Stillinger-Weber Parameters for InN: Application to $In_xGa_{1-x}N$*

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Abstract: By using a Stillinger-Weber (SW) type empirical potential for InN, the atomic structures of $In_xGa_{1-x}N$ alloys and the deformations induced by In-rich clusters in InGaN/GaN quantum wells are presented. The SW parameters are determined by fitting the lattice parameters and elastic constants of InN in wurtzite and zinc-blende structures. The energy of quantum wells containing In-rich clusters is investigated.

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1 Introduction

III-V nitride semiconductors (GaN, AlN, InN) are characterized by a direct band gap in the range of 0.7~6.2eV, which makes them excellent candidates for a large domain of optoelectronic applications[1]. In this manner, the first blue laser was produced with an $In_xGa_{1-x}N$ quantum well structure. Variation of the In concentration in these $In_xGa_{1-x}N$ alloys leads to different phenomena, such as In chemical inhomogeneity, phase separation, and partial ordering. The properties of In, Ga, and N phase systems have been previously investigated by empirical valence force field methods and confirmed by density functional theory[2~6]. However, for GaN/In_xGa_{1-x}N/GaN quantum wells, the mechanisms of light emission are still controversial: the formation of clusters due to indium segregation should result in the localization of carriers and be a centre for radiative recombination. One approach consists in measuring in HREM images the local deformation field in order to determine the chemical composition, but when this method was tried, InN clustering artefacts due to electron beam damage were found.

The simulation of these heterostructures requires the calculation of the atomic structure and strain energy. The size of the clusters can be large. Each cell must contain tens of thousands of atoms, and only empirical potentials are suitable. The choice of the Stillinger-Weber potential[7] is justified by our previous analysis of extended defects in GaN. A set of parameters for In and N atoms has been evaluated in order to reproduce the crystallographic parameters, bulk modulus and elastic constants of InN. Subsequently, the combination of the SW parameters for Ga, In and N atoms allows us to calculate the atomic structures and properties of $In_xGa_{1-x}N$ alloys with different In concentrations. In this paper, a set of Stillinger-Weber potential parameters for In-N and Ga-N is given, and a first investigation of the In-rich cluster in quantum wells is proposed. The computations are performed at "CRIHAN" (http://www.crihan.fr).

2 Modified Stillinger-Weber empirical potential

A modified Stillinger-Weber empirical poten-

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tial for Ga-N[8] has been largely used in the study of extended defects in GaN, such as dislocations, grain boundaries, stacking faults, and inversion domains. This potential has two terms, which describe respectively the two-body interaction between atoms and the three-body one involving the angle between the nearest neighbours. The adjustable parameters were generated by using some known properties such as the bulk modulus, binding energy, and lattice parameters. The modified parameters of the SW empirical potentials for Ga-N and In-N are presented in Table 1.

Table 1 Stillinger-Weber parameters for InN and GaN

SW potential parameter	Ga-N	In-N
A	7.7183	7.7546
B	0.6937	0.6986
a	1.8	1.8
γ	1.2	1.2
λ	23.0425	15.3604
ε/eV	2.2645	1.9925
σ/nm	0.17001	0.18790

These parameters give good crystallographic parameters of the materials: the calculated bond lengths of Ga—N and In—N are 0.1949 and 0.2156nm, respectively, similar to the experimental values. The calculated elastic constants and bulk modulus seem in fair agreement with the experimental data as well[9]. The most stable structures obtained with these parameters are wurtzite and zinc-blende structures. These parameters are thus suitable for calculating the atomic configurations in InGaN alloys.

In our calculation, the atomic structures were relaxed by using the Verlet algorithm. Periodic boundary conditions were used in the relaxation.

3 Quantum wells

Four MLs of InGaN were introduced into the GaN matrix as a QW. The QWs were created with respect to the phase decomposition according to the spinodal line in the phase diagram. Three cases were considered, which contained the same number of In, Ga, and N atoms in the 4ML quantum wells. The total InN concentration was about 29.65%. The first one contained 100% InN clusters (and was therefore named N100), the second (N95) had a concentration of 95% InN, and the last one (N80) 80%.

Only the deformations along the c axis were measured (Fig. 1). The deformation d is defined as

$$d = \frac{d_c}{d_0} - 1$$

where d_0 (= 0.25988nm) and d_c are the distances between the nearest metallic neighbours along the c axis in pure GaN and in the relaxed alloy, respectively. According to the measurements, the maximum deformation in the centre of the InN-rich cluster (N100) can reach 8.68%, which is close to experimental values (about 10%), confirming the experimental analysis of pure InN clusters in QWs by image processing[10].

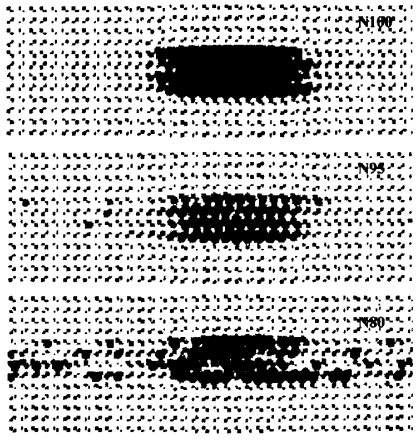

Fig. 1 Deformation maps of In-rich clusters in a QW
The size of the black balls is proportional to the deformation in the [0001] direction.

The energy differences with respect to a perfect GaN crystal vary from 1180eV for N80 to 1216eV for N100 with 16,238 atoms in the QW. The energy of a random distribution containing the same number of atoms is 1169eV. This result shows that the formation of In-rich clusters is not energetically favoured. With these potentials, the equilibrium distances in the bulk were found to be 0.194nm for GaN, and 0.215nm for InN bonds. In the QWs, the values for GaN are similar, with a slight spreading of the distribution (Fig. 2(a)). In the opposite, the distribution of the bond lengths in the QWs shows that the In—N bonds are shortened, and that the In-rich clusters thus are strained. In the pure InN clusters, and in N95, the mean bond length is close to 0.2075nm. This value goes up to 0.2095nm for N80, showing that it is less strained (Fig. 2(b)).

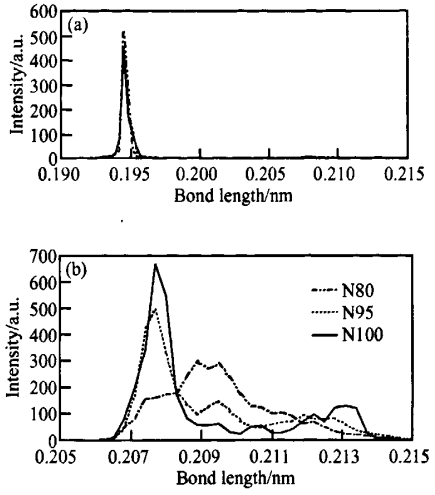

Fig. 2 (a) GaN bond length distributions in the QWs containing the clusters N80, N95 or N100; (b) InN bond length distributions in the QWs containing the clusters N80, N95 or N100

The analysis of the angle distribution shows two types of profiles, one for the In-rich clusters, N100 and N95 with three peaks, and the second one with only two peaks (Fig. 3). In the first one, the peak localized at 109.3° is close to the ideal value, 109.5°, and is likely due to the contributions of the atoms out of the clusters. The position of the peak is common to the three configurations. The two others, 108.9° and 109.8°, probably result from the deformation of the tetrahedra units in the clusters. In the configuration containing the

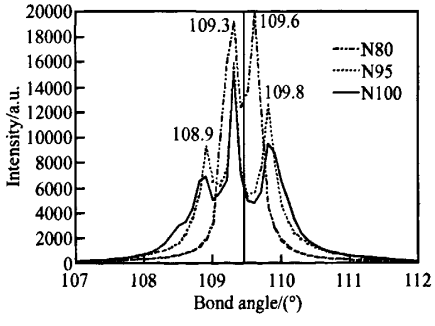

Fig. 3 Angular distribution of the QWs containing the configurations N80, N95 or N100

N80 clusters, the main peak at 109.3° is broader, and the other has shifted down from 109.8° to 109.6°, confirming that the deformation is less important. In these conditions, it is clear that the configuration N80 is the most likely structure in the hypothesis of the existence of In-rich clusters in QWs.

4 Conclusion

We have used a modified Stillinger-Weber potential to analyze InGaN quantum wells. Three cases were considered, with 100%, 95%, and 80% InN in the cluster. The clusters with the highest InN concentrations are not favourable, but it seems that the clusters with a low concentration could be possible.

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InN Stillinger-Weber 参数:用于 $In_xGa_{1-x}N$ 合金*

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摘要: 使用 Stillinger-Weber(SW)类型经典势,研究了 $In_xGa_{1-x}N$ 合金的原子结构以及富铟 Clusters 引起的 InGaN/GaN量子阱的形变.SW 参数来自氮化铟晶体常数和闪锌矿及铅锌矿结构中的弹性常数.还给出了含有富铟团簇的量子阱的能量.

关键词: 氮化铟; SW 参数; InGaN 量子阱; 富铟团簇
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