining a mobility of 60 100 cm^2/V s at 1.5 K in a $Al_{0.13}Ga_{0.87}N/GaN$ heterostructure grown on GaN single crystal with a sheet carrier density of 2.4×10^{12} cm^{-2} (symbol ♦ in Fig. 2). This sample is declared to be dislocation-free in the paper of Frayssinet *et al.*,[16] and this mobility value is one of the highest report ever in GaN-based semiconductors. Four other samples (symbol ▲ and ▼ in Fig. 2) show a mobility range of 10^3-10^4 cm^2/V s, and they may have dislocation densities in the typical range of 10^8-10^{10} cm^{-2}.

In conclusion, we have deduced a theory for dislocation core effect scattering in a quasitriangle $Al_xGa_{1-x}N/GaN$ heterostructure potential well. The dependence of mobility on carrier sheet density and dislocation density is imitated to be $N_s^{1.4734}/N_{\mathrm{dis}}$ approximately in the typical 2DEG density range of $1\times10^{12}-1\times10^{13}$ cm^{-2}. The results are compared with those obtained from a perfect 2DEG, and the reason for discrepancy is attributed to the different screening effect experienced by the ideal 2DEG and the electrons in a quasitriangle well.

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