First-principles calculation of atomic configurations in the vicinity of the boron atom in β-Ga_2O_3 irradiated with B^+ ions

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First-principles computer simulation of the local atomic configurations forming in the vicinity of boron atoms embedded into β-Ga_2O_3 by ion irradiation has been performed. It was assumed that after the dynamic stage is completed, the boron atom either occupies one of the interstitial sites or substitutes a gallium atom (which then relocates to a neighbouring interstitial site), followed by structural relaxation. It has been shown that the changes in configurations caused by relaxation can mainly be explained by the chemical interaction between boron and oxygen atoms and the tendency to establish a B-O bond length close to the sum of the ionic (or atomic) radii of these elements. The obtained results can be used for further calculations of the electronic structure and other parameters of ion-implanted boron-doped β-Ga_2O_3, that is important for the development of next-generation semiconductor device technologies.

Keywords: gallium oxide, ion implantation, boron ion doping, atomic structure, computer modeling.

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1. Introduction

Gallium oxide was of extreme interest among researchers and developers in the relevant pertinent arts (such as high current electronics, UV-photonics, gas sensorics, communications) due to the unique properties compliant with the modern requirements of these arts: large width of bandgap (~ 5 eV), high breakthrough voltages, radiation, chemical and thermal resistance, etc.

As it is known, one of the most popular and efficient methods of semiconductor microelectronics is ion implantation. Despite the fact that this method is already being used quite frequently by the developers of devices based on β-Ga_2O_3 [1–6], the physical and chemical basis of the method for this material are not yet developed well, especially when doped with chemically active elements.

One of the potentially popular elements for the gallium oxide technology is boron. Apart from rather toxic beryllium, boron has lowest atomic weight among chemically active elements, therefore accelerated B^+ ions, other things equal, develop less radiation damage and penetrate to deeper depth. Boron is isovalent to gallium, therefore, while substituting mainly the gallium points, it should not have electrical activity, it seems. However, the experiments have shown that layers ion-doped with boron may have a rather high conductivity [7]. Therefore, the ion doping with boron in the technology of semiconductor devices may be used both for the compensation of electrical activity of impurities by introduction of deed defect centers [8] and for the development of the conducting layers.

From the fundamental point of view, boron implantation is of great interest as a trivalent impurity with the least atomic number and least ion and atomic radii. Compared to gallium, boron has a stronger chemical bond to oxygen [9]. These factors may significantly affect the equilibrium atomic configuration in the surroundings of the boron atom and its interaction with the radiation defects. For example, it is interesting to find out the boron atom behavior when it enters the interstitial sites of different size. For the case of substitution of the interstitial gallium atom with the boron atom, strong local deformation may occur due to ion and atomic radii, which exceeds the potential energy and creates stimulus to change the atomic configuration.

The properties of boron-doped gallium are poorly known. Paper [10] studied the solid solution $(Ga_{1-x}B_x)_2O_3$ synthesized with sol gel method. Paper [11] studied the structural properties and profiles of element distribution in β-Ga_2O_3, irradiated with boron ions, and paper [7] together with the structure studied the optical and electrical properties of implanted layers β-Ga_2O_3:B. Paper [12] studied cathode luminescence, and paper [13] — phase transition β-Ga_2O_3 to γ-phase. The electron structure of β-Ga_2O_3 doped with boron was calculated ab inition in papers [14–16], but it did not take into account the true atomic configurations in case of ion radiation.

This paper is dedicated to the ab initio computer estimation of local atomic configurations implemented in the surroundings of the boron atom introduced in β-Ga_2O_3 by method of ion implantation, with account of structural relaxation — tuning caused by the principle of energy minimization. It was assumed that upon completion of the dynamic stage of accelerated ion movement, it gets into one of the interstitial sites or substitutes the gallium point (which at the same time was located in the adjacent interstitial site), and then relaxation takes place.

Table 1. Relaxation parameters and distances

Parameter	Interstitial site 1, small	Interstitial site 2, large	Interstitial site 3, medium
Boron atom displacement vector length, Å	0.50	0.72	0.74
Energy win under relaxation, eV	15.16	4.19	5.95
Distance from boron atom to closest oxygen atom before relaxation, Å	1.10	1.38	1.52
Distance from boron atom to closest oxygen atom after relaxation, Å	1.50	1.47	1.41

2. Calculation method

Use of software suites implementing the ab initio calculations of atomic configurations by pseudopotential method in case of study of the layers exposed to ion implantation seems to be feasible, since these suites make it possible to estimate the structural rearrangement of the non-equilibrium rearrangement of non-equilibrium atomic configurations.

This study used software suite Quantum Espresso [17]. The calculation was carried out using a model supercell β-Ga_2O_3, including four elementary cells (80 atoms) and one elementary cell obtained by replication (transmission) (dimensions $a = 12.45$ Å, $b = 3.08$ Å, $c = 5.88$ Å) [18]. For the calculation, Ultrasoft (US) [17] pseudopotential was used with Perdew, Burke, and Ernzerhof (PBE) functionality [19]. The cutoff energy was adopted to be equal to 400 eV [20], and the criterion of convergence of force fields corresponding to the relaxation of the equilibrium state lattice, was selected as equal to $2.6 \cdot 10^{-2}$ eV/A. At each step of the interactive process of finding the end equilibrium configuration of atoms, the coordinates and energy of crystallite were recorded.

3. Results and discussion

Further different variants were considered for the initial position of the implanted boron atom and defects located in its surroundings – Frenkel pair components. Since the review of all potential variants would have taken too much space, we limited ourselves to some cases only, which demonstrate typical features of the possible system behavior.

Variant 1. The boron atom before relaxation is located in one of the interstitial sites

Figure 1 shows the structure of the elementary cell β-Ga_2O_3. The presence of three types of interstitial sites is shown, which are notionally named „small“, „large“ and „medium“.

Figure 2 shows the initial positions of the boron atom (before relaxation) — in the centers of each interstitial site, and their position after relaxation. Table 1 shows the corresponding distances of these atoms to the closest atoms of gallium and oxygen, and also lengths of boron

Table 2. Ion and atomic radii of gallium, oxygen and boron atoms [21,22]

Atom	Ion radius, Å	Atomic radius, Å
Gallium	0.62	1.39
Oxygen	1.36	0.71
Boron	0.20	0.91

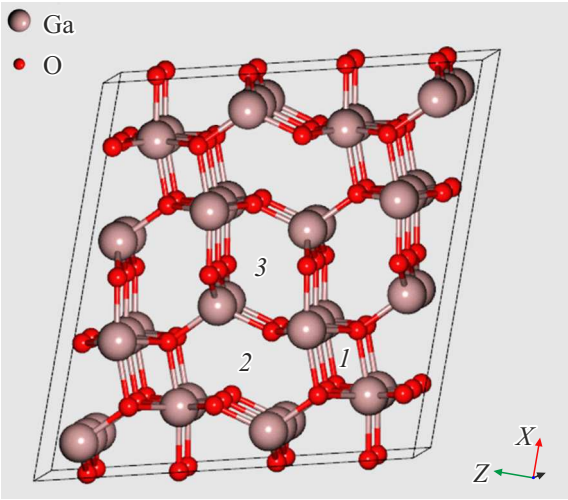

Figure 1. Atomic structure of modeled cell β-Ga_2O_3.

atom displacement vectors. You can see that relaxation led to significant displacement of the boron atom as such and adjacent atoms.

From Table 1 you can see that prior to relaxation the distance between the boron atom in the small interstitial site and the adjacent oxygen atom was smaller than the sum of ion (and atomic) radii of boron and oxygen (see Table 2). The increase of this distance under relaxation and its approaching the sum of radiii is quite explicable: it is accompanied with a significant win in energy. For the large and medium interstitial sites the deviation from the sum of radii to relaxation is significantly smaller, therefore the change of B-O distances under relaxation is also minor. It is, however, interesting that the length of the B atom

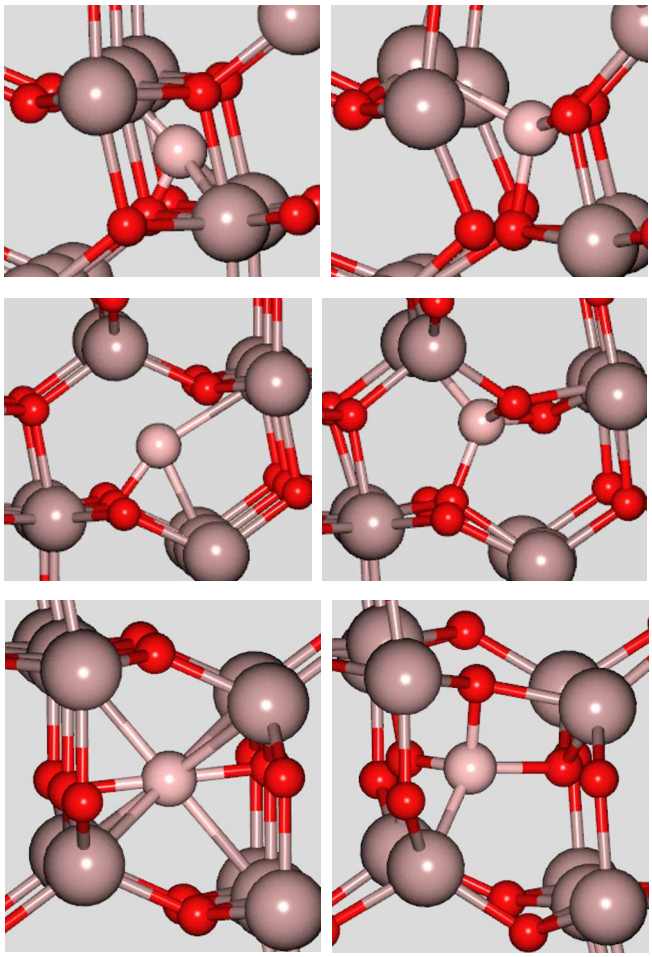

Figure 2. Atomic configuration for variant 1 before (left) and after (right) relaxation. Oxygen atoms — small red balls, gallium atoms — large pink and brown balls, boron atom — medium light pink ball. Initial positions of boron atom — in the center of small, large and medium interstitial sites (upper, middle and lower rows, accordingly).

displacement vector for the large and medium interstitial sites is larger than for the small interstitial site, i. e. the length of the vector does not correlate with the change of interatomic distances. Seemingly it is due to the fact that under relaxation the dominant is not the dimensional, but rather „the chemical“ facto — bond force.

Variant 2. Prior to relaxation the boron atom is located in one of the interstitial sites, and a vacancy of oxygen is located in the surroundings

It is evident that the probability of this variant increases with the growth of the dose, when the boron atom finds itself in the area saturated with vacancies created not only by this atom, but by overlapping of displacement cascades from other ions.

Figure 3 shows atomic configurations before and after relaxation, and Table 3 provides distances between the boron atom and the closest oxygen atom before and after relaxation, distances between the boron atom and oxygen vacancy before relaxation, distance between the boron atom after relaxation and the place of the initial location of the vacancy, boron atom displacement vector lengths and energy wins.

For this variant the behavior of boron before relaxation hardly differs from variant 1; boron atom displacement vector lengths for the small and medium interstitial sites are almost the same, and for the large interstitial site they are higher. This may still be explained with domination of the „chemical“ factor, and namely with the „attempt“ of boron to make a „normal“ bond with oxygen. The difference with variant 1 consists in the larger length of the boron atom displacement vector. Seemingly, this is due to the reduction of the local atomic density with the availability of the vacancy and, accordingly, by larger freedom of the atom

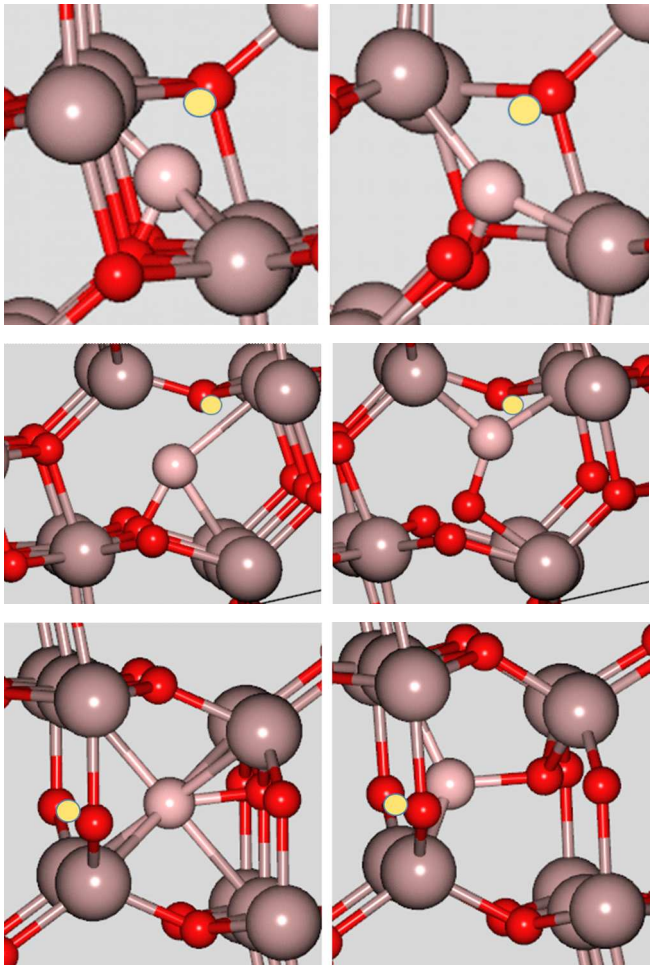

Figure 3. Atomic configuration for variant 2 before (left) and after (right) relaxation. Oxygen atoms — small red balls, gallium atoms — large pink and brown balls, boron atom — medium light pink ball. The position of the oxygen vacancy is marked with a yellow circle. Initial positions of boron atom — in the center of small, large and medium interstitial sites (upper, middle and lower rows, accordingly).

Table 3. Relaxation parameters for variant 2

Parameter	Interstitial site 1, small	Interstitial site 2, large	Interstitial site 3, medium
Boron atom displacement vector length, Å	0.66	1.00	0.68
Energy win under relaxation, eV	12.91	3.89	3.58
Distance from boron atom to O vacancy before relaxation, Å	1.89	2.07	1.52
Distance from boron atom to O vacancy after relaxation, Å	1.67	1.09	0.88
Distance from boron atom to closest oxygen atom before relaxation, Å	1.10	1.38	1.52
Distance from boron atom to closest oxygen atom after relaxation, Å	1.37	1.38	1.54

Table 4. Relaxation parameters for variant 3

Parameter	Interstitial site 1 small	Interstitial site 2 large	Interstitial site 3 medium
Boron atom displacement vector length, Å	1.03	1.16	0.66
Energy win under relaxation, eV	16.37	9.34	9.27
Distance from boron atom to Ga vacancy before relaxation, Å	1.97	2.95	2.40
Distance from boron atom to Ga vacancy after relaxation, Å	1.10	3.76	1.81

Table 5. Relaxation parameters for variant 4

Parameter	Interstitial site 1, small	Interstitial site 2, large	Interstitial site 3, medium
Boron atom displacement vector length, Å	1.29	1.32	1.15
Gallium atom vector displacement length, Å	1.46	1.13	0.92
Energy win under relaxation, eV	14.99	3.91	12.28
Distance from boron atom to closest oxygen atom before relaxation, Å	1.97	1.97	1.86
Distance from boron atom to closest oxygen atom after relaxation, Å	1.50	1.38	1.37

displacement. This also explains the reduction in the energy win.

Variant 3. Prior to relaxation the boron atom is located in one of the interstitial sites, and a vacancy of gallium is located in the surroundings

As you can see from Figure 4 and table 4, as a result of relaxation the boron atom in case of small and medium interstitial sites approaches the initial position of the vacancy, and in case of a large one — it moves further away. But in all three cases there is no substitution of the vacancy with the boron atom, i. e. formation of the substitution alloy. A trend is also seen to shorten the length of the B-O bond, which once again indicates the dominant effect of the „chemical“ factor.

Variant 4. Prior to relaxation, a gallium atom is located in one of the interstitial sites, and the boron atom is located in the gallium point

Such situation, as for the previous variant, is typical for the ion radiation.

As before, we considered the relaxation processes for three types of interstitial sites. The atom positions before and after the relaxation are shown in Figure 5, *and* Table 5

shows the lengths of boron atom displacement vectors, interatomic distances and energy win values.

From Figure 5 you can see that in case of the initial location of the boron atom in the small interstitial site, it was displaced with the gallium atom in the center of the interstitial site, and the gallium atom took the vacant place. At the same time the boron atom „left“ the interstitial site in the direction that is practically opposite to the interstitial site. For two other cases the configuration changes under relaxation are of less regular nature and are accompanied with a stronger local disorder, even though the lengths of boron displacement vectors for all three cases hardly differ.

As for energies, contrary to variants 1 and 2 the energy win under relaxation is significanly less. It is most important to note that the substitution of the vacant gallium point with the boron atom is not implemented for any of the initial configurations after relaxation: as if boron „avoids“ entering the vacancy. It may be explained by the fact that the chemical interaction between the boron atom and oxygen atom attempts to bring the length of B-O bond to the value close to the value of the sum of ion (or atomic) radii of these elements, if initially this value differs significantly from this sum.

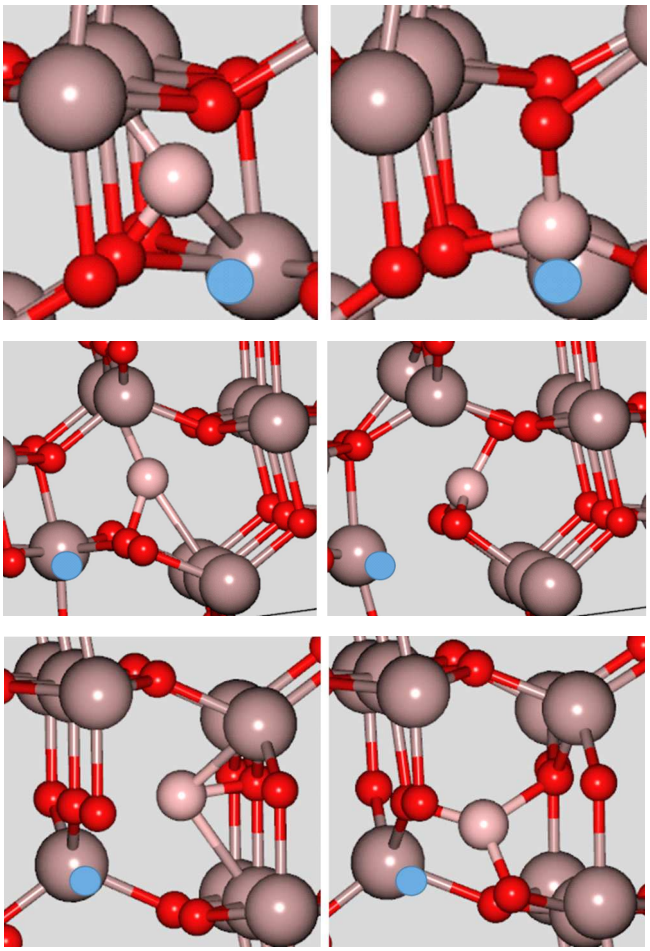

Figure 4. Atomic configuration for variant 3 before (left) and after (right) relaxation. Oxygen atoms — small red balls, gallium atoms — large pink and brown balls, boron atom — medium light pink ball. The position of the gallium vacancy is marked with a blue circle. Initial positions of boron atom — in the center of small, large and medium interstitial sites (upper, middle and lower rows, accordingly).

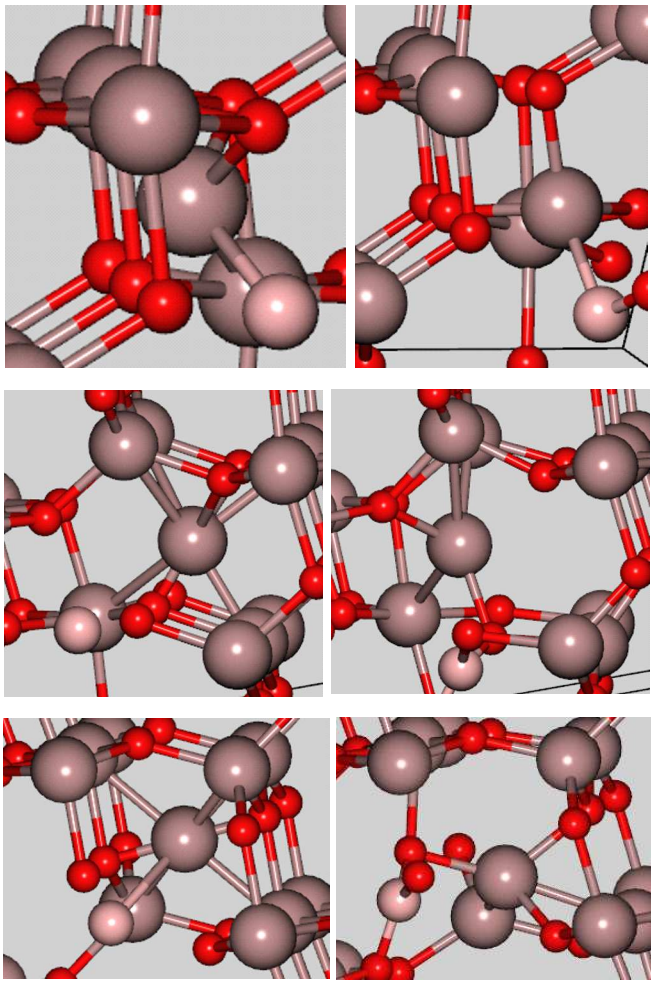

Figure 5. Atomic configuration for variant 4 before (left) and after (right) relaxation. Oxygen atoms — small red balls, gallium atoms — large pink and brown balls, boron atom — medium light pink ball. Initial positions of boron atom — in the center of the small, large and medium interstitial sites (upper, medium and bottom rows, accordingly).

4. Conclusion

The given results of the calculations make it possible to conclude that the ion implantation of boron in β-Ga_2O_3 around the boron atoms creates strong local deformations. This prevents considering the formed atomic configurations in „traditional“ terms of defects according to Frenkel or Schottky. Besides, of two intuitively suggested main factors causing transformation, — dimensional and chemical — the domination of the chemical factor is observed. This circumstance is seemingly due to high value of B-O

chemical bond, which is indicated by the fact that the value of B-O chemical bond in B_2O_3 compound is significantly higher than in Ga_2O_3 [9].

A question may arise — why the study of cathode luminescence spectra in β-Ga_2O_3 exposed to boron implantation [12] showed the presence of the same lines as in β-Ga_2O_3 not exposed to implantation. The answer is as follows. First, the concentration of boron implanted into β-Ga_2O_3 is substantially lower than the concentration of the generated Frenkel defects (in absence of annealing); under these conditions it is difficult to fix the lines of luminescence developed by groups of atoms localized around the boron atoms, even if such lines are available. Second, the specified groups seemingly are not the centers of luminescence, but centers of nonradiative recombination.

In any case the effect of boron implantation on the structure and properties of gallium oxide requires further research, including by ab initio calculations of the electron spectra. In particular, the question on the mechanisms of behavior of the structure and properties of implanted layers after thermal annealing remains open. Possibly, the effect of boron release from the lattice sites noted in paper [7] with the growth of the dose in the annealed samples reflects the found trend of energy unfavorableness of the boron atom staying in the gallium points.

The results obtained in the paper may be used for further calculations of electronic spectra and other properties of gallium oxide, ion-doped with boron.

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Conflict of interest

Authors declare no conflict of interest.

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