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Stress relaxation in III-V nitrides: investigation of metallic atoms interaction with the N-vacancy

ROFKA RAMDANI*, VIWANOU HOUNKPATI, JUN CHEN AND PIERRE RUTERANA

Normandie Univ, ENSICAEN, UNICAEN, CEA, CNRS, CIMAP, 14000 Caen, France

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Abstract – Molecular dynamics simulations have been carried out to study the interaction between two point defects in III-nitride materials (AlN, GaN and InN): a substitutional metal atom (Indium, Aluminum, Gallium) and the N-vacancy. The Stillinger-Weber (S-W) empirical potential is used. By calculating the potential energies of different configurations with these two defects, it is shown that the indium atom in AlN and GaN or aluminum and gallium in InN are stable in the immediate vicinity of the N-vacancy. In contrast, the gallium atom in AlN and the aluminum atom in GaN may be difficult to bring near the N-Vacancy. This behavior is related to the stress relaxation in the presence of these point defects. In AlN, the stability of indium atoms around the N-vacancy is the highest, indicating a good probability of aggregation, which may constitute a first explanation for the reported phase segregation during the growth of InAlN alloys.

Introduction. – Recent achievements in optoelectronics, namely III-V nitride-based light-emitting diodes (LEDs), laser diodes (LDs) and photodetectors, as well as high-frequency, high-power microelectronics (high electron mobility transistors (HEMTs)), are due to the rapid development of III-V semiconductors technology [1-4]. Interesting optical and electrical properties of III-V nitrides have led to extensive research worldwide for applications in optoelectronic devices operating in the visible and ultraviolet wavelengths [5-6]. With direct band gaps (0.67eV InN [7], 3.41eV GaN [8], 6.2eV AlN [9]), the alloy system offers a unique opportunity for device design. Indeed, the physical properties of III-V nitride materials (AlN, GaN and InN) and their alloys are very important and exceptional for potential device applications (absorption coefficients, high electron mobility, good thermal conductivity and high thermal stability) [9-12]. During recent years, the In-Al(Ga)N/GaN heterostructures have been extensively studied because of their superior potential for high-temperature and high-power electronics, but also as they represent a challenge for device fabrication [1,13]. Firstly, the binary compounds (AlN, GaN and InN) have very different physical properties (bond length, elastic properties, growth temperatures, thermal expansion coefficients, etc.) [9,10]. Secondly, the use of foreign substrates leads to the formation of a large number of extended defect densities (dislocations [14-16], stacking defects [17,18] and inversion domains [19,20]). Of course, point defects are also present and

they negatively affect the stability and performance of the devices [21-23]. Theoretical investigations based on first-principles calculations have shown that anti-sites and self-interstitials have a high formation energy in these wurtzite nitrides, while the vacancies are most stable [24-26]. The growth of III-V nitride alloys over the entire compositional range has been difficult with some degradation phenomenon which is still poorly understood and is a barrier to device fabrication.

Up to now, experimental observations have reported that In-rich clusters can form around threading dislocations with a screw component in InGaN films [27], while phase segregation in InAlN [28] and AlGaIn [29] alloys has been observed. Leonard et al. [30] proposed a continuum theory to explain the role of dislocations in alloys that undergo spinodal decomposition. However, an atomic scale exploration of these phenomena is still lacking.

These defects degrade the crystallographic quality of the deposited layers [16], [20], [31-33] and phenomena such as phase separation/segregation [34], or atomic ordering [35] have been reported. It is also expected, that the defects that form in the layers alter the local stress state and may lead to compositional inhomogeneity [36].

It is important to understand the origin of phase segregation in these alloys, due to stress relaxation generated by the different densities of point defects, such as vacancy, that may be encountered in the deposited layers. Their study is therefore essential to understand the

^(a)E-mail: rofka.ramdani@unicaen.fr

^(b)Present address: Normandie Univ, ENSICAEN, UNICAEN, CEA, CNRS, CIMAP, 14000 Caen, France.

R. Ramdani *et al.*

structural properties of the alloy, its chemistry and formation mechanisms, and eventually to contribute to the growth of optimal quality materials in order to improve device performance.

In this work, we have conducted a detailed study using molecular dynamics in the framework of modified empirical potentials (Stillinger-Weber) for the wurtzite structure [37,38], to analyze the interaction of metal atoms in III-V nitrides (AlN, GaN and InN) with the nitrogen vacancy. The aim has been to understand the stress relaxation around the nitrogen vacancy (N_v).

Calculation models. – Our calculations are based on the Stillinger-Weber potential [39] which has been previously modified in order to model the properties of the nitride compound [37], [40, 41]. The elastic constants and bulk modulus of AlN, GaN and InN wurtzite [40] calculated by this potential are given in the table 1. These theoretical results are in agreement with the first principle calculations [42] and experimental values [43-45]. One can notice that these 3 materials have different elastic behavior.

Table 1: Elastic constants and bulk modulus of the wurtzite AlN, GaN and InN calculated by the Stillinger-Weber potential [40] and experimental values [43-45].

Elastic constants (GPa)		AlN	GaN	InN
C_{11}^h	S-W	382	395	206
	Exp	345	390	220
C_{12}^h	S-W	129	134	109
	Exp	125	145	120
C_{13}^h	S-W	98	109	101
	Exp	120	106	91
C_{33}^h	S-W	413	419	214
	Exp	395	398	249
C_{44}^h	S-W	96	106	41
	Exp	118	105	36
B^h	S-W	203	213	139
	Exp	185	210	125

To relax the structures, we need to model the large number of atoms with defects and a large number of configurations and structures.

In this theoretical study, we started by choosing a 12 x 12 x 12 supercell with initial dimensions of 37.08Å x 32.11Å x 30.27Å (3456 atoms), large enough in the periodic boundary condition. This selection was made by finding an optimal compromise between results accuracy and computation time. Our objective was first to estimate the possible interaction of a substitute metal atom (In, Ga or Al atoms, denoted by M_s) with a nitrogen vacancy (N_v) in the center of an III-N supercell

(Figure 1). For example, In_s corresponds to an indium substitutional atom in a GaN or AlN matrix. In detail, considering AlN, a nitrogen atom N is removed and an indium atom is substituted to an Al, forming a pair of In_s and N_v point-defects in the AlN supercell. This configuration is referred to In-AlN. Since this interaction depends on the distance between the two defects, we considered all cases from the first N_v neighbor up to a distance of 27Å. For this study, 1728 structures were constructed for In-AlN, In-GaN, Ga-AlN, Ga-InN, Al-GaN and Al-InN, allowing to substitute a metal atom from the supercell periphery to the first neighbour of N_v in all three compounds. For each configuration, we replace all metal atoms in the III-N matrix one by one with a substitute metal, so we have more than 1728 structures containing a substitute metal and a N-vacancy with different distances. For the calculation of the potential energy containing M_s atoms, the cells were relaxed by using quenching algorithm [46] until the kinetic temperature goes down to 10^{-6} K. The Verlet algorithm [46, 47] is used to determine the atomic positions over time.

As all supercells contain the same number of atoms in a similar environment, the interaction energy (ΔE) of each substitute metal atom with N-vacancy can be estimated:

$$\Delta E = E_i - E_{ref} \quad (1)$$

It corresponds to the difference between the total energy E_i of the supercell that contains the sub-metal atom in a given position and the reference energy (E_{ref}) which is the energy of a supercell where M_s is sufficiently far from N_v that one can consider there is no interaction between these two defects. This energy difference is used to qualify the interaction between the defects.

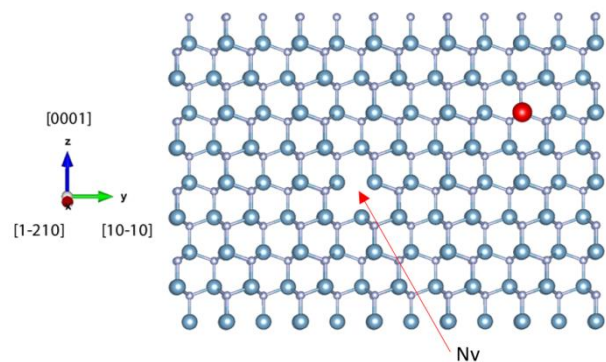


Fig. 1: A model of the supercells used to contain the N_v and one M_s atom (red).

Interaction energy. – The interaction energy deduced from the above calculation - Eqn. (1) is shown in Figure 2 for the three materials AlN, GaN and InN as a

function of the distance from the N_v to the M_s atom. One can observe that the interaction energy does not show a monotonous dependence on the distance, as observed by Lee et al. [48] in the case of In-In interaction in $In_xGa_{1-x}N$ layers. This non-monotonous behavior is due to the interaction of these two point defects.

- In zone (II), 6\AA to 9\AA , interaction energy shows small fluctuations
- Finally, the third zone (III), beyond 9\AA , is the zone where the interaction energy of the two defects is zero.

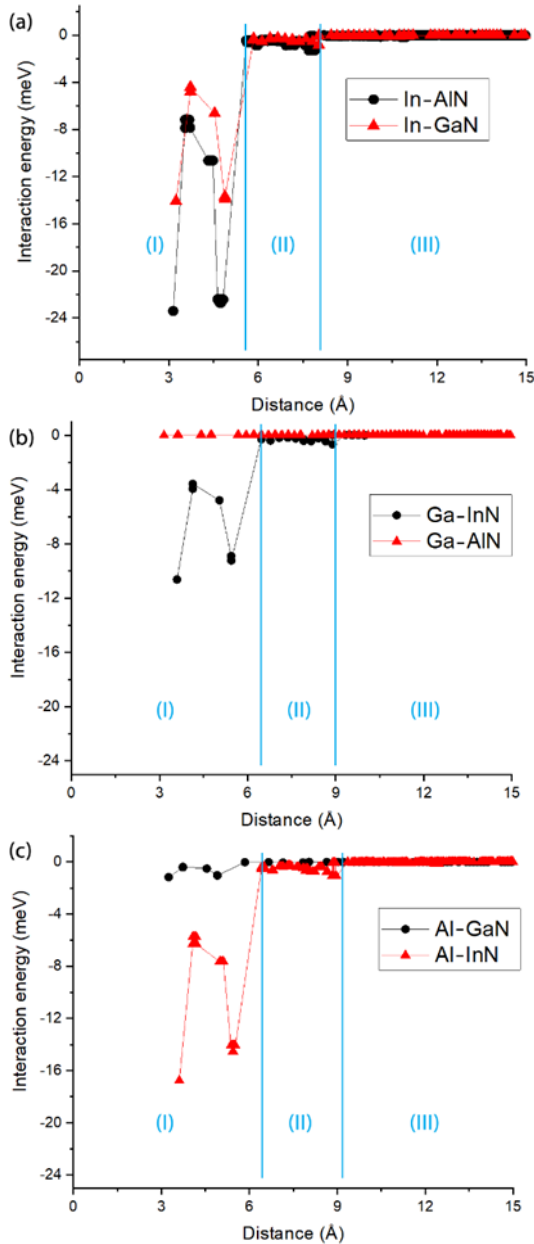


Fig. 2: Interaction energy as function of the distance between two defects: (a) substitutional In in AlN and GaN; (b) Ga in InN and AlN; (c) Al in GaN and InN.

In these curves, three zones are clearly exhibited:

- from the vacancy to about 6\AA (I), the interaction between the two defects is strong

Therefore, starting from a distance beyond 9\AA , any substitutional atomic position energy may be chosen as the reference for the calculation of interaction energy. In zone (II), the sub-metal atom positions are 5th to 12th neighbors of N_v , and the interaction gradually decreases to zero when the substitutional atom distance goes beyond 9\AA which may be set as the interaction range between the two point defects.

In the case of In-AlN, as can be seen in Figure 2a, this potential energy difference is always negative, and it changes noticeable from one position to the next. For discussion, we have named these neighbor positions G1, G2, G3, G4, and marked them in different colors (G1: green, G2: pink, G3: grey, G4: red) in figure 3. For the atoms in G4 and G1, we obtain the interaction energies of around -23meV , but, as can be seen, it is much less for the second (G2) and third neighbor sites (G3). The behavior of sub-In is similar in the case of GaN, but with smaller amplitude.

The substitutional Ga and Al have the same tendency in an InN matrix (Figure 2b and 2c), with Al-InN having slightly larger values of ΔE than Ga-InN. In summary, In-AlN exhibits the strongest interaction effect between the two point defects, followed by Al-InN, In-GaN, Ga-InN, Al-GaN and Ga-AlN. As a consequence of the relatively strong interaction between In_s and N_v , there could be an attraction of the two defects, as stabilized in G1 or G4 positions leading to a possible formation of In-rich clusters inside InAlN and InGaN alloys.

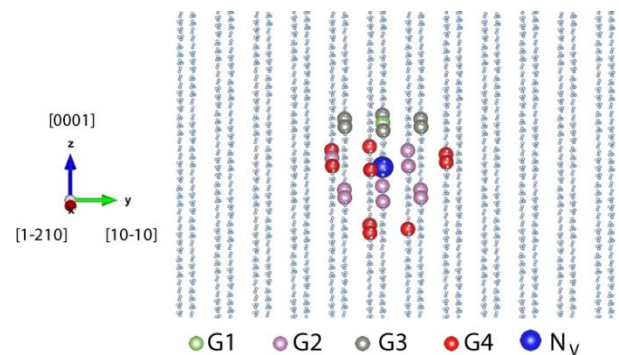


Fig. 3: Schematics of the four groups of atomic positions with most favourable energy.

The interactions between a N-vacancy and a Ga atom substituting for Al in AlN (Ga-AlN) are independent of their separation distance (Figure 2b). The interaction

R. Ramdani *et al.*

energy is practically zero. In the case of Al-GaN (Figure 2c), the interaction energy is very small but not zero. This is due to the elastic behavior of these two materials (AlN-GaN) which are very close (see table 1). For the other cases (In-AlN, In-GaN, Ga-InN, Al-GaN and Al-InN), the interaction energy depends on the distance between the N-vacancy and the substituting atom, especially in zone I. Indeed, in these cases, there is a large difference between the elastic properties of each couple of materials (AlN-InN and GaN-InN).

The empirical Stillinger-Weber potential used in this study, with the periodic condition, does not describe the charge state of the single nitrogen vacancy. Therefore, this calculation is an elastic field approach, i.e. the interaction energy results from the deformation of the bond lengths. When a substitutional metal (In, Ga or Al) is introduced in a III-N matrix (InN, GaN or AlN), the bonds are first deformed, creating a stress field around it. If this metallic atom is near a N-vacancy, the interaction of the two defects can generate a stress relaxation, which we will demonstrate later.

Strain relaxation. – In an attempt to better understand the above energy behavior and the strain relaxation processes, we analyzed the bond lengths and the angles for the metal atoms and the vacancies in the different configurations. Here we report only the bond lengths relaxations.

The introduction of the M_s atom (In, Al or Ga) into a III-N compound (InN, AlN or GaN), clearly leads to a local deformation of the bond length, compressive or extensive, as the size of the new metal atom is different. The local strain as undergone by the M_s is:

$$\varepsilon = \frac{\Delta l_1}{l_i} = \frac{l_s - l_i}{l_i} \quad (2)$$

Where l_i is the equilibrium bond length of the M_s in its binary compound with nitrogen (InN for example); l_s is the strained bond length in the III-N matrix without the interaction with N_v (Fig. 4). These initial strain ε values are given in the table 2.

For example, an InN bond is 3.24% compressed in AlN and the AlN bond is tensile by 2.44% in InN. As shown in table 2, the bonds of InN in In-AlN, InN in In-GaN and GaN in Ga-AlN are compressed from -0.64% to -3.24% and the bonds of AlN in Al-InN, GaN in Ga-InN and AlN in Al-GaN are under tensile strain, from 0.80% to 2.44%.

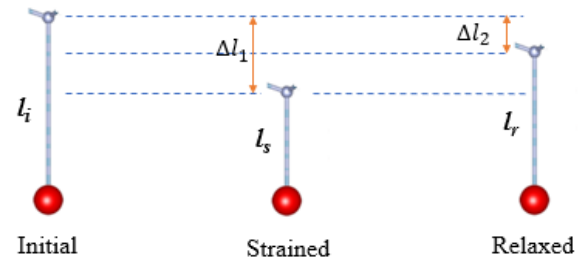


Fig. 4: Illustration of the deformation and the relaxation of M_s bond length.

For Al-GaN and Ga-AlN, the strains are very low. As explained in the previous section, this is due to the elastic properties of AlN and GaN and the very small initial strain when introducing the substituting metal atom. Therefore, the properties of these two materials being similar, neither AlN in GaN nor GaN in AlN are submitted to large strain.

When the nitrogen vacancy N_v is around, the strain is now defined as:

$$\gamma = \frac{\Delta l_2}{l_i} = \frac{l_r - l_i}{l_i} \quad (3)$$

where l_r (Fig. 4) is the relaxed bond length of M_s in the case of its interaction with N_v . The values of γ are given in table 2 for the atoms in G1-G4 positions. As can be seen, the strain γ (groups G1-G4) is smaller than the initial strain ε , meaning that the bonds undergo some relaxation in the presence of the N_v . The change is important in the case of In-AlN, In-GaN, Al-InN and Ga-InN and negligibly small for Al-GaN and Ga-AlN (Fig. 4).

As shown above, for the In-AlN which exhibits the largest strain ε with N-vacancy, the stress relaxation is the most important, which means that the indium atoms tend to sit close to the N-vacancy, and lead to the formation of In rich areas. This demonstration could be one of the mechanisms of indium precipitation in the growth of InAlN. The stress relaxation by the interaction between the sub atom and an N_v could thus be responsible of the degradation of the quality of deposited InAlN layers. For III-V nitrides materials with a given concentration of N-vacancies, these interactions can produce an effective stress relaxation in the materials.

Table 2: Strain of bond lengths of on M_s atoms in G1-G4 positions.

Bond of M_s		InN		AlN		GaN	
III-N matrix		In-AlN	In-GaN	Al-InN	Al-GaN	Ga-AlN	Ga-InN
Initial strain ε (%)		-3.24	-2.62	2.44	0.80	-0.71	1.73
Strain with N_v γ (%)	G1	-3.09	-2.50	2.32	0.77	-0.67	1.64
	G2	-3.19	-2.58	2.39	0.79	-0.69	1.69
	G3	-3.16	-2.56	2.38	0.79	-0.69	1.69
	G4	-3.09	-2.50	2.34	0.77	-0.68	1.66

Discussion. – The above study of the interaction between a substitutional metallic atom (M_s) and the N-vacancy (N_v) in III-N (AlN, GaN or InN) system shows that the metal atom could take a stable place in the vicinity of the vacancy in a radius of 6\AA (zone I) where the largest interaction energy (24meV for Indium in AlN) is obtained.

These results can be one of phase degradation explanations or segregation problems observed when producing these materials. Indeed, In the growth of InAlN at 18% In, a degradation of the quality of the deposited layers has been observed [49-51]. Previous studies highlighted the possible role of native defects generated during the growth of InAlN layers at 18% In [52, 53]. Moreover, phase separation was reported during the annealing treatment of an InAlN at 72% In, where In-rich clusters size started to increase from about 6\AA at 600°C as a function of time [28]. It may be pointed out that this radius of 6\AA corresponds to the size of the most stable In-rich cluster in InAlN in the above theoretical reports [52, 53].

On the other hand, the high stability of indium atoms around the N-vacancy indicates that the N-vacancy could have a role of segregation center in this type of material [52].

We also observe that between 6\AA to 9\AA (zone II), the interaction energy remains negative while decreasing substantially. Therefore, the N-vacancy can continue to interact weakly with metal atom located between 6\AA to 9\AA . In other words, the size of the cluster formed around the N_v could continue to increase beyond 6\AA up to 9\AA , although probably with a low indium composition.

Note that others defects (not investigated in this paper, dislocation for example) could also be a source of segregation in these materials. In fact, the deformation inside the InAlN/GaN heterostructures is not relaxed by the formation of interface defects such as dislocations [54]. Interestingly, the formation of interface dislocations in InGaN/GaN heterostructures has been reported [55], and, in this instance, the degradation of the crystalline quality is less pronounced than inside InAlN versus the indium composition.

Conclusion. – In summary, we have carried out a theoretical study of stress relaxation due to the interaction between two defects, the nitrogen vacancy and the substituted metal atoms (Al, Ga and In) in III-nitride matrices (AlN, GaN and InN). The interaction energies of the different cases In-AlN, In-GaN, Al-GaN, Al-InN, Ga-AlN and Al-InN have the same behaviors with varying amplitudes values. The In-AlN and Al-InN are two cases having the most important interaction. This can explain a possible mechanism of phases segregation in InAlN alloys where the first and the third metallic neighbors of the N-vacancy would be the most favorable position in the formation of the In-rich cluster. This effect, weaker for Al-GaN alloy and almost null for Ga-AlN alloy, which is due to the almost similar elastic properties (or stiffness) of GaN and AlN matrices, which reduces the deformation of AlN (or GaN respectively) in GaN (or AlN respectively) and also their small difference in lattice constants which produces an almost negligible initial strain.

The metal atoms located in the vicinity of the vacancy reduce the energy and exhibit a length deformation of the atomic positions with the vacancy defect which creates a stress field in the matrices studied. This interaction seems to be a driving force for these metal atoms to move to the vicinity of the vacancy and will be a start of the formation of dilute clusters in these III-N matrices.

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R. Ramdani *et al.*

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