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The size-quantized oscillations of the optical-phonon-limited electron mobility in AlN/GaN/AlN nanoscale heterostructures

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Abstract. We have studied the electron mobility in the AlN/GaN/AlN heterostructures with the nanometer scale thickness by taking into account multiple quantized electron subbands and the confined optical phonon dispersion. It was shown that the inter-subband electronic transitions play an important role in limiting the electron mobility in the heterostructures when the energy separation between one of the size-quantized excited electron subbands and the Fermi energy becomes comparable to the optical phonon energy. The latter leads to the oscillatory dependence of the electron mobility on the thickness of the heterostructure conduction channel layer. This effect is observable at room temperature and over a wide range of the carrier densities. The developed formalism and calculation procedure are readily applicable to other material systems. The described effect can be used for fine-tuning the confined electron and phonon states in the nanoscale heterostructures in order to achieve performance enhancement of the nanoscale electronic and optoelectronic devices.

1. Introduction

As the size of the electronic devices continues to decrease the accurate description of the electron mobility in the systems with confined electrons and confined phonons acquires particular importance [1]. It is well known that the electron – phonon scattering rates can undergo modification in the hetero- and nanostructures with the size-quantized electronic states and bulk phonons. Lee and Vassell [2] have shown theoretically that the low-field drift electron mobility in the thin quantum wells or narrow conduction channels decreases below the bulk semiconductor limit due to the electron state size quantization. At the same time, there exits an intermediate range of the quantum well thicknesses where the carrier mobility is enhanced. Their calculation was carried out in the relaxation time approximation for a single electron band and bulk acoustic and optical phonons. Fonoberov and Balandin [3] found that the low-field electron mobility in silicon nanowires with the barriers made of the "acoustically hard" materials can be increased via partial suppression of the deformation potential electron –acoustic phonon scattering. The mobility enhancement is more than an order of magnitude at low temperature, and about a factor of two at room temperature [3]. The results were obtained for the nanowires with the size-quantized electron states and confined acoustic phonon dispersion, which was modified due to the elastic mismatch at the interface between the nanowire and the barrier materials.

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In this paper, we examine the dependence of the electron mobility on the conduction channel thickness in the nanometer scale heterostructure by taking into account the (i) multiple size-quantized electron subbands; (ii) dispersion of the optical and acoustic phonons in such structures; and (iii) inelasticity of electron scattering on optical and acoustic phonons. The calculations have been carried out for AlN/GaN/AlN heterostructure with the nanometer thickness of the layers. It is known that GaN and AlN can form both wurtzite and zinc-blende crystal structure. The electron mobility in wurtzite AlN/GaN/AlN structures is strongly affected by the built-in electric field due to the spontaneous and piezoelectric polarization [4]. To separate the effect due to the built-in field from the nanoscale size-quantization and phonon dispersion effects we considered the zinc-blende AlN/GaN/AlN system. The large energy of optical phonons in GaN and AlN helps to better elucidate the effect.

2. Theoretical Model

We considered a generic three-layered heterostructure with the few nanometer thickness of each layer, which ensure the electronic state quantization and confinement of phonons. The electron relaxation rates were found from the solution of a system of the integral-differential Boltzman kinetic equations written as [5]

$$\sum_{\substack{\vec{p}',m=\pm1,\\ \lambda,n'=1,2,3}} [W(n,\vec{p}\to n',\vec{p}')\frac{(1-f^0(\varepsilon_n+m\cdot\hbar\omega_\lambda(q))}{(1-f^0(\varepsilon_n))}(\tau_n(\vec{p})-\tau_{n'}(\vec{p}')\frac{\vec{p}\,\vec{p}'}{p^2})]=1, \quad (1)$$

where $W(\gamma\to\gamma')=\frac{2\pi}{\hbar}\left|<\gamma\left|\hat{H}_{e-ph}\right|\gamma'>\right|^2\delta(E_\gamma-E_{\gamma'})$ is the probability of a transition of the electron-phonon system from the state γ with the energy E_γ to the state γ' with the energy $E_{\gamma'}$, $f^0(\varepsilon)=(\exp(\frac{\varepsilon-\varepsilon_F}{k_BT})+1)^{-1}$ is the Fermi – Dirac equilibrium distribution function, T is the absolute temperature, k_B is the Boltzman's constant, ε is the electron energy, q is the phonon wave number, $\vec{p}$ and $\vec{p}\,'$ are the electron momentum in the initial and final states, respectively, λ is the quantum number of the polar optical (interface or confined) or acoustic phonon modes, $\hat{H}_{e-ph}$ is the Hamiltonian of the electron interaction with the optical or acoustic phonon normal modes, which is given by Frohlich Hamiltonian for the case of the optical phonon modes and the deformation-potential Hamiltonian for the case of the acoustic phonon modes, $\tau_n(\varepsilon)$ (n=1,2,3) is the kinetic relaxation time of an electron with the energy ε in the subband n including intra- and intersubband scattering ($n \leftrightarrow n'$), where the index n' = 1,2,3. After the kinetic relaxation times were determined, we calculated the electron mobility by extending the standard formalism [6] to include the inter-subband and intra-subband transitions in the exited subbands, which led to the expression

$$\mu(T)=\frac{e}{k_BT}\frac{\sum_{n=1}^{3}\frac{1}{\bar{m}_n}\int_0^\infty \varepsilon\tau_n(\varepsilon)f^0(\varepsilon)(1-f^0(\varepsilon))d\varepsilon}{\sum_{n=1}^{3}\int_0^\infty f^0(\varepsilon_n^0+\varepsilon)d\varepsilon}, \quad (2)$$

where e is the electron charge, $\bar{m}_n$ is the effective electron mass averaged with the electron wave functions for the n-th energy level calculated by taking into account the electron penetration in the barrier layers [7]. The averaging procedure is needed in order to account for the finite wave function penetration to the barriers and the difference in the electron effective masses in the channel layer and the barriers. The details of the theoretical model and calculation procedure are reported by us elsewhere [8].

3. Results and Discussion

After finding the size-quantized electron states we calculated the energy separation $\Delta_{nF}(d, N_s) = \varepsilon_n^0 - \varepsilon_F$ between the confined states and the Fermi level as a function of the conduction channel thickness. The Fermi level position is determined by the given electron density. The maximum ($\hbar\omega_{\max}$ ~110 meV) and minimum ($\hbar\omega_{\min}$ ~66 meV) energies of the interface and confined optical phonons in AlN/GaN/AlN heterostructures set up the energy scale. The intersections of $\Delta_{nF}(d, N_s)$ curves with the maximum and minimum phonon energies $\hbar\omega_{\max,\min}$ establish the approximate values of the channel thickness when the electron mobility reaches its maxima values for the given carrier density. In figure 1 we present the mobility dependence on the heterostructure channel thickness d for several sheet carrier densities N_s. The results are shown for the temperature T=280 K.

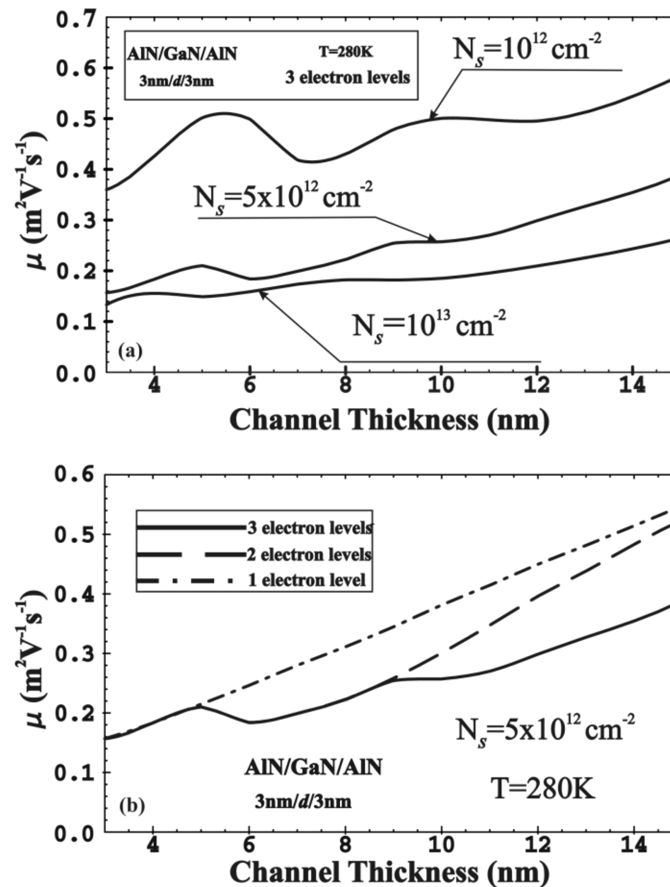

Figure 1: Room temperature electron mobility in the heterostructure limited by the optical phonons shown as a function of the conduction channel thickness for the different (a) values of the sheet electron concentration and (b) number of electron subband included in the model. The non-monotonic features are related to the enhancement of the inter-subband scattering when the energy difference between the subband and Fermi level coincide with the optical phonon energy.

One can see in figure 1 (a) that the mobility increases with the decreasing electron sheet carrier densities. The non-monotonic (oscillator) behaviour of the electron mobility curves for all considered densities is explained by the interplay of the intra- and intersubband scattering processes. The solid, dashed, and dashed-dotted lines in figure 1 (b) correspond to the electron mobility calculated by taking into account three (n=1, 2, 3), two (n=1, 2) and one (n=1) electron subbands, respectively. The electron mobility calculated by including only the intra-subband transitions (1←→1) increases

monotonically with the increasing channel thickness *d*. The latter dependence agrees with the result obtained by Anderson *et al.* [9]. For the small *d* when $\Delta_{nF}(d) > \hbar\omega$ and the intersubband transitions are absent, the solid, dashed and dashed-dotted curves coincide. Thus, the one-subband model calculation can only be valid for very thin channels (*d*<5 nm) when the subband separation is large (more than few $k_B T$). The electron scattering with the optical phonon accompanied by the optical phonon absorption and electron transition to the exited subbands starts when the phonon energy is somewhat smaller than the energy difference $\Delta_{nF}(d,N_s)$) owing to the partial populating of the electron states above the Fermi level. The onset of the inter-subband transitions limits the mobility increase even for thinner channel layers when the relatively small part of the electrons undergoes the inter-subband transitions (see figure 1 (a)). One can see from figure 1(a) that the mobility attains its maximum value at $d(N_s=10^{13}$ cm$^{-2})$ = 3.9 nm; $d(N_s=5\times10^{12}$ cm$^{-2})$ = 5 nm; and $d(N_s=10^{12}$ cm$^{2})$=5.5 nm. For the lower electron concentrations $(N_s = 5\times10^{12}\,cm^{-2};10^{12}\,cm^{-2})$ the onset of the inter-subband electron transitions appears at the larger thickness *d* due to the lager values of $\Delta_{nF}(d,N_s)$. The values of the material constants required for mobility simulation in AlN/GaN/AlN material system can be found in Refs. [10-12].

4. Conclusions

We have found that the low-field electron mobility in AlN/GaN/AlN heterostructures limited by the polar optical phonons manifest oscillatory behaviors as a function of the channel thickness. The oscillations appear in the wide range of temperatures and carrier densities. The effect is explained by the inter-subband electronic transitions, which play an important role when the energy separation between one of the size-quantized excited electron subbands and the Fermi energy becomes comparable to the optical phonon energy. The described mechanism can be used for fine-tuning the confined electron and phonon states to achieve performance enhancement of the nanoscale electronic and optoelectronic devices.

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