Built-in field effect on the electron mobility in AlN/GaN/AlN quantum wells

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The authors demonstrated theoretically that compensation of the built-in electric field in AlN/GaN/AlN heterostructures with the externally applied perpendicular electric field may lead to the increase of the in-plane electron drift mobility. It has been shown that two- to fourfold increase of the room temperature mobility can be achieved for both nondegenerate and degenerate electron densities. Their calculations clarified the role of the intersubband electron transitions mediated by optical phonons in limiting the carrier mobility in GaN-based heterostructures. The tuning of the electron mobility with the perpendicular electric field may impact design of the high-power GaN/AlGaN heterostructure field-effect transistors. © *2006 American Institute of Physics*.
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The electron mobility in polar semiconductors at room temperature (RT) and above is limited by the electron-phonon scattering.[1] The intensity of the electron-phonon interaction in semiconductor heterostructures depends on the electron wave function (w.f.) and energy spectrum as well as on the optical and acoustic phonon dispersions. Changing geometry and material parameters of heterostructures one can affect both the carrier and phonon spectra. Controlled modification of the electron spectrum is conventionally referred to as electron band-structure engineering,[1] while tuning the phonon modes has been termed as phonon engineering.[2]

In this letter we show that heterostructures made of wurtzite AlGaN/GaN/AlGaN offer an extra degree of freedom in tuning the electron-phonon interaction via adjustment of their built-in electric field. It has been established that the external electric field F_{ext} applied perpendicular to the heterostructure layers can alter the carrier mobility in a wide range. Depending on the electron concentration and applied field the mobility can manifest rather unexpected nonmonotonic character. This finding and the prospect of RT mobility enhancement may influence the design of the GaN-based optoelectronic devices or AlGaN/GaN heterostructure field-effect transistors (HFETs). Indeed, reduced scattering may lead to faster devices and better thermal management[3] while larger separation of the electron w.f. from the interface in the field-compensated heterostructures may decrease the flicker noise levels.[4]

The intensity of the built-in electric field $F_{\text{built-in}}$ due to the spontaneous and induced piezoelectric polarizations in AlN/GaN/AlN quantum wells (QWs) reaches several MV/cm.[5] The built-in electric field creates a triangular potential well in GaN layer. In Fig. 1 we show the electron w.f. for the ground $(n=1)$ and the first excited $(n=2)$ states in AlN(3 nm)/GaN(6 nm)/AlN(3 nm) QW, which are confined along z axis (growth direction). The z axis coincides with c crystallographic direction and originates in the middle of QW. The electric field value indicated in Fig. 1 is the difference between the built-in and external fields, i.e., $\mathcal{F}=F_{\text{built-in}}-F_{\text{ext}}$. The value of $\mathcal{F}$ determines the slope of the potential well in the GaN layer. When $\mathcal{F}=0$, the built-in electric field is entirely compensated by the perpendicular external field: $F_{\text{built-in}}=F_{\text{ext}}$. To better elucidate the effect it is assumed that the carrier concentration is not affected by the external field. Since the barrier height is ~1.918 eV the electrons do not spill over and can move only along the QW layer. As the QW slope increases, the electron w.f. for the ground $\varphi_{n=1}(z)=\varphi^{s}_{n=1}(z)$ and excited $\varphi_{n=2}(z)=\varphi^{a}_{n=2}(z)$ states is squeezed to the heterostructure interface.

The energy of the ground and the first excited electron states in the flat QW $(\mathcal{F}=0)$ with the width $d_1=6$ nm is equal to $\varepsilon^0_1=40.8$ meV and $\varepsilon^0_2=163.3$ meV, respectively. In QW with the uncompensated field $\mathcal{F}=2000$ kV/cm, it is $\varepsilon^0_1=388$ meV and $\varepsilon^0_2=731.6$ meV, respectively. The confined optical phonon energies in such heterostructure are in the intervals of 69.2–69.34 and 90.8–91.9 meV, while the interface optical phonon energies are in the intervals of 69.2–81.6 and 91.8–110.4 meV. We determined the optical phonon spectra in such heterostructure using equations from Ref. 6. Our calculations show that for relevant carrier concentrations $(N_s=10^{12}\ \text{cm}^{-2}-N_s=10^{13}\ \text{cm}^{-2})$ the mobility in QW with the compensated field $(\mathcal{F}=0)$ is limited by the intersubband transitions $(1\leftrightarrow 2)$ rather than the intrasubband transitions $(1\leftrightarrow 1)$. The latter is true even in the case when the phonon energy $\hbar\omega_{\max}$ only slightly exceeds the energy $\varepsilon^0_2-\bar{\varepsilon}$ required

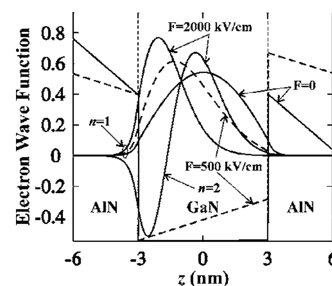

FIG. 1. Electron wave functions for the ground and first excited subbands in AlN/GaN/AlN heterostructure with different values of the perpendicular electric field $\mathcal{F}$, which is defined as the difference between the built-in (spontaneous and induced polarizations) and the compensating external field, i.e., $\mathcal{F}=F_{\text{built-in}}-F_{\text{ext}}$.

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for the intersubband transition. For the nondegenerate electron gas (NEG) the energy $\bar{\varepsilon}$ is defined as $\bar{\varepsilon}=\varepsilon_1^0+k_BT$ (k_B is Boltzmann's constant and T is the absolute temperature) while for the degenerate electron gas (DEG) $\bar{\varepsilon}$ is equal to the Fermi energy ε_F. Since the third subband is much higher in energy (ε_3^0=367.4 meV for $\mathcal{F}=0$) its effect is negligible. Thus when the optical phonon energy is comparable with the energy difference $\varepsilon_2^0-\bar{\varepsilon}$ the intersubband transitions dominate the scattering.

To account for the intersubband transitions in QWs we derived the system of two integral equations for the electron kinetic relaxation times. This system is the extension of the Boltzmann transport equation introduced in the convenient form in Ref. 7. The system of two integral equations has been modified to include the phonon dispersion. The modified equations, derived under the assumption of a spherical electron Brillouin zone, are written as

$$\sum_{\substack{\mathbf{p}',m=\pm1,\\ \lambda,n'=1,2}}\left[W(n,\mathbf{p}\rightarrow n',\mathbf{p}')\frac{1-f^0(\varepsilon_n+m\hbar\omega_\lambda(q))}{(1-f^0(\varepsilon_n))}\left(\tau_n(\mathbf{p})-\tau_{n'}(\mathbf{p}')\frac{\mathbf{p}\mathbf{p}'}{p^2}\right)\right]=1, \quad (1)$$

where $n=1,2$. In Eq. (1) $W(\gamma\rightarrow\gamma')=2\pi/\hbar|<\gamma|\hat{H}_{\mathrm{IF}}^S+\hat{H}_{\mathrm{IF}}^A+\hat{H}_C^S+\hat{H}_C^A|\gamma'>|^2\delta(E_\gamma-E_{\gamma'})$ is the probability of a transition of the electron-phonon system from the state γ with energy E_γ to the state γ' with the energy $E_{\gamma'}$, $f^0(\varepsilon)=(\exp((\varepsilon-\varepsilon_F)/k_BT)+1)^{-1}$, ε is the electron energy, q is the phonon wave vector, **p** and **p**′ are the electron momentum in the initial and final states, respectively, λ is the polarization index (quantum number) of the confined and interface optical phonon branches, $\tau_1(\varepsilon)$ is the kinetic relaxation time of an electron with energy ε in the first (ground) subband, which includes electron transitions within the fist subband $(1\leftrightarrow1)$ and transitions from the first to the second subband $(1\rightarrow2)$, and $\tau_2(\varepsilon)$ is the kinetic relaxation time of an electron in the second subband, which includes transitions from the second to the first subband $(2\rightarrow1)$ and the transitions within the second subband $(2\leftrightarrow2)$.

The Hamiltonians of interaction of electrons with the symmetric (S) and asymmetric (A) confined (C) and interface (IF) optical phonon modes, i.e., $\hat{H}_{\mathrm{IF}}^S$, $\hat{H}_{\mathrm{IF}}^A$, $\hat{H}_C^S$, and $\hat{H}_C^A$, in AlN/GaN/AlN heterostructure were taken from Ref. 8. In the framework of our theoretical approach one can make the following observations. The intrasubband scattering in the ground state $(1\leftrightarrow1)$ is determined by the matrix element $M_{11}=\int_{-d/2}^{d/2}\varphi_{n=1}^2V_{\mathrm{IF},C}^{S,A}dz$, where d is the width of the whole heterostructure and $V_{\mathrm{IF},C}^{S,A}$ is the potential for the S, A, C, and IF optical phonon modes. With increasing electrical field this matrix element increases mostly due to the w.f. $\varphi_{n=1}(z)$ shift to the QW interface and growth of its maximum (see Fig. 1). For $\mathcal{F}=0$, only S phonon modes contribute to the matrix element. The intensity of the intersubband electron transitions $(1\leftrightarrow2)$ is determined by (i) the value of the energy difference $\varepsilon_2^0-\bar{\varepsilon}$ and (ii) the matrix element $M_{12}=\int_{-d/2}^{d/2}\varphi_{n=1}\varphi_{n=2}V_{\mathrm{IF},C}^{S,A}dz$. When $\varepsilon_2^0-\bar{\varepsilon}$ becomes larger than the phonon energy $\hbar\omega$ the intersubband transitions stop. For $\mathcal{F}=0$, w.f. $\varphi_{n=2}$ is antisymmetric and, correspondingly, transitions are generated by antisymmetric phonon modes. A perpendicular electric field squeezes $\varphi_{n=2}$: for $\mathcal{F}$=2000 kV/cm both extremes are in one-half of the GaN layer (-3 nm$<z<0$), which reduces the matrix element M_{12}. The latter, together with the increased gap between subbands, reduce the electron transitions with increasing field. The electron mobility was calculated using the expression

$$\mu(T)=\frac{e}{m^*k_BT}\frac{\int_0^\infty\varepsilon\tau_1(\varepsilon)f^0(\varepsilon)(1-f^0(\varepsilon))d\varepsilon+\int_0^\infty\varepsilon\tau_2(\varepsilon)f^0(\varepsilon)(1-f^0(\varepsilon))d\varepsilon}{\int_0^\infty f^0(\varepsilon_1^0+\varepsilon)d\varepsilon+\int_0^\infty f^0(\varepsilon_2^0+\varepsilon)d\varepsilon}, \quad (2)$$

where e is the electron charge and m^* is the effective electron mass. Note that Eq. (2) takes into account both the intrasubband and intersubband transitions.

To solve Eq. (1) we generated a mesh with the step of 0.2 meV. The upper boundary energy of $\varepsilon_{\max}$=600 meV was chosen from the condition $\varepsilon_{\max}>>\hbar\omega_{\mathrm{opt}}$. The system of $2N$ (N=3001) liner equations for the values of τ_1 and τ_2 in the nodal points ε_l $(l=1,\ldots,N)$ has been solved numerically. The system of the equations was terminated with the condition $\varepsilon_l+\hbar\omega(q)\approx\varepsilon_N$ when $\varepsilon_l+\hbar\omega(q)>\varepsilon_N$ ($\varepsilon_N=\varepsilon_{\max}\gg\hbar\omega_{\mathrm{opt}}$). The calculated relaxation times were plugged into Eq. (2) to obtain the mobility.

The results for RT mobility with the low, medium, and high electron densities are shown in Fig. 2. The first observation is that increasing electron density reduces the electron mobility due to enhancement of the inequality $\hbar\omega>\varepsilon_2^0-\varepsilon_F$,

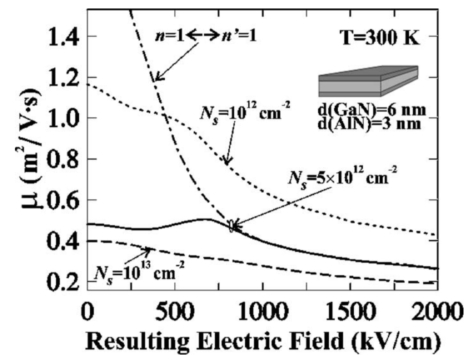

FIG. 2. Electron mobility vs perpendicular electric field in AlN/GaN/AlN heterostructure for three values of the electron concentration. Dash-dotted curve shows the mobility calculated by taking into account scattering in the ground state subband only ($N_s=5\times10^{12}$ cm^{-2}).

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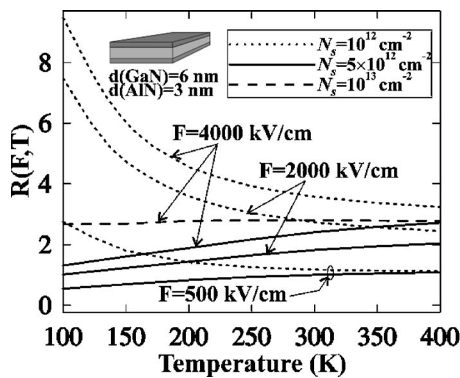

FIG. 3. Mobility enhancement coefficient $R(\mathcal{F},T)$ as a function of temperature for three values of the electron concentration.

which make the intersubband transitions more intensive. With increasing $\mathcal{F}$ the energy gap between subbands widens and the intrasubband scattering becomes the only scattering mechanism. The effect of the uncompensated field $\mathcal{F}\neq 0$ is twofold. From one side, the field reduces intersubband scattering $(1\leftrightarrow 2)$, but enhances intrasubband scattering $(1\leftrightarrow 1)$. In NEG case ($N_s=10^{12}$ cm^{-2}) in the field range $\mathcal{F}=250-300$ kV/cm the transitions $(1\rightarrow 2)$ weaken and the reduction of μ slows. In the limit of high fields ($\mathcal{F}=2000$ kV/cm), μ is defined by the transitions $(1\leftrightarrow 1)$ with absorption of a phonon (the phonon-emission limited mobility is approximately three times larger). For $N_s=5\times 10^{12}$ cm^{-2} the range of the fields when transitions $(1\rightarrow 2)$ dominate is wider. Weakening of the intersubband transitions leads even to a moderate growth of μ and appearance of a maximum near $\mathcal{F}\sim 700$ kV/cm. For fields $\mathcal{F}\sim 2000$ kV/cm the intrasubband transitions with the absorption and emission of a phonon became approximately equal in strength. In DEG case ($N_s=10^{13}$ cm^{-2}) with the externally compensated built-in field ($\mathcal{F}=0$) intrasubband transitions $(1\leftrightarrow 1)$ with phonon emission become important, while the interval of switching on the intersubband transitions $(1\rightarrow 2)$ extends in energy. Strengthening of the electron-phonon interaction leads to nearly monotonic reduction in the carrier mobility with increasing $\mathcal{F}$.

Figure 3 shows the ratio of the mobility in QW with the compensated field to that with uncompensated field $\mu(\mathcal{F}=0,T)/\mu(\mathcal{F}_0,T)$ as a function of temperature T. The results are presented for three values of the uncompensated field, $\mathcal{F}_0=500$ kV/cm, $\mathcal{F}_0=2000$ kV/cm, and $\mathcal{F}_0=4000$ kV/cm, and three electron concentrations. For NEG ($N_s=10^{12}$ cm^{-2}) the mobility at $\mathcal{F}=0$ is larger than that at $\mathcal{F}_0\neq 0$ since the electron-phonon interaction is stronger in the tilted QW with the uncompensated built-in electric field. With increasing T, the mobility ratio monotonically decreases from $\sim$8–9 at $T=100$ K to $\sim$3 at $T=300$ K. One should note here that $T<100$ K range requires separate consideration since at low temperatures the electron mobility is limited by acoustic phonons and impurity scattering.[9,10] For higher $N_s=5\times 10^{12}$ cm^{-2}, the RT mobility is enhanced by a factor of $\sim$2 for GaN QWs with the compensated electric field (with the initial built-in field between 2000 and 4000 kV/cm). In DEG case ($N_s=10^{13}$ cm^{-2}) we observe the mobility enhancement of a factor of $\sim$3 in the whole temperature range.

A direct comparison of the calculated μ with experiment is currently not possible since the available data for AlGaN/GaN HFETs is affected by the electron spillover, parallel conduction channels, defects, etc.[11,12] It is meaningful though to validate the model using data reported for similar structures. Levinshtein *et al.*[13] reported $\mu=0.14$ m^2/V s for GaN-based HFETs with additional SiO_2 barrier layer for improved carrier confinement. Our calculated value for $N_s=10^{13}$ cm^{-2} and uncompensated 2000 kV/cm field is only 25% higher, which can be explained by the neglected surface roughness and defect scattering.

In conclusion, we have shown that the mobility in GaN-based QWs with the strong built-in field can be substantially enhanced by compensating the built-in field with the external perpendicular electric field. The enhancement is strong even at $T=300$ K for a wide range of the carrier densities. The intriguing nonmonotonic dependence of the mobility on electric field is explained by the interplay of the intra- and intersubband scattering processes, which are affected by the external field in an opposite way.

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