Reducing Mg Acceptor Activation-Energy in Al\(_{0.83}\)Ga\(_{0.17}\)N Disorder Alloy Substituted by Nanoscale (AlN)\(_5\)/(GaN)\(_1\) Superlattice Using Mg\(_{Ga}\) \(\delta\)-Doping: Mg Local-Structure Effect

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Improving p-type doping efficiency in Al-rich AlGaN alloys is a worldwide problem for the realization of AlGaN-based deep ultraviolet optoelectronic devices. In order to solve this problem, we calculate Mg acceptor activation energy and investigate its relationship with Mg local structure in nanoscale (AlN)\(_5\)/(GaN)\(_1\) superlattice (SL), a substitution for Al\(_{0.83}\)Ga\(_{0.17}\)N disorder alloy, using first-principles calculations. A universal picture to reduce acceptor activation energy in wide-gap semiconductors is given for the first time. By reducing the volume of the acceptor local structure slightly, its activation energy can be decreased remarkably. Our results show that Mg acceptor activation energy can be reduced significantly from 0.44 eV in Al\(_{0.83}\)Ga\(_{0.17}\)N disorder alloy to 0.26 eV, very close to the Mg acceptor activation energy in GaN, and a high hole concentration in the order of 10\(^{19}\) cm\(^{-3}\) can be obtained in (AlN)\(_5\)/(GaN)\(_1\) SL by Mg\(_{Ga}\) \(\delta\)-doping owing to GaN-monolayer modulation. We thus open up a new way to reduce Mg acceptor activation energy and increase hole concentration in Al-rich AlGaN.

Al-rich AlGaN alloys are ideal materials for deep ultraviolet (DUV) optoelectronic devices with operating wavelength down to 200 nm due to their large direct band gaps\(^1\)–\(^4\). They have potential applications in sterilization, water and air purification, biological and chemical agent detection, high-density data storage and medical research\(^3\)–\(^6\). However, the external quantum efficiency of AlGaN-based DUV light-emitting diodes (LEDs) is extremely low around 0.1%\(^7\)–\(^8\). Generally, three main factors, that is, the high dislocation density (10\(^{10}\) cm\(^{-2}\)), the low p-type doping efficiency, and the AlN-like valence-band maximum (VBM), i.e., the crystal-field split-off hole band as the VBM other than the heavy hole band (see Figure 2.12 in Ref. 9), contribute to this overall small value. We will here focus on improving p-type doping efficiency in Al-rich AlGaN. It is well-known that realizing p-type doping in Al-rich AlGaN is extremely difficult due to the following three major reasons, i.e., the high acceptor activation energy \(E_A\), the compensation by nitrogen vacancies, and the limited acceptor solubility\(^7\). For the most widely used Mg acceptor dopant, its \(E_A\) increases monotonically with Al composition from 0.16–0.25 eV in GaN to \(>0.50\) eV in AlN\(^9\). Therefore, realizing p-type Al-rich AlGaN has become one of the most challenging tasks in the nitride community.

Great efforts have been devoted to improve p-type conduction in group-III nitrides\(^10\)–\(^16\). Polarization doping has been proposed to increase the hole concentration in compositionally graded AlGaN alloys, in which Mg acceptor is ionized by the polarization field\(^10\)–\(^12\). Alternative acceptor-donor co-doping has also been developed to reduce the acceptor activation energy\(^13\)–\(^14\). The non-equilibrium growing with pulse doping has been proved to increase the hole concentration\(^15\). Furthermore, Mg \(\delta\)-doping, an impurity-growth mode by closing Ga and Al flow and leaving N and Mg flow, enhances the p-type conductivity of AlGaN alloys\(^16\). To the best of our knowledge, only several experiments are focused on the p-type conduction of Al-rich AlGaN alloys\(^3\)–\(^5\),\(^7\)–\(^18\). The related theoretical work is still absent at present. Our purpose here is to overcome the p-type doping bottlenecks in Al-rich AlGaN.
We note that nanometer scale compositional inhomogeneity has an important influence on the luminescence efficiency of group-III nitride semiconductors. It has been found that the nanoscale islands or quantum dots observed in AlGaN can improve its internal quantum efficiency. Moreover, atomic-scale compositional superlattice (SL) has also been observed in Al-rich AlGaN thin films grown by molecular-beam epitaxy (MBE). Recent theoretical and experimental works prove that the nanoscale (AlN)5/(GaN)1 SL, substituting for the Al-rich AlGaN disorder alloy, can convert the VBM from the crystal-field split-off hole to heavy hole band, which directly leads to the increase of the desired transverse electric (TE) polarized light emission efficiency in the DUV spectral region (Ref. 27 and Jiang, X.-h., et al., unpublished data). Compared with Al-rich AlGaN alloy, the SL structure has an obvious advantage because it can combine the high TE polarized light emission efficiency of GaN and the wide energy gap of AlN.

According to the tight-binding approximation, we know that the electronic structures of Mg atom doped in AlGaN can be modified significantly by its nearest and next-nearest (NN) atoms. We will thus pay our attention to the nearest and NN atoms and investigate their influence on Mg electronic structures in nanoscale (AlN)5/(GaN)1 SL and Al0.83Ga0.17N uniform alloy. Generally, the formation energy can be calculated as follows:

\[
E_f = E_{tot} - E_{VBM} - E_{corr}
\]

where \( E_{VBM} \) is the energy of the valence band maximum, \( E_{tot} \) is the total energy of the supercell containing the defect, and \( E_{corr} \) is the correction term, which is the energy of N in the N2 molecule. Otherwise, for the N-poor case, \( E_{Al(Ga)} = \mu_{Al(Ga)} - (\mu_{Al(Ga)} + \mu_{N}) \), i.e., the energy of Al (Ga) in bulk Al (Ga). The Mg acceptor level \( E_F \) in the band gap decreases. The Mg acceptor activation energy can be reduced significantly by its nearest and next-nearest atoms. We will thus pay our attention to the nearest and NN atoms and investigate their influence on Mg electronic structures in nanoscale (AlN)5/(GaN)1 SL and Al0.83Ga0.17N uniform alloy. Generally, \( E_F \) of a defect D in charge state \( q \) can be calculated as follows:

\[
E_F = E_{tot}[D\{q\}] - E_{tot}[\text{bulk}]
\]

\[
= \sum_i n_i \mu_i + q(E_V + E_F + \Delta V[D])
\]

where \( E_{tot}[D\{q\}] \) is the total energy of the supercell containing the defect D in charge state \( q \), \( E_{tot}[\text{bulk}] \) is the total energy in the same supercell without the defect, \( n_i \) is the number of the \( i \)-th constituent, which has been added to \( n_i > 0 \) or removed from \( n_i < 0 \) the host material, and \( \mu_i \) is its chemical potential. \( E_F \) is the Fermi level referenced to the VBM \( E_V \) of the bulk. The range of \( E_F \) is taken to be the band gap of the bulk. A correction term \( \Delta V[D] \) is introduced in order to align the reference electrostatic potential in the charged defect supercell with that in the bulk. For the finite supercell calculation, a correction term \( E_{corr} \) is also needed due to the dispersion of the defect level, especially for the shallow level. It can be inferred from the energy difference between the highest occupied state at the \( \Gamma \) point and the average value at several special \( k \) points. The chemical potentials \( \mu \) closely depend on the growth conditions and can be determined by:

\[
\mu_{Al} + \mu_{N} = \mu_{AlN}
\]

\[
\mu_{Ga} + \mu_{N} = \mu_{GaN}
\]

\[
3\mu_{Mg} + 2\mu_N = \mu_{MgN_2}
\]

\[
\mu_N \leq \mu_{N(N_2)}
\]

Because the group-III nitride semiconductors are usually grown under the N-rich and N-poor conditions, which directly determine the kind and concentration of defects in semiconductors, we thus consider these two limited cases to calculate the Mg acceptor formation energy. For the N-rich case, \( \mu_N = \mu_{N(N_2)} \) (the energy of N in a N2 molecule). Otherwise, for the N-poor case, \( \mu_{Al(Ga)} = \mu_{Al(Ga)}[\text{bulk}] \), i.e., the energy of Al (Ga) in bulk Al (Ga). The Mg acceptor level \( E_F \) is defined as the position where the charge states of \( q = 0 \) and \( -1 \) have equal formation energy and can be calculated from the following formula:

\[
E_A = E_{tot}[D^-] - E_{tot}[D^0] - E_V - \Delta V[D] + E_{corr}
\]

Our calculated formation energies as a function of \( E_F \) are shown in Figure 2 for MgGa in nanoscale (AlN)5/(GaN), SL, and MgAl and MgGa in Al0.83Ga0.17N uniform alloy under N-poor and -rich conditions. We can see from Figure 2 that the \( E_F \) of Mg2+ under p-type condition (EF close to the VBM) is larger than that of Mg+ under n-type condition (EF close to the bottom of the conduction band). We can thus understand that the Mg acceptor concentration is low in thermodynamic equilibrium due to its large \( E_F \) in p-type (AlN)5/(GaN) SL and Al0.83Ga0.17N alloy, which is consistent with the

![](image)
previous experiment\textsuperscript{11}. The formation energy as a function of \(E_F\) under N-poor is similar to that under N-rich. The \(E_F\) of Mg\(_{Ga}\) and Mg\(_{Al}\) decreases by 0.94 eV approximately from N-poor to rich conditions because of the negative formation enthalpy of GaN and AlN. Moreover, we can see from Figure 2(a) that Mg\(_{Ga}\) in (AlN\(_5\))/(GaN\(_1\)) SL has two stable charge states, i.e., neutral 0 and −1, which induces a shallow acceptor level (0.26 eV). Figure 2(b) shows that \(E_F\) of Mg\(_{Ga}\) is about 0.20 eV lower than that of Mg\(_{Al}\) in Al\(_{0.83}\)Ga\(_{0.17}\)N uniform alloy. The Mg atom thus tends to replace Ga atom other than Al atom. This can be attributed to the weak bond strength between Ga and N atoms compared to that between Al and N atoms.

The Mg atom can also substitute Al atom to form an acceptor in (AlN\(_5\))/(GaN\(_1\)) SL except for the aforementioned Mg\(_{Ga}\). In order to know the preferable position of Mg\(^{2+}\) dopant, we further calculate its formation energy (see Figure 3(a)) for the chosen four special cation positions. The difference of sites 1–4 mainly concentrates on the nearest and NN neighbours of Mg, i.e., local structure around Mg atom (see Figure 3(c)). For the chosen four special positions, the NN Ga-atom numbers \(N_{Ga}\) are 6, 3, 0 and 0 from site 1 to 4, respectively. We can see from Figure 3(a) that the formation energy \(E_F\) increases monotonously from site 1 to 4 in (AlN\(_5\))/(GaN\(_1\)) SL, which is larger than \(E_F\) of Mg\(^{2+}\) in GaN and smaller than that in AlN, as it should be. The \(E_F\) rapidly increases from site 1 to 2, then slowly increases from site 2 to 4. This is because the Ga–N bond is weaker than the Al–N bond. We can conclude that Mg atom tends to occupy Ga site to form Mg\(_{Ga}\) acceptor in (AlN\(_5\))/(GaN\(_1\)) SL. This can be realized by means of Mg 6-doping technique, i.e., closing Al flow and leaving Ga and Mg flow\textsuperscript{30}.

We further calculate Mg acceptor activation energy \(E_A\) in GaN, AlN, and Al\(_{0.83}\)Ga\(_{0.17}\)N uniform alloy (see Table 1). For the sake of comparison, some previous theoretical and experimental results are also given. We can see from Table 1 that our calculated \(E_A\) is 0.21 eV in GaN, which is within the range of well-accepted theoretical results (0.198–0.26 eV)\textsuperscript{32,33} and experimental values (0.16–0.25 eV)\textsuperscript{31,34,35}. For Mg dopant in AlN, excellent agreement of \(E_A\) (0.48 eV) with the previous theoretical calculations (0.40–0.78 eV)\textsuperscript{14,33,36} and experiments (0.5 eV)\textsuperscript{32,33,34,35} is also confirmed. This clearly indicates that our current calculations with the AM05 exchange-correlation (XC) functional\textsuperscript{14} are accurate and reliable for the acceptor activation energy. Moreover, we calculate \(E_A\) of Mg\(_{Ga}\) and Mg\(_{Al}\) acceptors in Al\(_{0.83}\)Ga\(_{0.17}\)N uniform alloy and find that they have equal \(E_A\) (0.44 eV) despite different cation sites occupied by Mg atom, which is in the range of the reported experimental values from 0.40 eV for Al-content \(x = 0.7\) to 0.50 eV for \(x = 1.0\). It is worthwhile to note that, in spite of the Al-site or Ga-site occupied by Mg atom, \(E_A\) in Al\(_{0.83}\)Ga\(_{0.17}\)N uniform alloy is always large and approaches the corresponding value of AlN. Therefore, it is extremely difficult to reduce Mg acceptor activation energy in Al-rich AlGaN. We will turn our attention to Mg dopant in (AlN\(_5\))/(GaN\(_1\)) SL substitution for Al\(_{0.83}\)Ga\(_{0.17}\)N disorder alloy and seek a new way to reduce \(E_A\) in the following text.

Figure 3(b) shows our calculated Mg acceptor activation energies \(E_A\) in GaN, AlN, and Al\(_{0.83}\)Ga\(_{0.17}\)N uniform alloy (see Table 1). For the sake of comparison, some previous theoretical and experimental results are also given. We can see from Table 1 that our calculated \(E_A\) is 0.21 eV in GaN, which is within the range of well-accepted theoretical results (0.198–0.26 eV)\textsuperscript{32,33} and experimental values (0.16–0.25 eV)\textsuperscript{31,34,35}. For Mg dopant in AlN, excellent agreement of \(E_A\) (0.48 eV) with the previous theoretical calculations (0.40–0.78 eV)\textsuperscript{14,33,36} and experiments (0.5 eV)\textsuperscript{32,33,34,35} is also confirmed. This clearly indicates that our current calculations with the AM05 exchange-correlation (XC) functional\textsuperscript{14} are accurate and reliable for the acceptor activation energy. Moreover, we calculate \(E_A\) of Mg\(_{Ga}\) and Mg\(_{Al}\) acceptors in Al\(_{0.83}\)Ga\(_{0.17}\)N uniform alloy and find that they have equal \(E_A\) (0.44 eV) despite different cation sites occupied by Mg atom, which is in the range of the reported experimental values from 0.40 eV for Al-content \(x = 0.7\) to 0.50 eV for \(x = 1.0\). It is worthwhile to note that, in spite of the Al-site or Ga-site occupied by Mg atom, \(E_A\) in Al\(_{0.83}\)Ga\(_{0.17}\)N uniform alloy is always large and approaches the corresponding value of AlN. Therefore, it is extremely difficult to reduce Mg acceptor activation energy in Al-rich AlGaN. We will turn our attention to Mg dopant in (AlN\(_5\))/(GaN\(_1\)) SL substitution for Al\(_{0.83}\)Ga\(_{0.17}\)N disorder alloy and seek a new way to reduce \(E_A\) in the following text.

![Figure 3](image_url)
be further reduced owing to the high Mg acceptor activation energy if the Ga atoms are not restricted to a single atomic layer.

**Discussion**

Why does Mg acceptor activation energy sensitively depend on the local structure around Mg dopant and can be reduced significantly in nanoscale (AlN)$_5$/(GaN)$_1$ SL? According to the band offset explanation, Mg activation energy $E_A$ is dominated by the position of the VBM state of the host material. The higher the VBM is, the lower the $E_A$ is. In our current Mg doping calculations in (AlN)$_5$/(GaN)$_1$ SL, $E_A$ has a significant variation with different Mg doping positions, whereas the VBM is always fixed. Obviously, the previous viewpoint cannot explain our results anymore. In order to have a deep understanding for the results of Figure 3(b), we further calculate the partial density of states (PDOS) of Mg atom near the Fermi energy in (AlN)$_5$/(GaN)$_1$ SL for different Mg doping-sites (see Figure 3(c)).

![Figure 4](image) The Mg PDOS near Fermi level $E_F$ in p-type (AlN)$_5$/(GaN)$_1$ SL for different Mg doping-sites (see Figure 3(c)).

We can find from Figure 4 that the localization of the Mg defect state sensitively depends on Mg site or local structure around it. The Mg impurity state changes markedly from the delocalized state to highly localized one from site 1 to 4 (see Figure 4(a–d)). According to the definition of shallow and deep levels in semiconductors, we know that the Mg$_{Ga}$ acceptor level, corresponding to the delocalized state in site 1, is a shallow level. The acceptor level goes deeper from site 2 to 4 due to the strong localization of the Mg defect state. We thus can understand the results of Figure 3(b). Hence the Mg$_{Ga}$ acceptor has the strongest delocalization, which results in the smallest acceptor activation energy in the SL.

Considering that the localization of Mg defect state is closely related to its local structure, we thus pay our attention to the relationship between the local structure and the localization of Mg defect state in order to explore the real physical origin of reducing Mg acceptor activation energy in nanoscale (AlN)$_5$/(GaN)$_1$ SL. Figure 5 shows the local structure around Mg acceptor, i.e., the Mg-centered tetrahedron, for the chosen four different Mg doping-sites. We find that the volumes $V$ of Mg-centered tetrahedrons, indicating the average interaction strength between N and Mg atoms, are 4.317, 4.348, 4.360, and 4.374 Å$^3$ for Mg sites 1–4, respectively. The volume related to site 1 (4) is the smallest (largest). This is owing to the GaN-monolayer strong modulation effect, which is originated from the larger covalent radius of Ga atom than that of Al atom as the NN neighbors of Mg dopant. It is the variation of the local structure that leads to the difference of the interaction between N and Mg atoms, which directly modify the localization of the Mg defect state and Mg acceptor activation energy. The smaller $V$ is, the stronger the N-Mg interaction is. The corresponding Mg defect state thus becomes more delocalization, and the activation energy is reduced due to the strong interaction between N and Mg atoms. We thus can understand that the local structure in Figure 5(a) has the smallest volume, the strongest N-Mg interaction, the most obvious delocalization of the Mg defect state (see Figure 4), and the smallest acceptor activation energy among the four different Mg doping-sites (see Figure 5| Local-structure around Mg acceptor for the chosen four different Mg doping-sites (see Figure 3(c)). The calculated bond/edge length (in Å) and the tetrahedron volume $V$ (in Å$^3$) are indicated.)

![Figure 5](image) The calculated bond/edge length (in Å) and the tetrahedron volume $V$ (in Å$^3$) are indicated.
increase from 4.317 to 4.374 Å (smaller the activation energy is. When the volume

1019 cm

The hole concentration can be significantly enhanced up to the realization of AlGaN-based DUV optoelectronic devices. We

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