Lithuanian Journal of Physics, Vol. **55**, No. 1, pp. 10–16 (2015)

INFLUENCE OF VACANCIES ON INDIUM ATOM DISTRIBUTION IN InGaAs AND InGaN COMPOUNDS

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Received 15 August 2014; revised 27 October 2014; accepted 10 December 2014

It has been theoretically ascertained that for defect-free InGaAs and InGaN compounds the uniform distribution of indium atoms is more energetically preferable than the clustering distribution. The presence of gallium and arsenic vacancy in InGaAs and nitrogen vacancy in InGaN facilitates indium atom clustering distribution. It has been shown that the increase in the indium content in InGaAs and InGaN compounds leads to the decrease of the formation energy of gallium, arsenic and nitrogen vacancies.

Keywords: InGaN, InGaAs, defect formation energy

PACS: 61.72.uj, 61.72.Bb

1. Introduction

$In_xGa_{1-x}As$ and $In_xGa_{1-x}N$ compounds with the indium content up to 0.3 are materials widely used in fabrication of laser diodes and light-emitting diodes. Optical properties of such devices are dependent to a greater extent on the indium atom spatial distribution within the device active layer, especially when the last is a quantum well one[1, 2].

The peculiarities of the indium spatial distribution in InGaAs and InGaN compounds were investigated experimentally [3–7]. The theoretical study of possible spatial distribution types of the indium atoms in InGaN was carried out only for the defect-free crystal [8, 9]. Indium atom spatial redistribution in the presence of InGaAs and/or InGaN crystal lattice point defects was not considered in detail.

Among the defects formed in InGaAs and InGaN compounds, the gallium, arsenic and nitrogen vacancies are widespread. The defects can change the crystal structure near the first or even the second coordinate sphere relative to the defect centre [10]. This may have an appreciable effect on the indium atom distribution layout. In addition to that, the defect properties, e. g. formation energy, can be markedly dependent on the indium content in InGaAs and InGaN compounds [11, 12].

The aim of this article is the investigation of peculiarities of the indium atom spatial distribution within InGaAs and InGaN compounds in the presence of point defects and the evaluation of influence of the indium content on the point defect (gallium, arsenic and nitrogen vacancies) formation energy in the compounds.

2. Computation methods

The indium atoms spatial distribution and the energy characteristics of the vacancies in InGaAs and InGaN compounds depending on the indium content have been simulated in the framework of the cluster approach. The model clusters were formed by "cutting" the bounded fragment from the GaAs and GaN crystal volume [13, 14]. The initial positions of atoms of the clusters were given as the positions of these atoms in real crystal lattice sites. The GaAs and GaN lattice constants were taken from [15] at the temperature of 300 K. The dangling bonds arisen at the cluster border during "separation" of the fragment from the crystal volume were closed by the hydrogen atoms in order to simplify the self-consistency calculation procedure [13, 16].

Two calculation methods have been used for the investigation of indium atom distribution and the evaluation of vacancy formation energy. The first method

was a quantum-mechanical first-principles (Hartree-Fock) method of the self-consistent field which represents each molecular orbital as a linear combination of atomic orbitals. The atomic orbitals were described using the MINI basis set [17]. This method was realized with the help of the software package GAMESS [18, 19]. The second calculation method was a semi-empirical method with the PM7 modelling Hamiltonian realized using the program package MOPAC 2012 [20, 21].

70-atom (35 Ga + 35 As) GaAs and 68-atom (34 Ga + 34 N) GaN model clusters were selected for the simulation. The cluster size was chosen on the grounds of the appropriate cluster symmetry and calculation precision as well as machine time minimization. Gradient convergence tolerance for GAMESS calculations was taken as 0.00001 Hartree/Bohr. For the MOPAC calculations a Pulay's procedure was used [22]. The PM7 accuracy is described in [21]. Modelling of the indium atom spatial distribution was performed by the substitution of some gallium atoms in the GaAs or GaN cluster for indium atoms (see Fig. 1). Two types of the indium atom spatial distribution within the InGaAs and InGaN model clusters, namely, the clustering distribution and the uniform distribution were considered. The first distribution type is characterized by minimal distances between indium atoms. In the case of the second/uniform distribution type the distances between indium atoms were taken maximally possible within the model cluster.

The geometry optimization was conducted for each indium atom and the crystal atoms within the first coordinate sphere relative to each indium atom. The optimization of atoms within two coordinate spheres leads to almost the same geometry obtained with optimization of the atoms within only one coordinate sphere. It has been found for our model approach that the difference in the positions of the same atom calculated taking into account one and two coordinate spheres is less than 0.02 Å.

The numerical calculations were conducted, first, for the three InGaAs model clusters: 1) defect-free cluster (IGA_{DF}), 2) InGaAs cluster with gallium vacancy (IGA_{Ga}), and 3) InGaAs cluster with arsenic vacancy (IGA_{As}). Then, the calculations were made as applied to the three types of the InGaN cluster: 1) defect-free cluster (IGN_{DF}), 2) InGaN cluster with gallium vacancy (IGN_{Ga}), and 3) InGaN cluster with nitrogen vacancy (IGN_{N}). The IGA_{As} and IGN_{N} clusters are illustrated in Fig. 2. The vacancies in IGA_{Ga}, IGA_{As}, IGN_{Ga} and IGN_{N} model clusters were allocated within the first coordinate sphere relative to the centre of the indium atom group.

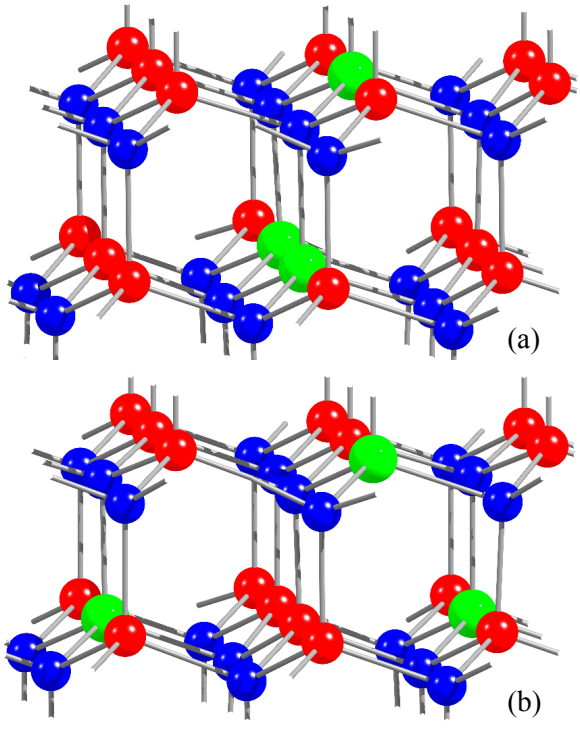

Fig. 1. Clustering (a) and uniform (b) distributions of indium atoms in the $In_{0.09}Ga_{0.91}As$ model cluster (green balls are In atoms, red balls are Ga atoms and blue balls are As atoms). The distance between each indium atom and the end atom of the cluster (InGaAs and InGaN) is no less than two coordinate spheres.

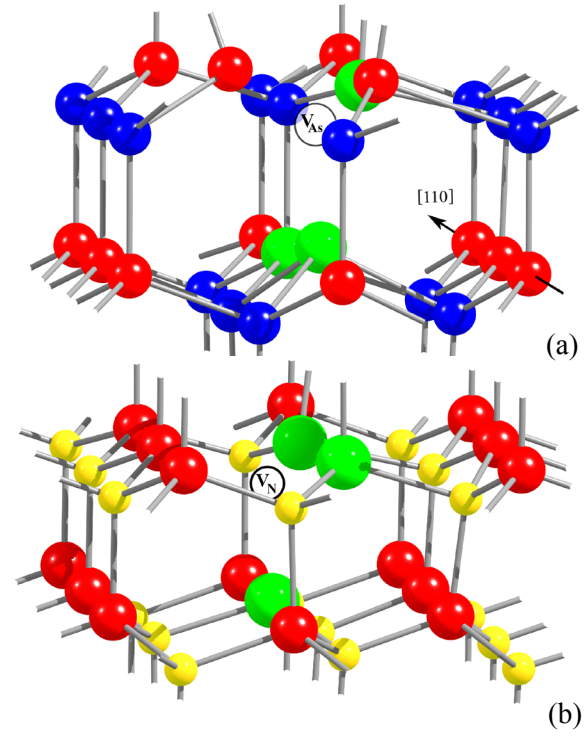

Fig. 2. IGA_{As} (a) and IGN_{N} (b) clusters (yellow balls are nitrogen atoms). The distance from the vacancy to the cluster surface is no less than three coordinate spheres.

To evaluate the effect of the indium content in InGaAs and InGaN compounds on the vacancies formation energy 68 and 66 atom clusters were used, respectively. In our article the term "defect formation energy" means the energy required for formation of the defect in the existing cluster, and the sum energies of isolated atoms for both the defect and defect-free clusters are equal due to an identity of their atom content. It should be noted that vibrational processes and cluster enthalpy changes are not taken into account in our modelling.

Gallium, arsenic and/or nitrogen vacancies were formed by removing the corresponding atom from the crystal lattice site. The vacancies were placed at the centre of the model clusters and the distance from the vacancy to the cluster surface is no less than three coordinate spheres. The structure parameters of the defect clusters with different indium content were optimized relative to the total energy minimum using the above-mentioned quantum-mechanical first-principles and semi-empirical calculation methods. The calculated lattice constants for the defect-free InGaAs and InGaN compounds are presented in Ref. [23].

Table 1. The calculated r_c and r_u (in Å) as well as E_c–E_u (in eV) values for the $In_{0.09}Ga_{0.91}As$ compound.

	GAMESS			MOPAC		
Cluster	r_c	r_u	E_c–E_u	r_c	r_u	E_c–E_u
IGA_{DF}	4.08	6.88	0.121	4.01	6.85	0.084
IGA_{As}	3.96	6.06	–0.366	3.95	6.34	–0.448
IGA_{Ga}	4.03	6.76	–0.109	4.01	6.71	–1.120

3. Indium atom spatial distribution

The results of calculations of the maximum distance between indium atoms for the clustering distribution r_c and uniform distribution r_u as well as the difference between the total energies of model clusters with the clustering and uniform indium atom distributions E_c–E_u are given in Tables 1 and 2 for InGaAs and InGaN compounds. It should be noted that both values E_c and E_u are negative by their physical nature.

As seen from Table 1, for the defect-free $In_{0.09}Ga_{0.91}As$ compound the uniform indium atom distribution is more energetically preferable than the clustering one. (The magnitude of E_u is 0.121 eV (GAMESS) or 0.084 eV (MOPAC) greater than that for E_c). Addition of indium to the IGA_{DF} cluster leads to an increase of the E_c–E_u difference. In particular, for the $In_{0.11}Ga_{0.89}As$ compound E_c–E_u = 0.189 eV (GAMESS) or 0.117 eV (MOPAC). These data are in agreement with the result of studying the $In_{0.12}Ga_{0.88}As$ quantum wire properties performed using cross-sectional scanning tunnelling microscopy [3]. No indium clustering phenomenon was observed under that experimental condition.

In the presence of the arsenic vacancy the clustering distribution is more energetically preferable for InGaAs than the uniform one (as can be seen from Table 1, the energy difference E_c–E_u changes the sign as one goes from the IGA_{DF} to IGA_{As} cluster). This can be explained in the following way. Indium atoms introduce strains into the GaAs crystal lattice. If V_{As} is arisen near the indium atom, it facilitates the relaxation of strains. When the arsenic vacancy is allocated within the first coordinate sphere relative to the centre of the indium atom clustering group, it reduces the strains introduced by all indium atoms (see Fig. 2(a)). This strain release effect manifests itself weaker in the case of the uniform indium atom distribution because the vacancy is located near only one indium atom.

Another situation occurs when the arsenic vacancy is outside the first coordinate sphere of the indium atoms group related to the clustering distribution. In this instance for InGaAs the E_c–E_u is positive in the sign and equal to 0.206 eV (GAMESS) or 0.132 eV (MOPAC). The positive value of E_c–E_u means that the uniform distribution is energetically more preferable than the clustering one.

Table 2. The calculated r_c and r_u (in Å) as well as E_c–E_u (in eV) values for the $In_{0.09}Ga_{0.91}N$ compound.

	GAMESS			MOPAC		
Cluster	r_c	r_u	E_c–E_u	r_c	r_u	E_c–E_u
IGN_{DF}	3.29	5.03	1.770	3.60	5.00	1.175
IGN_{N}	3.04	4.88	–1.599	2.93	4.94	–2.020
IGN_{Ga}	3.17	4.26	2.755	3.03	4.38	0.332

According to our calculation (see Table 1), the gallium vacancy affects the indium atom distribution for InGaAs in the same manner as the arsenic vacancy, but the relaxation of strains introduced by indium atoms is realized via the relaxation of arsenic atoms which are bonded with the indium atoms and gallium vacancy.

The same tendency for the vacancies influence on the indium atoms distribution was observed in the results of the modelling using the density functional theory (DFT). For the IGA_{DF} cluster E_c–E_u = 0.003 eV, r_c = 4.11 Å and r_u = 6.91 Å, for the IGA_{As} cluster E_c–E_u = –0.013 eV, r_c = 4.00 Å and r_u = 6.20 Å, and for the IGA_{Ga} cluster E_c–E_u = –0.008 eV, r_c = 4.06 Å and

r_u = 6.72 Å. For DFT calculations the hybrid functionals B3LYP with Hay-Wadt effective core potentials for all heavy atoms in a combination with the Hay-Wadt valence basis were used and realized in the GAMESS program [19].

For the defect-free $In_{0.09}Ga_{0.91}N$ compound the uniform indium distribution is energetically more preferable than the clustering one by 1.770 (GAMESS) or 1.175 eV (MOPAC) (see Table 2). For the $In_{0.12}Ga_{0.88}N$ compound the E_c–E_u energy difference is 1.891 (GAMESS) or 1.242 eV (MOPAC), and r_c = 4.51 Å. These values are close to E_c–E_u = 1.04 eV obtained theoretically for the $In_{0.17}Ga_{0.83}N$ compound using first-principles calculations [8]. This conclusion is also supported by the fact that the indium clusterization phenomenon was not revealed experimentally for $In_xGa_{1-x}N$ compounds with x < 0.3 [6] and for $In_{0.22}Ga_{0.78}N$ [4, 5] using the electron microscopy with the electron energy less than 0.4 MeV.

The indium clustering distribution for the $In_{0.09}Ga_{0.91}N$ compound becomes energetically preferable in the presence of the nitrogen vacancy (see Table 2). The indium clustering was observed experimentally in the $In_{0.22}Ga_{0.78}N$ compound irradiated by the electron beam with the 0.4 MeV energy [4, 5]. As it was ascertained in [24], the isolated nitrogen vacancies are formed in the InGaN compounds at the electron beam energy of about 0.4 MeV. Thus, our calculation results may help to explain partially the experimentally observed indium atom clustering under the electron beam irradiation. The size of the indium atom clusters observed in the experiments [4, 5] is about 1 nm. Based on the data given in Table 2, the size of the indium clustering area in the $In_{0.09}Ga_{0.91}N$ compound is roughly specified by the value of $r_c \approx 3$ Å. The difference between the experimental and calculated indium cluster sizes is likely conditioned by two reasons. Firstly, the greater is the indium content value for the InGaN compound the higher can be the indium atom clustering size in the presence of the nitrogen vacancies. The indium content used in our calculations is less by two times than the one in the experiments [4, 5]. Partially, that assumption is confirmed by the value of E_c–E_u = –1.631 eV (GAMESS) or –2.113 eV (MOPAC) calculated for $In_{0.12}Ga_{0.88}N$ (this value is less than E_c–E_u given in Table 2 for $In_{0.09}Ga_{0.91}N$). Secondly, the nitrogen vacancies distribution in the InGaN irradiated by the electron beam may be nonuniform which can lead to vacancies complex formation and larger size of the indium clustering area.

As contrasted to the InGaAs compound, the presence of the gallium vacancy in the InGaN compound does not change the indium distribution within the model cluster (see Table 2). This result can be explained by the difference between the crystal lattices of GaN (wurtzite) and GaAs (zincblende). The tendency for the vacancies influence on the indium atoms distribution in the InGaN compound remains with the DFT calculations (the hybrid functionals B3LYP with Hay-Wadt effective core potentials in a combination with Hay-Wadt valence basis).

Table 3. The calculated formation energy E_f for gallium (V_{Ga}) and arsenic (V_{As}) vacancy calculated using GAMESS and MOPAC for different In content in InGaAs.

	E_f, eV (GAMESS)		E_f, eV (MOPAC)	
In content	V_{Ga}	V_{As}	V_{Ga}	V_{As}
GaAs	5.223	4.916	4.351	2.117
$In_{0.12}Ga_{0.88}As$	4.931	3.814	4.224	1.457
$In_{0.20}Ga_{0.80}As$	4.735	2.764	4.153	1.104
$In_{0.32}Ga_{0.68}As$	4.503	1.218	4.041	0.994

4. Vacancy formation energy

The vacancy formation energy E_f is given in Tables 3 and 4 for the $In_xGa_{1-x}As$ and $In_xGa_{1-x}N$ compounds depending on the indium content value.

The gallium vacancy formation energy calculated for GaAs using the computation packages GAMESS and MOPAC was found to be 5.223 and 4.351 eV, respectively (see Table 3). These values are close to E_f obtained for GaAs by different calculation methods, namely, (2.69–4.89) eV [25–29] as well as to that derived using the experimental approach (3.2 ± 0.5 [30], 4 ± 0.5 eV [31]). It was shown theoretically [27] that the V_{Ga} formation energy for the $In_{0.5}Ga_{0.5}As$ compound was equal to 3.0 eV. According to the results of our modelling the value of E_f for the $In_{0.31}Ga_{0.69}As$ compound is 4.503 (GAMESS) or 4.041 eV (MOPAC). The last E_f values are also in agreement with the above mentioned data.

Table 4. The calculated formation energy E_f for gallium (V_{Ga}) and nitrogen (V_N) vacancy calculated using GAMESS and MOPAC for different In content in InGaN.

	E_f, eV (GAMESS)		E_f, eV (MOPAC)	
In content	V_{Ga}	V_N	V_{Ga}	V_N
GaN	8.957	2.704	7.955	1.652
$In_{0.12}Ga_{0.88}N$	8.282	2.035	7.235	1.467
$In_{0.21}Ga_{0.79}N$	7.899	1.745	6.572	1.211
$In_{0.32}Ga_{0.68}N$	7.521	1.535	5.902	1.003

According to different papers [25, 27, 29, 32, 33] the values of the arsenic vacancy formation energy for GaAs are in the range (2.08–5.21) eV. The E_f value

for the arsenic vacancy in the $In_{0.5}Ga_{0.5}As$ compound was theoretically evaluated as 2.52 [32] and 2.6 eV [27]. As follows from Table 3, our results for the V_{As} formation energy both for GaAs and InGaAs are in agreement with the E_f presented in the above-mentioned papers.

The results of the calculations of gallium vacancy formation energy for GaN (8.957 eV for GAMESS or 7.955 eV for MOPAC, see Table 4) are close to that (7–8.40) eV obtained theoretically by different methods [34–36]. The values of the nitrogen vacancy formation energy for GaN obtained in papers [34–36] are in the range of (0.89–3.16) eV. As follows from Table 4, the results of our calculations of both V_{Ga} formation energy and V_N formation energy for GaN are close to the E_f calculated in other papers.

Both for the InGaAs and InGaN compounds the gallium, arsenic and nitrogen vacancy formation energy decreases with an increase in the indium content, but for the arsenic and nitrogen vacancies the decrease rate is greater than that for the gallium vacancy.

An increase of the indium content in the InGaAs compound leads to a decrease in the Ga and As vacancies formation energies and hence facilitates indium clustering (see Section 3). As for the InGaN compound, this effect is not so unambiguously apparent. With an increase of the indium content the Ga and N formation energies are decreased. But the indium clustering in the presence of Ga vacancy (as opposed to the N vacancy) does not take place. Thus, the In clustering effect in the InGaN compound should be studied taking into account the mutual interaction between the Ga and N vacancies.

5. Conclusions

It has been theoretically ascertained that for defect-free InGaAs and InGaN compounds the uniform distribution of indium atoms in the crystal lattice is more energetically preferable than the clustering distribution. The presence of gallium or arsenic vacancies in InGaAs and nitrogen vacancy in InGaN within the first coordinate sphere relative to the centre of the indium atom group facilitates the indium atom clustering distribution.

The effect of the indium content on the properties of vacancies arising in InGaAs and InGaN compounds has been evaluated in the framework of the cluster approximation using first-principles and semi-empirical quantum mechanical calculations. It has been shown that the increase in the indium content in InGaAs and InGaN compounds leads to the decrease in the formation energy of gallium, arsenic and nitrogen vacancies. This phenomenon facilitates the indium clustering in InGaAs and InGaN compounds.

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VAKANSIJŲ ĮTAKA INDŽIO ATOMŲ PASISKIRSTYMUI InGaAs IR InGaN JUNGINIUOSE

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