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Micro Characteristics of InGaN/GaN Quantum Wells

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Abstract: InGaN/GaN quantum well exhibits a series of unusual optical properties. However, the physics of quantum well on the micro scale is subjected to large uncertainties. Little is known on the discontinuities of energy band structure and local states on the atomic level in the case of different In atoms distribution in the $In_xGa_{1-x}N$ layers caused by In compositional fluctuation and phase separation, which intensively alters the optical and electronic properties. Using the efficient and accurate total energy and molecular-dynamics package VASP which is based on the density functional method, we performed the first principles calculations on InGaN/GaN quantum wells. The calculated results exhibit discrete bands around the conduction band minimum and the valence band maximum that vary with the In atom distributions. Moreover, the local states with the discrete bands are likely to appear the quantum confined Stark effect in the InGaN/GaN interface enhanced by the polarization field in the crystal. The control and further understanding of those micro characteristics may lead to the improved performance of InGaN QWs.

Key words: InGaN; quantum well; VASP; energy band structure

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1 Introduction

In recent years, GaN based semiconductors have been considered as an potential candidate material for short wavelength light emitting applications[1,2] due to their wide band gap[3], high breakdown field, large electron saturation velocity, and chemical stability at high temperatures. Of particular interest is all kinds of $In_xGa_{1-x}N$/GaN quantum well (QW) structures which play a pivotal role in devices such as active region of the light-emitting[4~7].

In spite of many works of QW structures, there remain a number of open questions related to the physics of QW on a micro scale. Little is known on the discontinuities of band structures and local states near different atoms under different In distribution caused by In compositional fluctuation in $In_xGa_{1-x}N$ layers, which intensively influence on the optical and electronic properties. Hence, unveiling the mechanism of electronic behavior at the atomic level is essential for assessing the degree of carrier confinement and designing electronic and optoelectronic devices under precise control. In this paper, we performed the first principles calculations with the help of an efficient and accurate simulation package, VASP (Vienna *Ab-Initio* Simulation Package), and systematically explored the characteristics of InGaN/GaN QW under the micro scale.

2 Computational Details

VASP is based on the density functional method with the molecular dynamics. The calculations reported here were carried out by employing the projector augmented wave method (PAW) for its reasonable accuracy and efficiency. Both Ga and In 3d electrons are treated as part of the valence band, and the plane-wave cutoff energy is taken to be 36.75Ry. An 8×8×8 Gamma centered Monkhost-

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Pack mesh[8] was used to sample the Brillouin zone. In addition, the geometry optimizations were preformed by relaxing all degrees of freedom using the conjugate gradient algorithm.

GaN has an wurtzite structure in which Ga-N bilayers were arranged in ABAB … stacking sequence[9] correspondence to hexagonal phase. We designed two kinds of InGaN/GaN QWs, as Model Ⅰ and Ⅱ shown in Fig. 1. To fully diminish the coupling between wells in the periodic supercells, their geometry structures of repeating supercells were constructed with strip cuboid supercells composed of 1 × 1 × 16 unit cells with 64 atoms. InGaN QWs were separated by a thicker GaN barrier of about 7.5 nm. The different In distributions were constituted by inserting one Ga-N bilayer into In-N layers as shown in Model Ⅱ. For comparison, the bulk GaN and InN as the same size are also calculated.

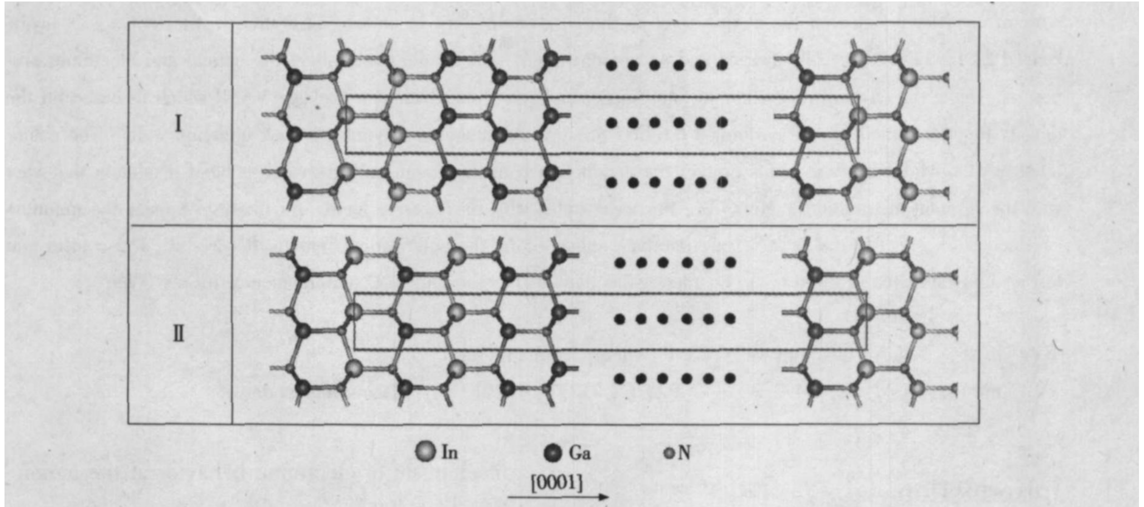

Fig. 1 Geometry structures of InGaN/GaN QWs with 64-atom supercells of Model Ⅰ and Ⅱ.

3 Results and Discussion

3.1 Lattice Structure

In the relaxation calculations, it is seen that the errors of the calculated lattice constants of the bulk GaN and InN are within 1% compared to the experimental values, which confirms the reliability of the computational method.

The calculated lattice constants a are 0.3235 and 0.3236 nm for Model Ⅰ and Ⅱ, respectively. These values are a little larger than that of bulk GaN, which is reasonable due to GaN barrier subjecting to a biaxial in-plane tensile stress when some Ga layers are substituted by larger radius In. In contrast, the lattices are reduced in InGaN to release the misfit stress, which appear more distinct in Model Ⅰ. These lattice distortions are attributable to larger difference of lattice constants between GaN barrier and InGaN well in Model Ⅰ, which is accompanied by the phase separation[10] and compositional disorder[11, 12].

On the contrary, the lattice of GaN barrier is correspondingly reduced along c axis, as shown in Fig. 2. It is obvious that when In atoms enlarge the lattice in a axes, the interplanar crystal spacing in c direction is simultaneously reduced, which may lead to the difference of electronic structures.

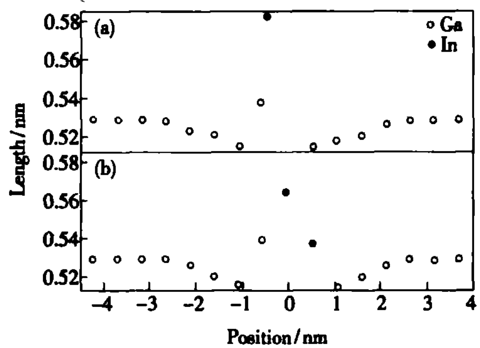

Fig. 2 The unit cell length as a function of position along c axis for Model Ⅰ (a) and Ⅱ (b).

3.2 Band Structure

The optical and electrical properties of semiconductors fundamentally depend on their band

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structure. In general, quantum confinement occurs when the well-width of QW approach the size of Bohr radius. For a comprehensive understanding on the quantum confinement effect, we have the aid of solving the effective mass Schrödinger equation for the simplified square potential well shown in Fig. 3

$$\left[-\frac{\hbar^2}{2m_e^*}\nabla^2 + V(z) \right] \Psi = E\Psi \qquad (1)$$

where m_e^* is the effective mass of the electron. From Eq. (1), the energy levels at Γ point for the electrons at the bottom of the conduction bands are

$$E = E_e + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_e^*} + \frac{\hbar^2 n^2 \pi^2}{2m_e^* L^2} \qquad (2)$$

where $n = 1, 2, 3, \cdots$. In Eq. (2), electrons have quantized kinetic energy and possess discrete energy

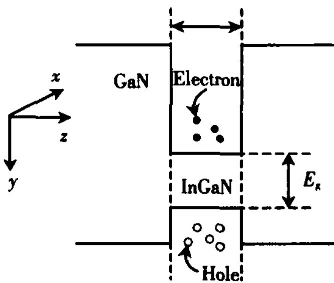

Fig. 3　The simplified square potential well of InGaN/GaN QW.

levels along z direction.

In Fig. 4, it is obvious that the band structures take discrete constant energy at both the conduction band minimum (CBM) and the valence band maximum (VBM) perpendicular to the interfacial plane (in c axis), whereas the band structures keep on parabola for both Model Ⅰ and Ⅱ. Our results indicated that the electrons parallel to the interfacial plane behaved very much as the free electrons, whereas perpendicular to the interfacial plane, the kinetic energy of the electrons, which were not approximately continuous, were quantized and subject to the discrete confined states giving birth to the two-dimensional electron gas. Along the high symmetry lines from Γ to A, the CBM in Model Ⅰ and Ⅱ are 1.53 eV, 1.41 eV lower than that in Bulk GaN, respectively. Attributed to the reduction of the symmetry from C_{6v} to C_{3v} caused by the insertion of InGaN QW, the 2-fold degenerated CBM of Bulk GaN is split into 2 subbands in the case of Model Ⅰ and Ⅱ. While at VBM, the heavy hole band and light hole band in Model Ⅰ and Ⅱ are 0.065 eV, 0.42 eV lower than those in Bulk GaN. It is obvious that the closer In atoms stand, the smaller band gap will approach.

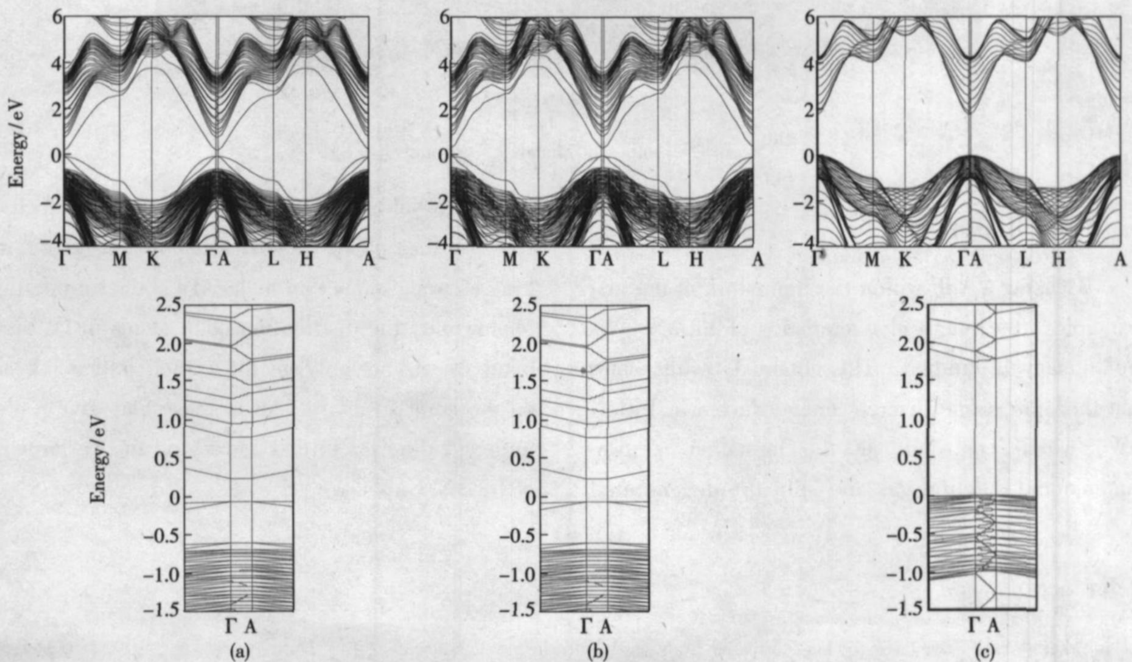

Fig. 4　Band structures of Model Ⅰ (a), Model Ⅱ (b) and bulk GaN (c) with their magnifications around Γ and A points.

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3.3 Density of States

The DOS profiles of each Ga-N and In-N bi-layers along [0001] direction are shown in Fig. 5. In the manner of speaking, it can illuminate the band structure of QW in real space. In Fig. 5, the formation of confinement states are ascribed to In-N bi-layers, which have a confining effect on the electrons and holes. Meanwhile, in tune with the aforementioned lattice distortions near InGaN/GaN interfaces, some Ga-N bilayers have the similar local DOS to adjacent In-N bilayers, which imply the interaction between In and vicinal Ga atoms. Nevertheless, the asymmetric interaction also suggests the influence of other potential field on local DOS.

Furthermore, we can observe that the bands bend along *c* axis and their trends are consistent with the affection of polarization field. This also accounts for that the polarization field results in the asymmetric interaction between In and vicinal Ga atoms. Due to the band bending[13], the electrons and holes are separated apart to the opposite sites of the well, which will bring about the quantum confined stark effect (QCSE)[14,15]. Meanwhile, the electron-hole spatial overlap wave function is decreased, the recombination rate is suppressed, the light emission efficiency is decreased, and the threshold current density is enhanced.

The states at the bottom of the conduction band in Model II are fewer than that in Model I, which will result in lower internal quantum efficiency. In addition, the interaction between In and vicinal Ga atoms help shape a wider QW and enlarge the space between electrons and holes, which would further reduce the recombination rate. Consequently, thinning down the thickness of InGaN QW is an effective way to overcome the bottleneck of the electron-hole spatial separation[16] and to improve the light emission efficiency and the wavelength stability.

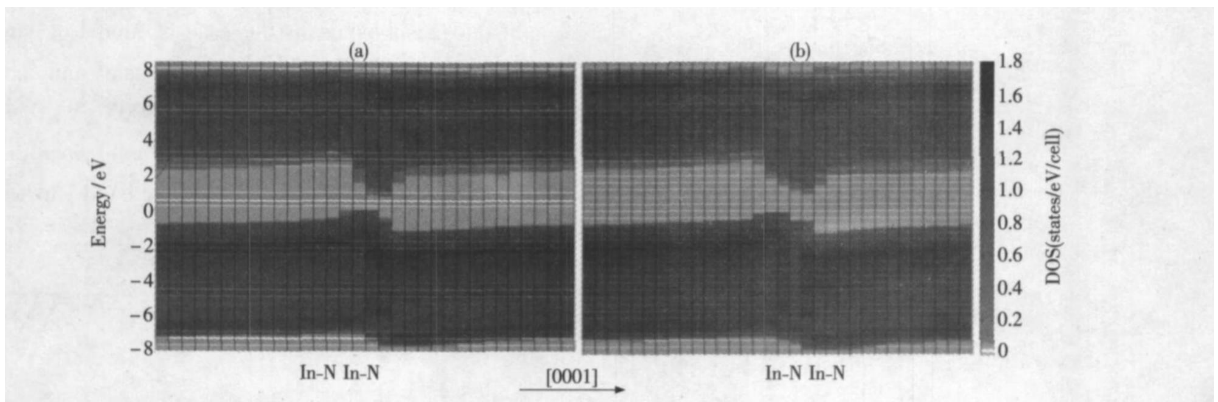

Fig. 5 PDOS profiles of Model I (a) and II (b).

4 Conclusion

By using VASP within the framework of the first principles, the micro characteristics of InGaN QWs are intensively studied. The obtained results show that there are some discrete energy levels in InGaN QW, which contribute to the formation of two-dimensional electron gas and split the degenerated band into subbands. The internal field induced by QCSE brings about the band bending in well, making a strong impact on material's optical properties. Meanwhile, the distribution of In atoms in QW have many effects not only on the crystal lattice but also on the band structure. All of those may give a clear understanding for further improving the performance of InGaN/GaN QWs.

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InGaN量子阱的微观特性

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摘要: 采用 VASP程序包模拟计算 InGaN量子阱的能带, 精细展示了量子阱实空间能带结构。计算结果表明, In原子所在区域出现局域束缚态, 导带底与价带顶的简并能级发生分裂, 同时量子阱沿垂直结面方向存在分立的能级。此外, 针对影响能带的 In组分波动、能带弯曲等问题进行探讨, 以准确描述其电子行为, 从而深入系统地了解 InGaN/GaN量子阱的电学光学等特性。

关　键　词: InGaN; 量子阱; VASP; 能带结构

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