Optical phonon influence on the mobility of electrons in wurtzite and zincblende AlN/GaN quantum wells

X M Jia and S L Ban
Department of Physics, Inner Mongolia University, Hohhot 010021, P.R. China
E-mail: slban@imu.edu.cn

Abstract. Based on the dielectric continuum phonon model, uniaxial model and force balance equation, the electronic mobility parallel to the interfaces of wurtzite and zincblende AlN/GaN quantum-wells (QWs) is discussed in consideration of the scattering from the confined and interface optical phonon modes. The dependence of the mobility on the well width within temperature region that optical phonons play a main role is presented. It is shown that the total electronic mobility for a wurtzite QW is lower obviously than that for a zincblende QW due to the structure anisotropy effect. The main contribution to the mobility is from the confined optical phonon modes for a wide QW, whereas that is from the interface optical phonon modes for a narrow QW. It is also found that the electron effective mass is the main reason to reduce the mobility among the many factors such as the dielectric constants, band offsets between the well and barrier materials, etc. for a wurtzite QW.

1. Introduction
The group III nitrides have recently attracted much attention due to their large band gap and favorable material properties. GaN and AlN crystals have not only a wurtzite (WZ) structure (hexagonal symmetry), but also a zincblende (ZB) structure (cubic symmetry). The electron-phonon (e-p) interaction in the former structure is substantially different from that in the latter one. A series work was done by Stroscio’s group to investigate the complicated e-p interaction in layered WZ structures. The Fröhlich-like electron-optical-phonon interactions in WZ structures with single and double hetero-interfaces were derived [1]. Afterwards, they [2] studied the optical phonon spectra for the Al$_{0.15}$Ga$_{0.85}$N/GaN QW, AlN/GaN QW, and GaN dielectric slab in detail. It is known that so-called confined and half space modes can not be “confined” entirely inside one layer, but can penetrate into the surrounding materials.

The early work about electronic mobility in GaN-based materials was given by Littlejohn et al. [3]. Hsu and Walukiewicz [4] presented the electron mobility in Al$_{1-x}$Ga$_x$N/GaN heterostructures, and indicated that only the lowest subband is occupied for the electron concentrations below $4.5 \times 10^{12}$cm$^{-2}$. Yao et al. [5] performed a calculation of mobility in AlGaN/GaN heterostructures by applying the force balance equation, which has been proved to be useful and convenient for studying carrier transport. At a high temperature, the main mechanism that influences electron transport is well known to be the scattering from polar optical phonons. Komirenko et al. [6] calculated the electron scattering of energy-dependence via interaction with optical confined and interface (IF) modes in WZ QWs. It is emphasized that it is sufficient to take only the scattering from optical confined and IF modes in an AlN/GaN QW into account. However, to our knowledge, the studies on transport in nitride compounds
have not been on the same level as those for GaAs-based materials, and the dependence of the mobility on the well width which has been discussed for GaAs-based materials \cite{7,8} and on temperature in WZ AlN/GaN QWs has not been presented. In this paper, the electronic mobility parallel to the interfaces of WZ and ZB AlN/GaN QWs is discussed in consideration of the scattering from the confined and IF optical phonon modes.

2. Electronic mobility
We consider a single QW with the WZ structure whose $z$ axis is collinear with the c-axis and perpendicular to the interfaces. The direction parallel to the interface is denoted as $\perp$ and the origin of the coordinates is located at the geometrical center of the well. Material 1 (well material) is between $z = \pm \frac{1}{2} d$ and material 2 (barrier materials) occupies the space $z > \frac{1}{2} d$.

Based on the approximation of effective mass and finite deep QW, the electron wave function of subband $n$ \cite{9} can be obtained by solving the Schrödinger equation with Ben-Daniel boundary conditions.

We only consider the scattering from the confined and IF modes in both WZ and ZB QWs, since the propagating modes do not exist in a AlN/GaN QW, and the half-space modes nearly have no contribution to the e-p interaction except for a very narrow QW \cite{9}. In a WZ AlN/GaN QW, the IF modes can be classified into symmetric and anti-symmetric modes. For the symmetric IF mode, its potential is given by \cite{1}

$$
\phi_{\perp, q}^i = \left[ \frac{4\pi \hbar S^{-1}}{\partial \omega} \left( \sqrt{\varepsilon_{11}} \varepsilon_{11} \tanh(\sqrt{\varepsilon_{11}} / \varepsilon_{11} q d / 2) - \sqrt{\varepsilon_{21}} \varepsilon_{21} \right) \right]^{1/2} \frac{1}{\sqrt{2} q} \times \begin{cases} \cosh(\sqrt{\varepsilon_{11}} / \varepsilon_{11} q z / \varepsilon_{11} q d / 2) & |z| < d / 2 \\ \varepsilon^{-\sqrt{\varepsilon_{21}} / \varepsilon_{21} q d / 2} & |z| > d / 2 \end{cases}
$$

(1)

The potential of the anti-symmetric IF mode can be written as

$$
\phi_{\parallel, q}^i = \left[ \frac{4\pi \hbar S^{-1}}{\partial \omega} \left( \sqrt{\varepsilon_{11}} \varepsilon_{11} \coth(\sqrt{\varepsilon_{11}} / \varepsilon_{11} q d / 2) - \sqrt{\varepsilon_{21}} \varepsilon_{21} \right) \right]^{1/2} \frac{1}{\sqrt{2} q} \times \begin{cases} \sinh(\sqrt{\varepsilon_{11}} / \varepsilon_{11} q z / \varepsilon_{11} q d / 2) / \varepsilon^{-\sqrt{\varepsilon_{21}} / \varepsilon_{21} q d / 2} & |z| < d / 2 \\ \text{sgn}(z) e^{-\sqrt{\varepsilon_{21}} / \varepsilon_{21} q d / 2} & |z| > d / 2 \end{cases}
$$

(2)

Here $\varepsilon_{\perp} (\omega)$, $\varepsilon_{\parallel} (\omega)$ are the direction-related dielectric constants, $q$ is the two-dimensional wave vector of the phonon modes in the $x$-$y$ plane, $S$ is the normalization area of the quasi-two-dimensional electron gas.

Since the dielectric constants depend on the orientation, the confined phonon modes in a WZ AlN/GaN QW are more complex than that in a ZB one. For the symmetric confined mode, the potential is \cite{1}

$$
\phi_{\perp, k}^\pm = \left[ \frac{4\pi \hbar S^{-1}}{\partial \omega} \left( \varepsilon_{11} q^2 + \varepsilon_{21} k_{in}^2 \right) d / 2 - 2 q \cdot f_s (\omega) \cos(k_{in} d / 2) \right]^{1/2} \times \begin{cases} \cos(k_{in} z), & |z| < d / 2 \\ \cos(k_{in} d / 2) e^{-\sqrt{\varepsilon_{21}} / \varepsilon_{21} q d / 2}, & |z| > d / 2 \end{cases}
$$

(3)

for the anti-symmetric confined mode, the potential is
\[ \phi_{k_{\text{in}}}^{d} = \left[ \frac{4\pi h S}{\partial (\varepsilon_{j} + \varepsilon_{j}^{k_{\text{in}}}) d / 2 - 2q \cdot f_{j}(\omega) \sin(k_{\text{in}} d / 2)} \right]^{1/2} \times \begin{cases} \sin(k_{\text{in}} z), & |z| < d / 2 \\ \text{sgn}(z) \sin(k_{\text{in}} d / 2) e^{-|z|d_{z}/2}, & |z| > d / 2 \end{cases} \]  

where \( f_{j}(\omega) \), \( f_{j}(\omega) \), \( k_{\text{in}} \), and \( k_{\text{c}} \) were given by Ref. [1], respectively.

In a ZB AlN/GaN QW, the potentials of the symmetric and anti-symmetric IF modes [10] can be obtained from Equations (1)-(2) by neglecting the structure anisotropy (i.e., \( \omega_{\perp} = \omega_{\parallel}, \omega_{\parallel} = \omega_{z}, \varepsilon_{\perp} = \varepsilon_{z} \)). Similarly, the potentials for confined modes [10] can also be obtained by Equations (3)-(4) with \( \omega = \omega_{\parallel} \).

According to Lei and Ting’s force-balance equation [11] the linear mobility \( \mu \) of the quasi-two-dimensional electron gas is given by

\[ \frac{1}{\mu} = \frac{2\hbar}{e n_{0} k_{B} T} \sum_{n, n'} \left| M_{n, n'}(\mathbf{q}, \omega, \lambda) \right|^{2} q_{z}^{2} \left( 1 - e^{\frac{\hbar \omega_{\parallel}}{k_{B} T}} \right)^{2} \Pi_{z}(n, n', \mathbf{q}, \omega). \]  

where \( n_{0} \) is the electron sheet density, \( k_{B} \) the Boltzmann constant, \( \left| M_{n, n'}(\mathbf{q}, \omega, \lambda) \right| \) the Fröhlich interaction matrix between subbands \( n \) and \( n' \) coupling to the \( \lambda \) th branch of phonons, and \( \Pi_{z}(n, n', \mathbf{q}, \omega) \) the imaginary part of the two-dimensional density-density correlation function of the zeroth order [12].

3. **Numerical results and discussion**

Here we consider the situation that only the lowest subband is occupied and the inter-subband transition is neglected for the areal electronic density \( n_{0} < 4.5 \times 10^{12} \text{cm}^{-2} \) [4]. \( n_{0} = 1.0 \times 10^{12} \text{cm}^{-2} \) is adopted in our computation so that we can confine ourselves only to the \( n'=n=0 \) terms.

**Figure 1.** The contributions to the electronic mobility from the confined (dashed lines) and IF phonon (dot-dashed lines) scattering for WZ and ZB AlN/GaN QWs as functions of well width \( d \), at temperature \( T=300\text{K} \). The total mobility is denoted by the solid lines.

**Figure 2.** The total electric mobility as a function of temperature \( T \) for the given well width \( d=60\text{Å} \). The total mobility, the mobility limited by the confined and IF phonons in WZ(ZB) AlN/GaN QWs are denoted by curves 1(4),2(5),3(6), respectively.

Figure 1 gives the contributions to the electronic mobility from the confined and IF phonon scattering for WZ and ZB AlN/GaN QWs as functions of well width \( d \), at temperature \( T=300\text{K} \), but
the IF modes are dominant in narrow ones for both the WZ structure and ZB structure, and the tendency of corresponding curves for WZ QWs is the same as that for ZB QWs. The mobility limited by the confined modes decreases significantly with increase of well width, finally goes to a saturation, and the one corresponding to the IF modes first decreases towards a small valley, then increases significantly. As a result, the total mobility reduces weakly and then increases to the saturation slowly as the well width increases. The reason is that the electron is confined in the well, the probability near the vicinity of the interfaces and penetrating into the barriers can be neglected for wider QWs, so that the scattering is mainly from the confined phonons. While, as the well width decreases, the probability of electron appearing in the vicinity of interfaces becomes bigger due to the confinement of barriers, and the scattering from the IF phonons becomes stronger, at the same time, the scattering from confined phonons becomes weaker. The contribution from the IF modes is dominant if the well width decreases below a critical value. It is also found that the total mobility in a WZ AlN/GaN QW is lower than that in a ZB one. The scattering from confined modes in the former structure is stronger than that in the latter within the range of well width considered. But for the IF modes, the properties are similar to the confined modes only for a narrower QW. As the well becomes wider, the interaction of electron-IF-phonons in the WZ structure is weaker than that in the ZB structure. It can be seen that the structure anisotropy increases the e-p interaction and reduces the total electron mobility.

The electronic mobility as a function of the temperature $T$ for the given well width $d=60\,\text{Å}$, corresponding to the two structures discussed above, is shown by figure 2. Obviously, the electronic mobility decreases as the temperature increases for both WZ and ZB QWs. This is because the lattices oscillate strongly at high temperature to increase scattering from phonons. In addition, it can be seen that the confined phonons scattering is dominant in wider WZ and ZB QWs, and the structure anisotropy effect causes a large reduction on the total electronic mobility. We also did the calculation by considering the variation of separate parameters. It was found that the variation of electron effective mass plays a more important role to decide the mobility, while the influence of the dielectric constants and the phonon frequencies and the offset of conduct bands on the mobility is smaller.

4. Conclusions
The electronic mobility parallel to the interfaces in WZ and ZB AlN/GaN QWs is presented and the dominant scattering mechanisms at the temperature range of optical phonons being available are considered. It is shown that, there is a large reduction of the total electronic mobility in WZ QWs comparing with that in ZB QWs due to the structure anisotropy, and the variation of electron effective mass influences the mobility significantly. The main contribution to the mobility is from the confined optical phonon modes for a wide QW, whereas that is from the IF optical phonon modes for a narrow QW.

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