Microelectronics Journal 40 (2009) 342–345

Contents lists available at ScienceDirect

Microelectronics Journal

journal homepage: www.elsevier.com/locate/mejo

Microstructure analysis in strained-InGaN/GaN multiple quantum wells

Huaping Lei [a,b], Jun Chen [c,*], Xunya Jiang [b], Gérard Nouet [a]

[a] Centre de Recherche sur les Ions, les Materiaux et la Photonique (CIMAP), 6 Boulevard Maréchal Juin, 14050 Caen, France
[b] State Key Laboratory of Functional Materials for Informatics, SIMIT, CAS, Changning Road 865, Shanghai 200050, China
[c] Laboratoire de Recherche sur les Propriétés des Matériaux Nouveaux, Université de Caen, IUT d'Alençon, 61250 Damigny, France

ARTICLE INFO

Available online 19 September 2008

PACS:
61.43.Bn
61.46.Bc
68.65.Fg

Keywords:
Computational simulation
Multiple quantum wells
InGaN
Strain

ABSTRACT

The barrier thickness effect on the energy and microstructure properties of InGaN/GaN multiple quantum wells is investigated with Stillinger–Weber potential. The calculation indicates that the energy of a quantum well increases as the GaN barrier thickness rises, and that Ga–N and In–N bonds are shrunk with respect to those of random InGaN alloy. Moreover, a critical value of the barrier thickness exits. If the barrier thickness exceeds the critical value, the bond length of Ga–N in quantum wells reduces as a function of indium concentration. This singular behavior of Ga–N bond is analyzed with a force balance model.

1. Introduction

The narrow band gap of InN, 0.7 eV, has given a new impact to the wavelength range of the III-nitrides [1,2]. Thus, the InGaN heterostructures are very attractive for light-emitting diodes, laser diodes and solar cell devices working within a wide spectrum range. In reality, the light-emission mechanism of InGaN/GaN heterostructures is still controversial: the formation of In-rich clusters in InGaN quantum wells (QWs) due to Indium segregation should result in the localization of the excitons for the radiative recombination [3,4]. But recent experiment based on the three-dimensional atomic-probe technique indicates that no In-rich clusters exist in InGaN QWs [5]. The controversy about the existence of these clusters is still relevant by involving the effect of the electron beam damages in transmission electron microscopy (TEM) experiments [6,7] or equilibrium phase separation. Moreover, the large biaxial strain due to the lattice mismatch (10.7%) between GaN and InN remains a key parameter in InGaN/GaN heterostructures. Actually, there are still few works concerning the strain effect on the stability of wurtzite InGaN/GaN MQWs. In this paper, Stillinger–Weber (SW) potential is applied to investigate the energy and microstructure properties of InGaN/GaN MQWs with different barrier thicknesses.

2. Simulation method and model

SW potential only considers the two- and three-body interactions of the nearest neighbor atoms and it is suitable to describe the properties of the tetrahedral semiconductors [8]

$$\Phi(1,\ldots,N)=\sum_{i,j(i<j)}^{N}\phi_2(i,j)+\sum_{i,j,k(i<j<k)}^{N}\phi_3(i,j,k). \tag{1}$$

The two-body interaction term is

$$\phi_2(i,j)=\varepsilon f_2(r_{ij}/\sigma), \tag{2}$$

with

$$f_2(r)=\begin{cases}A(B/r^4-1)\exp[1/(r-a)], & r<a,\\ 0, & r>a\end{cases} \tag{3}$$

and the three-body interaction term is

$$\phi_3(i,j,k)=\varepsilon f_3(\vec{r}_i/\sigma,\vec{r}_j/\sigma,\vec{r}_k/\sigma), \tag{4}$$

$$f_3(\vec{r}_i,\vec{r}_j,\vec{r}_k)=h(r_{ij},r_{jk},\theta_{ijk})+h(r_{ji},r_{ik},\theta_{jik})+h(r_{jk},r_{ki},\theta_{jki}), \tag{5}$$

$$h_{ijk}(r_{ij},r_{jk},\theta_{ijk})=\lambda\exp[\gamma/(r_{ij}-a)+\gamma/(r_{jk}-a)](\cos\theta_{ijk}+1/3)^2. \tag{6}$$

ε and σ are energy and length units, respectively. α is the cut-off distance. $\theta(i,j,k)$ is the angle formed by the $\vec{r}_{i,j}$ and $\vec{r}_{j,k}$ vectors. A, B, λ and γ are the bond-strength factors. The modified SW potential parameters for Ga–N and In–N are presented in Table 1.

In order to validate the SW parameters, the crystallographic parameters and elastic constants of GaN and InN are calculated and compared with the experimental and first-principle calculation values [9–11]. The values calculated with SW potential are in fair agreement with the experimental and first-principle calculation data (Table 2). The periodic boundary condition and Verlet algorithm are used. The size of the supercell along $[1\bar{2}10]$ and

* Corresponding author.
E-mail address: jun.chen@unicaen.fr (J. Chen).

0026-2692/$ - see front matter © 2008 Elsevier Ltd. All rights reserved.
doi:10.1016/j.mejo.2008.07.068

Table 1
SW potential parameters for Ga–N and In–N

	A	B	λ	α	γ	ε (eV)	σ (Å)
Ga–N	7.718	0.694	28.5	1.8	1.2	2.265	1.700
In–N	7.755	0.699	18.5	1.8	1.2	1.993	1.879

Table 2
Crystallographic parameters (Å) and elastic constants (GPa)

		Bond length	Lattice constant	C11	C12	C13	C33	C44	B
GaN	Expt. [a]	1.949	3.189	390	145	106	398	105	210
	Present	1.949	3.183	394	133	109	419	106	212
InN	Cal. [b]	2.156	3.538	220	120	91	249	36	125
	Present	2.156	3.521	206	109	101	214	41	139

[a] Ref. [10].
[b] Ref. [11].

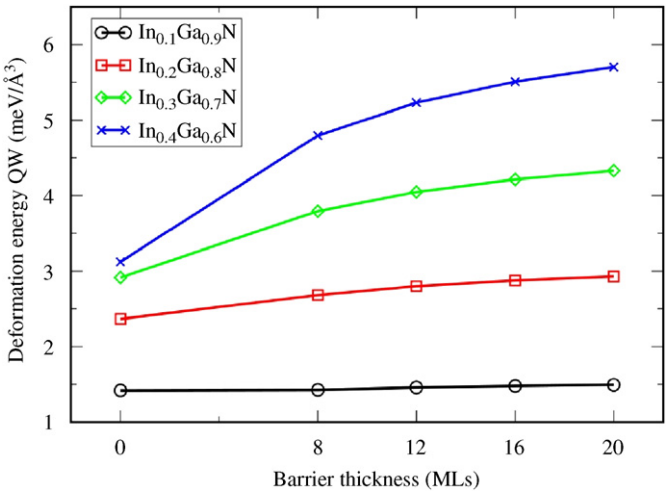

Fig. 2. (Color online) Deformation energy of InGaN QWs with different Indium concentration as a function of barrier thickness. 0 MLs indicates the random InGaN alloy.

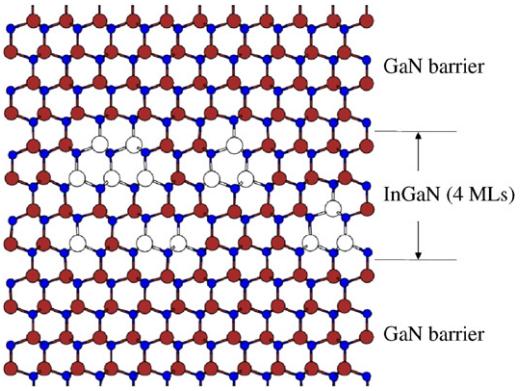

Fig. 1. (Color online) Schematic diagram of InGaN/GaN MQWs along $[1\bar{2}10]$ direction (red, white and blue circles represent Ga, In and nitrogen atoms, respectively).

$[10\bar{1}0]$ is $40a \times 24\sqrt{3}a$. The width of InGaN QWs is typically taken as 4 monolayers (MLs) and In atoms randomly distribute inside (Fig. 1). In the first stage of this analysis, no GaN barriers are considered, and the whole system is equivalent to a pure random InGaN alloy. Secondly, the heterostructure is formed with the insertion of 8, 12, 16 and 20 MLs GaN (2 MLs = $1c_{GaN}$) as barriers regularly spaced along the c-axis. The atom number in the supercell is in the order of magnitude 10^4.

3. Results and discussion

As shown in Fig. 2, the deformation energy of QWs in InGaN/GaN heterostructure is calculated as a function of the barrier thickness for different Indium concentration. The formation of random InGaN alloy (0 MLs) results in the energy increase from 1.4 to 3.1 meV/Å^3 when Indium concentration changes from 10% to 40%. With the effect of the barriers, the deformation energy of InGaN QWs in InGaN/GaN heterostructure is higher than that of the alloy with the same Indium concentration. For example, when the GaN barrier is 8 MLs thick, the energy is higher 0.007 meV/Å^3 (0.5%) for $In_{0.1}Ga_{0.9}N$ QWs and 1.671 meV/Å^3 (53%) for $In_{0.4}Ga_{0.6}N$ QWs than that of the InGaN alloys with the corresponding Indium concentration. Meanwhile, the energy of QWs depends on the barrier thickness. The thicker barrier results in the higher deformation energy of QWs. But the barrier thickness effect is less pronounced for the low Indium concentration. As the barrier thickness increases from 0 to 20 MLs, the deformation energy increases 0.073 meV/Å^3 for $In_{0.1}Ga_{0.9}N$ QWs but 2.578 meV/Å^3 for $In_{0.4}Ga_{0.6}N$ QWs.

The barrier thickness effect on the microstructure properties of QWs is investigated. As a function of Indium concentration, Ga–N and In–N bond lengths of MQWs with different barrier thicknesses are shown in Figs. 3(a) and (b), respectively. The inset within Fig. 3(a) is the variation of Ga–N bond length in the barrier region. Compared with those of the random InGaN alloy (dash lines in Figs. 3(a) and (b), respectively), Ga–N and In–N bonds are compressed in MQWs. And Ga–N bonds in the barriers are different from those in QW region. Taking $In_{0.3}Ga_{0.7}N$ ($2c_{InGaN}$)/GaN($4c_{GaN}$) MQWs for example, the bond length of Ga–N in the barriers and QWs, respectively, reduces to −0.46% and −0.79%, and In–N bond length reduces to −0.89% compared with those of $In_{0.3}Ga_{0.7}N$ alloy (1.967 Å for Ga–N and 2.117 Å for In–N). The compression of In–N bond in the strained InGaN has been validated through EXAFS experiments [12] (Fig. 3(b)). And both of Ga–N and In–N bonds are compressed more by the thicker barriers.

Furthermore, when the barrier is thin, Ga–N and In–N bond lengths increase normally as a function of Indium concentration like those of InGaN alloy. However, as shown in Fig. 3(a), there is a critical value of the barrier thickness, above which the bond length of Ga–N in QWs behaves singularly and inversely decreases as Indium concentration increases. For the 4 MLs thick InGaN QWs, the critical barrier thickness is estimated to $6c_{GaN}$. Meanwhile, In–N bonds keep increasing as a function of Indium concentration. We change the width of InGaN QWs to 2 MLs and 6 MLs. The results indicate that the abnormality of Ga–N bonds still occurs, but the critical barrier thickness shifts to $3c_{GaN}$ for 2 MLs and $9c_{GaN}$ for 6 MLs thick InGaN QWs. The strain, defined as $\varepsilon(x) = (a(x) - a_0(x))/a_0(x)$ where $a(x)$ and $a_0(x)$ are, respectively, the lattice constant of QWs and the alloy with the same Indium composition is introduced to describe the abnormality of Ga–N bonds. As shown in Fig. 4, independent of the width of the QWs, there is a critical value of the strain, over which Ga–N bonds decreases as a function of Indium concentration. Thus, the strain would be responsible for the abnormality of Ga–N bonds. The