The Quantum Calculation for Valence Band Structure of Strained Zinc-blende GaN Using Six-Band Based k-p Method

Yaqun Liu, Everett X. Wang, Gary Zhang and Xiyue Li*

School of Information Engineering, Guangdong University of Technology, Guangzhou, China

lixiyue915@gdut.edu.cn

Abstract. The variations of valence band energy with stress effects in zinc-blende GaN are proposed in this paper. The calculations are based on a six-band strain dependent k-p Hamiltonian, and can be self-consistently solved by Schrödinger-Poisson equation. Accurate physical pictures are given for the quantized valence sub band structure under biaxial and uniaxial stress in (001) surface along the [110] direction accounting the quantum confinement effect. The warping of the energy profile results in carrier distribution change. This research will be beneficial for improving the hole mobility and the selective of optimum stress for group-III nitride semiconductor based devices.

1. Introduction

As one of the representatives of the Wide-Bandgap semiconductor materials, GaN have attracted significant amounts of attention in the past several decades due to the promising electrical and optical properties [1-3]. It is known that the polarization charge in zinc-blende GaN is less than wurtzite form, and the studies focus on valence band structure is also relatively few. However, as GaN play a crucial role in 5G devices and LEDs, and the zinc-blende structure is superior to the wurtzite structure in terms of symmetry, ease of doping, and low phone scattering. Therefore, it is still very important to study the potential of zinc-blende form, especially for the properties in heterostructure taking the stress effect which is caused by AlGaN substrate into account.

In the earlier, the band structure of GaN has been calculated by using methods such as first-principles calculation [4], the empirical pseudopotential method (EPM) [5], quasiparticle calculation [6] and so on. In this work, we use the six-band stress-dependent quantum k-p method to calculate the valence band structure of zinc-blende GaN. With this method, both biaxial and uniaxial effects are investigated. Quantum confinement effect is also included. The energy band structure is the foundation in fully appreciating the properties of materials, and the dispersion relation of the valence band in strained materials is also the theoretical basis for understanding the valence band properties and calculating hole mobility. This analysis will provide a physical explanation for the variation of valence band structure under different stress conditions.

2. Calculation for valence band structure

The k-p method provides a powerful approach for calculating valence band structure in stressed zinc-blende GaN. According to Luttinger-Kohn theory, the valence band structure for Bulk zinc-blende GaN can be obtained by the following 6×6 Hamiltonian matrix [7][8]:

\[
\begin{pmatrix}
E_1 & k_x \mu & k_y \mu & k_z \mu & \frac{1}{2} \alpha \mu^2 & \frac{1}{2} \alpha \mu^2 \\
0 & E_1 & k_z \mu & k_y \mu & \frac{1}{2} \alpha \mu^2 & \frac{1}{2} \alpha \mu^2 \\
0 & 0 & E_1 & k_x \mu & \frac{1}{2} \alpha \mu^2 & \frac{1}{2} \alpha \mu^2 \\
0 & 0 & 0 & E_1 & \frac{1}{2} \alpha \mu^2 & \frac{1}{2} \alpha \mu^2 \\
0 & 0 & 0 & 0 & E_1 & \frac{1}{2} \alpha \mu^2 \\
0 & 0 & 0 & 0 & 0 & E_1
\end{pmatrix}
\]
where

\[
Q = Q_x + Q_s, \quad T = T_x + T_s
\]

\[
R = R_x + R_s, \quad S = S_x + S_s
\]

\[
Q_x = -\frac{\hbar^2}{2m_0} \left[ (\gamma_1 + \gamma_2)(k_x^2 + k_y^2) + (\gamma_1 - 2\gamma_2)k_z^2 \right]
\]

\[
T_x = -\frac{\hbar^2}{2m_0} \left[ ((\gamma_1 - \gamma_2)(k_x^2 + k_y^2) + (\gamma_1 + 2\gamma_2)k_z^2 \right]
\]

\[
S_x = i\frac{\hbar}{m_0} \sqrt{3}\gamma_3 (k_x - ik_y)k_z
\]

\[
R_x = -\frac{\hbar^2}{2m_0} \sqrt{3}[\gamma_3(k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y]
\]

\[
Q_s = a_x(e_{xx} + e_{yy} + e_{zz}) + 0.5b(e_{xx} + e_{yy} - 2e_{zz})
\]

\[
T_s = a_y(e_{xx} + e_{yy} + e_{zz}) - 0.5b(e_{xx} + e_{yy} - 2e_{zz})
\]

\[
R_s = \frac{\sqrt{3}}{2} b(e_{xx} - e_{yy}) - i d e_{xy}
\]

\[
S_s = -d(e_{xz} - i e_{xy})
\]

\[
\left(\begin{array}{cccc}
Q & S & R & 0 \\
S^* & T & 0 & R^* \\
R^* & 0 & T & -S \\
0 & R^* & -S^* & Q
\end{array}\right) \left(\begin{array}{c}
\frac{i}{\sqrt{2}} (Q-T) \\
\frac{i}{\sqrt{2}} S \\
\frac{i}{\sqrt{2}} (Q-T) \\
\frac{i}{\sqrt{2}} S^*
\end{array}\right) = \frac{1}{2}(Q+T) - \Delta_s
\]

m_0 denotes to free electron mass, \( \gamma_1, \gamma_2 \) and \( \gamma_3 \) are Luttinger parameters proposed in [7], \( \Delta_s \) is the spin-orbit interaction, \( a_x, b \) and \( d \) are Bir-Pikus deformation potential. In this work, we restrict ourselves to the special case of a biaxial stress and a uniaxial stress along x-y plane, namely,

\[
\begin{align*}
\varepsilon_{xx} &= \varepsilon_{yy} \\
\varepsilon_{xy} &= 0 \\
\varepsilon_{yz} &= \varepsilon_{zz} = 0
\end{align*}
\]

thus

\[
S_x = 0
\]

Therefore, the relationship between strain \( e_{ij} \) and stress \( s_{ij} \) can be written as

\[
\begin{align*}
\varepsilon_{xx} &= s_{11} \cdot s_{xx} + s_{12} \cdot (s_{yy} + s_{zz}) \\
\varepsilon_{xy} &= s_{11} \cdot s_{yy} + s_{12} \cdot (s_{xx} + s_{zz}) \\
\varepsilon_{zz} &= s_{11} \cdot s_{zz} + s_{12} \cdot (s_{xx} + s_{yy}) \\
\varepsilon_{zy} &= s_{44} \cdot s_{yy}
\end{align*}
\]

and \( s_{11}, s_{12}, s_{44} \) can be related to the elastic constants [9] with the description of

\[
\begin{align*}
s_{11} &= \left[ 1 / (c_{11} + 2 \cdot c_{12}) + 2 / (c_{11} - c_{12}) \right] / 3 \\
s_{12} &= \left[ 1 / (c_{11} + 2 \cdot c_{12}) - 1 / (c_{11} - c_{12}) \right] / 3 \\
s_{44} &= 1 / c_{44}
\end{align*}
\]
In this work, the valence band along (001) is classified by angular momentum due to the fourfold rotation symmetry in zinc blende crystals. Solving for the eigenvalue of the Hamiltonian matrix including the spin-orbit interaction, the basis of Bloch states consist of six angular momentum Eigen states, which representing heavy-hole, light-hole and spin-orbit split-off valence band state with spin up and down, can be obtained. However, if the quantization is not included, only 6 subbands can be observed. It is not enough for the researches in electrical and optical properties.

In order to accurately realize the subband structure for zinc-blende GaN, an investigation has been undertaken by using the k-p model approach, which is simple enough to be solved by Schrödinger equations and rigorous enough to include the effect of arbitrary stress. This method has also been used in strained bulk and quantum well structures with zinc-blende symmetry [10].

In GaN/AlGaN heterojunction interface, the $k_z$-direction is quantized because of the quantum well produced by the gate filed in a (001) wafer. By replacing $k_z$ with an operator $(i\varepsilon\partial/\partial z)$, the quantized valence hole subband energy can be calculated by using (6):

$$H(k_{x,y},k_z) + V(z) \cdot \varphi_{k_{x,y}}(z) = E(\zeta) \cdot \varphi_{k_{x,y}}(z)$$  

where $H(k_{x,y},k_z)$ is the quantized k-p Hamiltonian matrix including the strain component. The (6) yield negative eigenvalues $E(k)$, and below the sign convention appropriate to analyze transport [positive kinetic energies $E(k)$] will be employed.

Equation (6) can be discretized on a mesh in the z-direction with $N_z$ nodes and turn into an eigenvalue problem of a $6N_z \times 6N_z$ complex band Hermitian matrix to propose the iso-energy contours. With the use of non-uniform mesh which can reduce the computation time effectively, a matrix with 12 non-zero length tridiagonal block form can be obtained and the calculation in this work includes the lowest 30 subbands. As the relative fine discretization employed, the subband structure requires the solution of eigenvalue problem of Schrödinger equations and its discretized form to obtain the quantized subband energies. A self-consistent, two-dimensional solution of the Schrödinger and Poisson equations is utilize d in order to analyze a much wider range of account for band profile as rigorously as possible. This method is very efficient in finding Eigen-states that extend over a relatively large spatial area without loss of accuracy.

3. Result and discussion

3.1 Bulk Zinc-blende GaN Valence Band Structure

In this section, we will describe the main effect on the valence band of bulk zinc-blende GaN. The (001) is chosen as the transport plane and [110] as the current direction since it is currently the case for the similar PMOS technology. Two kinds of stress are considered, including the biaxial stress due to lattice mismatch and uniaxial stress along the current channel.

In Fig. 1(a) and (b), we can see the three-dimensional heavy-hole (HH) iso-energy structure near $\Gamma$ point without applied stress. The HH band is consist of 12 “wings” including four “in-plane” wings located in the plane of the channel and eight “out-of-plane” wings understood as perpendicular to the channel. In no-stress case, all wings are equivalent at energy, and also be equally populated by hole carriers. The calculated HH band with biaxial tensile, uniaxial tensile and uniaxial compressive are shown in Fig. 1(c) ~ (e), describing that the energies are not equivalent at all. The effects causing by biaxial and uniaxial stress will be discussed later.
3.2 Quantized Subband Structure

To further illustrate the quantum well structure including the effects of biaxial and uniaxial stress, the discretized E-k dispersion of zinc-blende GaN under a gate field are calculated, taking quantum confinement effect into account. By solving (6), the quantized subband energy level can be obtained. Fig. 2(a) – (f) shows iso-energy contours of the lowest 6 quantized subbands. We can see that only the shapes of first and second subbands are similar to Fig.1 (b), and the more the energy, the more the shapes deviates. Therefore, it is feasible to simulate the properties of quantum well by using the first pair subbands.

From Fig. 2(a), we can observe the strong anisotropy of iso-surface. In $k_z \neq 0$ case, all the shapes which can be observed in the bulk bands are still visible in the picture, while the band below the plane...
cannot be seen because it is the same as the band above the plane. When these “out-of-plane” wings are occupied and there is a vertical confinement field in the $z$-direction, effective coupling can be provided.

Fig.3 shows the iso-energy contour of the first subband in $k_z=0$ plane is markedly four-angle star shape. The reason for choosing this plane is we can only focus on the four “in-plane” wings which play the most important role in transport behavior.

![Figure 3](image)

Figure 3. Iso-energy contours of the first subband separated by 25meV in $k_z=0$ plane without applied stress. It clearly shows high curvature (small effective mass) at A, C, and low curvature (high effective mass) at B, D.

It is clearly that along current channel direction of [110], A and C have more curvature than B and D. Therefore, the effective mass of carriers sitting on A and C is lighter than that sitting on B and D, while the carriers on the out-of-plane wings have medium effective mass. Under different stress, wings energy can be moved up and down. Some wings will become dominant when their energy is lowered by stress. Since all the wings have their minima at $\Gamma$ point. The dominant wing with the lowest energy has the highest population concentration at and around the $\Gamma$ point. Therefore, we expect that the band shape of the leading wings also determines the hole distribution and mobility behavior.

Next, we examine the effects induced by biaxial and uniaxial stress. The lattice mismatch between the epitaxially grown GaN and AlGaN substrate will generate biaxial stress. Fig. 4 shows the biaxial tensile ($s_{xx}=s_{yy}=1\text{GPa}$) case (the solid contours) and unstressed case (the dotted contours). An interesting phenomenon is that the innermost solid contours are circular rather than four-angle star shaped. It is revealed that the energy of light hole (LH) band is now below the heavy hole (HH) band under biaxial tensile stress, and the rotation symmetry along the $z$ axis is unchanged.

![Figure 4](image)

Figure 4. Iso-energy contours of the first subbands separated by 25 meV in $k_z=0$ plane under 1GPa biaxial tensile stress
The uniaxial stress consists of biaxial and shear part, therefore the model has to be able to treat both biaxial and shear stress to be accurate. When the GaN/AlGaN heterojunction is stressed along the channel direction, the uniaxial stress includes the $s_{xx}$ component along the channel, the $s_{yy}$ component perpendicular to the channel, and $s_{xy}$, which is a shear. The presence of the $s_{xy}$ component describes the main difference between biaxial and uniaxial stresses, and it can also induce the carrier repopulation among the “in-plane” wings. Fig. 5 and Fig. 6 show the iso-energy contours of the first subbands in (001) plane for lowest energy hole band under 1GPa uniaxial compressive stress ($s_{xx}=s_{yy}=s_{xy}=-500\text{MPa}$) and uniaxial tensile stress ($s_{xx}=s_{yy}=s_{xy}=500\text{MPa}$) in [110] direction, respectively. The dotted contours on each plot also show the non-stress case. Uniaxial stress changes the rotation symmetry about the $z$-direction to twofold. When the 1GPa uniaxial stress is applied, the iso-energy contours of the innermost region are close to an “ellipsoid-like” shape. The distortion of the iso-contour present that energy distribution will change. In particular, Fig. 5 shows an energy lowering in A and C, while a rise can be seen in B and D with uniaxial compressive stress. This results a carrier repopulation from B and D to A and C, causing a mobility enhancement because the lighter effective mass is advantageous to transport characteristics. On the other hand, with the uniaxial tensile stress in Fig.6, the result is opposite, the carrier are redistributed from A and C to B and D, leading the mobility degradation. The same results can be also certified in Fig. 7. Presenting that under the uniaxial compressive stress condition, the energy of the A-C line is much closer to $\Gamma$ point than B-D line. Therefore, uniaxial compressive stress is considered to be the most efficient way to enhance hole mobility with the combined effects by biaxial compression and shear components.

![Figure 5](image1.png) Iso-energy contours of the first subbands separated by 25 meV in $k_z=0$ plane under 1GPa uniaxial compressive stress

![Figure 6](image2.png) Iso-energy contours of the first subbands separated by 25 meV in $k_z=0$ plane under 1GPa uniaxial tensile stress
Figure 7. Energies of the first subband in A-C line and B-D line with no stress, 1GPa biaxial tensile stress, 1GPa uniaxial compressive stress and 1GPa uniaxial tensile stress condition, respectively.

4. Conclusion
In this work, a concise overview of the quantized subbands model and applicable for zinc-blende GaN/AlGaN heterojunction quantum well has been presented by employing a six-band based stress-dependent k-p method, and presented their respective work mechanisms. Based on this model, comprehensive analysis of the energy dispersion for the valence band structure under biaxial and uniaxial stress in (001) surface along [110] direction has been given. The variation of subband energies is illustrated by two-dimensional iso-energy diagram. Uniaxial compression in the [110] direction can enhance hole mobility through the combination of biaxial compressive and the shear stress. The biaxial compression component can make the holes redistribute into four “in-plane” wings, and the shear component further move holes into the wings perpendicular to the channel, reducing the effective mass greatly. Such combined effects are considered to make uniaxial compressive stress as the most efficient way for the hole mobility enhancement in zinc-blende GaN/AlGaN heterojunction.

The method in this work will be very useful for the calculation of valence band in strained quantum well structure, which has a great potential for applications to optical and electronic devices.

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5. References
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