

## DEFECTS AND DOPING IN III-V NITRIDES

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### Abstract

We present a theoretical study of point defects and impurities in GaN. Sources of *n*-type doping are investigated: nitrogen vacancies are too high in energy, but silicon and oxygen readily incorporate. The properties of oxygen, including *DX*-center formation, support it as the main cause of unintentional *n*-type conductivity. Gallium vacancies are the likely source of the yellow luminescence. An investigation of various acceptor impurities indicates that Mg is still the acceptor of choice for *p*-type doping. The role of hydrogen during acceptor doping is discussed. We also find that compensation of acceptors by nitrogen vacancies may occur, likely leading to the observed persistent photoconductivity.

### 1. Introduction

GaN is successfully being used for green, blue, and UV light emitters and for high-temperature or high-power applications [1]. Light-emitting diodes [2] are already being produced in large quantities for use in applications ranging from traffic lights to full-color displays. Nakamura and coworkers have also achieved various milestones in the fabrication of laser diodes, including room-temperature CW (continuous wave) operation [3]. In addition, GaN is a very promising material for high-frequency and high-power devices [4] and for solar-blind detectors [5]. The ability to control doping is crucial for all of these applications; wide-band-gap semiconductors such as GaN have long suffered from lack of control of the doping levels. In this paper we discuss how a theoretical approach for native defects and dopant impurities, combined with state-of-the-art first-principles calculations, can be used to understand the various factors that govern doping.

Native defects have often been invoked to explain doping problems. Specifically, in GaN the nitrogen vacancy has traditionally been thought to be the source of *n*-type conductivity. Our first-principles investigations, however, indicate that nitrogen vacancies are high-energy defects in *n*-type GaN, and thus are unlikely to form in large concentrations [6]. We have proposed that unintentional impurities such as oxygen and silicon are the actual cause of the observed unintentional *n*-type doping [7]. These impurities are calculated to be shallow donors with high solubilities. Additional support for this assignment comes from the finding that oxygen (but not Si) behaves as a *DX* center in GaN under pressure, in agreement with recent experimental observations [8].

After a description of the theoretical approach in Section 2, we will summarize our main results for native defects in Section 3. In Section 4 we will discuss *n*-type doping and the behavior of oxygen and silicon. A major concern for optoelectronic devices is the presence of alternate

recombination channels, such as the “yellow luminescence” (YL), which occurs mainly in *n*-type GaN. Gallium vacancies are the most likely source of this YL [9].

*p*-type doping of GaN has become possible through a post-growth activation step in MOCVD-grown material. Hydrogen plays a crucial role in this process. The behavior of hydrogen in GaN is broadly similar to that in other semiconductors, including the stability of  $H^+$  in *p*-type material and the negative- $U$  character (in this case with a very large magnitude of  $U$ ) [10, 11]. Intriguing differences occur, however, for instance in the structure of hydrogen-acceptor complexes. In Section 5 we will summarize results for hydrogen in GaN. Results for interactions between hydrogen and native defects will also be presented.

The specific role of hydrogen in *p*-type doping will be addressed in Section 6. This section also discusses other aspects of acceptor doping in GaN. *p*-type doping levels are still lower than desirable for low-resistance cladding layers and ohmic contacts. Achieving higher hole concentrations with Mg as the dopant has proved difficult; various explanations have been proposed for this limitation. Our investigations of compensation mechanisms [12] have revealed that the determining factor is the solubility of Mg in GaN, which is limited by competition between incorporation of Mg acceptors and formation of  $Mg_3N_2$ ; incorporation of Mg on interstitial or substitutional nitrogen sites was found to be unfavorable. We will also discuss the prospects of other acceptor impurities for achieving higher doping levels [13]. We have also studied the interaction between O and Mg acceptors. The presence of oxygen during growth is detrimental to achieving *p*-type doping in the nitrides.

## 2. Theoretical approach

Key parameters in our approach are obtained from first-principles calculations that do not require any adjustable parameters or any input from experiment. The computations are founded on density-functional theory [14], using a supercell geometry and soft Troullier-Martins pseudopotentials [15]. The effect of *d* electrons in GaN is taken into account either through the so-called non-linear core correction [16] or by explicit inclusion of the *d* electrons as valence electrons; the latter proved to be necessary for obtaining accurate results in certain cases [17]. Further details of the computational approach can be found in Refs. [6], [18], and [19].

A key quantity describing the behavior of defects and impurities is their *formation energy*,  $E^f$ . The formation energy determines the equilibrium concentration of impurities or native defects according to the expression

$$c = N_{\text{sites}} \exp^{-E^f/k_B T} \quad (1)$$

where  $N_{\text{sites}}$  is the number of sites the defect or impurity can be incorporated on,  $k_B$  the Boltzmann constant, and  $T$  the temperature. Equation (1) shows that defects with a *high* formation energy will occur in *low* concentrations.

The formation energy is not a constant but depends on the growth conditions. For example, the formation energy of an oxygen donor is determined by the relative abundance of O, Ga, and N atoms, as expressed by the chemical potentials  $\mu_O$ ,  $\mu_{Ga}$  and  $\mu_N$ , respectively. If the O donor is charged (as is expected when it has donated its electron), the formation energy depends further on the Fermi level ( $E_F$ ), which acts as a reservoir for electrons. Forming a substitutional O donor requires the removal of one N atom and the addition of one O atom; the formation energy is therefore:

$$E^f(\text{GaN:O}_N^q) = E_{\text{tot}}(\text{GaN:O}_N^q) - \mu_O + \mu_N + qE_F \quad (2)$$

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Formation Energy (eV)

where  $E_{\text{tot}}(\text{GaN}:\text{O}_N^q)$  is the total energy derived from a calculation for substitutional O, and  $q$  is the charge state of the O donor.  $E_F$  is the Fermi level. Similar expressions apply to other impurities and to the various native defects. We refer to Refs. [6] and [20] for a more complete discussion of formation energies and their dependence on chemical potentials.

Note that the Fermi level  $E_F$  is not an independent parameter, but is determined by the condition of charge neutrality. However, it is informative to plot formation energies as a function of  $E_F$  in order to examine the behavior of defects and impurities when the doping level changes. As for the chemical potentials, these are variables which depend on the details of the growth conditions. For ease of presentation, we set these chemical potentials to fixed values in the figures shown below; however, a general case can always be addressed by referring back to Eq. (2). The fixed values we have chosen correspond to Ga-rich conditions [ $\mu_{\text{Ga}} = \mu_{\text{Ga(bulk)}}$ ], and to maximum incorporation of the various impurities, with solubilities determined by equilibrium with  $\text{Ga}_2\text{O}_3$ ,  $\text{Si}_3\text{N}_4$ , and  $\text{Mg}_2\text{N}_3$ .

### 3. Native defects

Our first-principles results for native defects were described in detail in Ref. [21]. One general conclusion is that self-interstitial and antisite defects are high-energy defects in GaN, and are thus unlikely to occur. Nitrogen vacancies ( $V_N$ ) behave as donors, which means that their formation energy is higher in  $n$ -type material than in  $p$ -type [see Eq. (2)]. Nitrogen vacancies are therefore unlikely to form in  $n$ -type GaN, and hence they cannot be responsible for  $n$ -type conductivity. The low formation energy of  $V_N$  in  $p$ -type GaN, however, makes it a likely compensating center for acceptor doping, as will be discussed in Section 6. In  $n$ -type GaN the lowest-energy native defect is the gallium vacancy ( $V_{\text{Ga}}$ ), a triple acceptor. This defect plays a role in donor compensation, as well as in the frequently observed yellow luminescence. Both aspects will be discussed in the next section.

### 4. $n$ -type doping

Figure 1 summarizes our results for native defects and impurities relevant for  $n$ -type doping. As discussed in Section 3, nitrogen vacancies have too high a formation energy to be responsible for  $n$ -type conductivity in GaN. In contrast, Fig. 1 shows that O and Si have relatively low formation energies in  $n$ -type GaN, and can thus be readily incorporated. Both O and Si form shallow donors in GaN. The slope of the lines in Fig. 1 indicates the charge state of the defect or impurity [see Eq. (2)]:  $\text{Si}_{\text{Ga}}$ ,  $\text{O}_N$ , and  $V_N$  all appear with slope +1, indicating single donors.

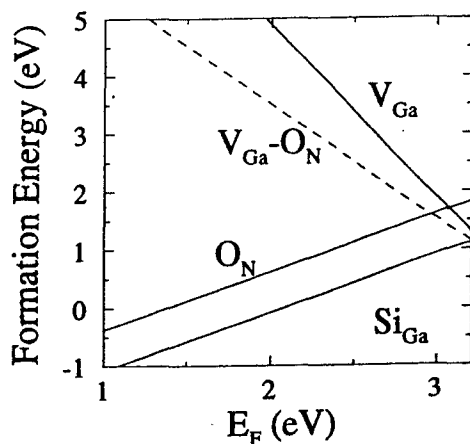


Figure 1: Formation energy vs. Fermi energy for native defects (nitrogen and gallium vacancies), donors (oxygen and silicon) and the  $V_{\text{Ga}}\text{-O}_N$  complex. The zero of Fermi energy is located at the top of the valence band.

Oxygen had been considered a potential source of  $n$ -type conductivity in GaN by Seifert *et al.* [22] and by Chung and Gershenson [23]. Still, the prevailing conventional wisdom, attributing the  $n$ -type behavior to nitrogen vacancies, proved hard to overcome. Recent experiments have now confirmed that unintentionally doped  $n$ -type GaN samples contain silicon or oxygen concentrations high enough to explain the electron concentrations. Götz *et al.* [24] reported electrical characterization of intentionally Si-doped as well as unintentionally doped samples, and concluded that the  $n$ -type conductivity in the latter was due to silicon. Götz *et al.* have also recently carried out SIMS (secondary-ion mass spectroscopy) and electrical measurements on hydride vapor phase epitaxy (HVPE) material, finding levels of oxygen or silicon in agreement with the electron concentration [25].

High levels of  $n$ -type conductivity have always been found in GaN bulk crystals grown at high temperature and high pressure [26]. It has recently been established that the characteristics of these samples (obtained from high-pressure studies) are very similar to epitaxial films which are intentionally doped with oxygen [27, 28]. The  $n$ -type conductivity of bulk GaN can therefore be attributed to unintentional oxygen incorporation. The high-pressure experiments have also shown that freezeout of carriers occurs at pressures exceeding 20 GPa [8, 26, 28, 29]. Originally this observation was interpreted as consistent with the presence of nitrogen vacancies, since the  $V_N$  donor gives rise to a resonance in the conduction band, which emerges into the band gap under pressure. However, the observations are also entirely consistent with a “DX-like” behavior of the oxygen donor.

We have carried out extensive calculations for oxygen in GaN under pressure, as well as in AlGa<sub>x</sub>N alloys [30]. Under compression the oxygen impurity assumes an off-center configuration: a large outward relaxation introduces a deep level in the band gap [31]. This behavior explains the carrier freezeout in GaN under pressure. Silicon donors do not exhibit this transition, consistent with experiment [8]. Alloying with AlN increases the band gap similar to the application of hydrostatic pressure; one therefore expects that the behavior of the impurities in AlGa<sub>x</sub>N would be similar to that in GaN under pressure. Explicit calculations for oxygen in AlN indeed produce DX behavior [30]. These results are consistent with the observed decrease in  $n$ -type conductivity of unintentionally doped Al<sub>x</sub>Ga<sub>1-x</sub>N as  $x > 0.4$  [32].

As a final comment on Fig. 1 we note that gallium vacancies ( $V_{Ga}^{3-}$ ) have relatively low formation energies in highly doped  $n$ -type material ( $E_F$  high in the gap); they could therefore act as compensating centers. Yi and Wessels [33] have found evidence of compensation by a triply charged defect in Se-doped GaN. We have also proposed that gallium vacancies are responsible for the “yellow luminescence” (YL) in GaN, a broad luminescence band centered around 2.2 eV [9]. The origins of the YL have been extensively debated; as discussed in Refs. [9] and [34], the calculated properties of the gallium vacancy are in good agreement with experimental results.

## 5. Hydrogen

Hydrogen also has strong effects on the properties of GaN. Many growth techniques, such as metal-organic chemical vapor deposition (MOCVD) or hydride vapor phase epitaxy (HVPE) introduce large concentrations of hydrogen in the growing material. The behavior of hydrogen in GaN was analyzed in detail in Refs. [10] and [11]. We found that hydrogen incorporates more readily in  $p$ -type than in  $n$ -type GaN. In  $p$ -type GaN H behaves as a donor ( $H^+$ ), compensating acceptors. Hydrogen can bind to the Mg acceptors with a binding energy of 0.7 eV. The structure of the resulting complex is unusual in that H does not sit next to the Mg, but

actually binds to a N atom which is a neighbor of the acceptor. As a direct consequence the vibrational frequency of the complex is *not* representative of a Ga-H bond, but rather of a N-H bond. The calculated vibrational frequency is  $3360\text{ cm}^{-1}$ . This value does not include anharmonic effects; these may lower the frequency considerably in the case of N-H vibrations, by as much as  $170\text{ cm}^{-1}$  [35]. Götz *et al.* [36] have reported a value of  $3125\text{ cm}^{-1}$  for this local vibrational mode.

We have recently also studied the interactions of hydrogen with native point defects in GaN [37]. Since antisites and self-interstitials are very unlikely to form in GaN (see Section 3) we have focused on H interacting with vacancies. This interaction is often described in terms of tying off of dangling bonds. This picture does not apply in the case of the nitrogen vacancy, which is surrounded by Ga atoms at a distance of  $1.95\text{ Å}$  from the center of the vacancy; a typical Ga-H bond distance is too large for more than one H to fit inside the vacancy. The calculated binding energy of the  $(V_NH)^{2+}$  complex, expressed with respect to interstitial H in the positive charge state, is  $1.56\text{ eV}$ ; the formation energy of this complex is included in Fig. 2. We have proposed that this complex is involved in the appearance and disappearance of photoluminescence (PL) lines during post-growth annealing of Mg-doped layers grown by MOCVD [38].

For the Ga vacancy ( $V_{Ga}$ ), we find that one, two, three or four H atoms can be accommodated in the vacancy, and levels are removed from the band gap as more hydrogens are attached. Distinct N-H bonds are formed, with a bond length of about  $1.02\text{ Å}$  and vibrational modes between  $3100\text{ cm}^{-1}$  and  $3500\text{ cm}^{-1}$ . Hydrogenated gallium vacancies with one or two H atoms behave in much the same way as the unhydrogenated kind; they may therefore contribute to compensation of donors as well as to the yellow luminescence.

## 6. p-type doping

Magnesium has emerged as the acceptor dopant of choice in GaN. It has been found, however, that hole concentrations obtained with Mg doping are limited. In addition, it is well known that Mg-doped GaN grown by MOCVD needs to be subjected to post-growth treatments such as low-energy electron-beam irradiation [39] or thermal annealing [40] in order to activate the acceptors. All of these features can be addressed by our first-principles results, which are summarized in Fig. 2.

The Mg acceptor ( $Mg_{Ga}$ ) has a low enough formation energy to be incorporated readily in GaN. We have also investigated other positions of Mg in the lattice, such as on substitutional N sites ( $Mg_N$ ) and on interstitial sites ( $Mg_i$ ), always finding much larger formation energies [12]. We therefore conclude that Mg overwhelmingly prefers the Ga site in GaN, the main competition being with formation of  $Mg_2N_3$ , which is the solubility-limiting phase. It would be interesting to investigate experimentally whether traces of  $Mg_2N_3$  can be found in highly Mg-doped GaN.

Other potential sources of compensation are also illustrated in Fig. 2. The nitrogen vacancy, which had a high formation energy in *n*-type GaN (see Fig. 1), has a significantly lower formation energy in *p*-type material, and could act as a compensating center. Figure 2 shows that  $V_N$  can occur in a  $3+$  as well as a  $+$  charge state; the  $+/3+$  transition is characterized by a large lattice relaxation [21]. Compensation by nitrogen vacancies may therefore be responsible for the observed persistent photoconductivity effects [41]. The metastability is associated with the different position of the  $A_1$  state near the valence band in the  $+1$  and  $+3$  charge states; this state is occupied with two electrons the  $+1$  charge state, and empty for the  $3+$  charge state.

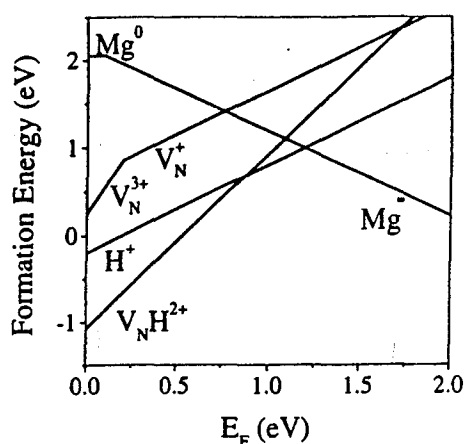


Figure 2: Formation energy as a function of Fermi level for Mg in different configurations (Ga-substitutional, N-substitutional, and interstitial configuration). Also included are the native defects and interstitial H.

Figure 2 also shows that hydrogen, when present, has a formation energy much lower than that of the nitrogen vacancy. In growth situations where hydrogen is present (such as MOCVD or HVPE) Mg-doped material will preferentially be compensated by hydrogen, and compensation by nitrogen vacancies will be suppressed. The presence of hydrogen is therefore beneficial – at the expense, of course, of obtaining material that is heavily compensated by hydrogen! Fortunately, the hydrogen can be removed from the active region by treatments such as low-energy electron-beam irradiation [39] or thermal annealing [40]. A more complete discussion of the role of hydrogen in GaN is given in Refs. [10] and [11].

For Mg, we thus conclude that achievable doping levels are mainly limited by the solubility of Mg in GaN. We have investigated other candidate acceptor impurities, and evaluated them in terms of solubility, shallow *vs.* deep character, and potential compensation due to incorporation on other sites [13]. None of the candidate impurities exhibited characteristics exceeding those of Mg. In particular, we perceive no noticeable advantage in the use of Be, which has been suggested as a superior dopant.

Last but not least we note the importance of avoiding any type of contamination during growth of *p*-type GaN. For instance, the oxygen formation energy shown in Fig. 1 clearly extrapolates to very low values in *p*-type GaN. Any oxygen present in the growth system will therefore be readily incorporated during *p*-type growth. In addition, complex formation between oxygen and magnesium can make oxygen incorporation even more favorable: we find that oxygen binds to Mg with a binding energy of 0.6 eV.

## 7. Conclusions

To maintain the rapid progress in development of GaN-based devices, a fundamental understanding is required of the behavior of point defects and dopants. First-principles calculations can greatly assist in providing a framework for understanding doping problems. Specific results for donor and acceptor doping have been presented in this paper. The main conclusions for *n*-type GaN are that (i) nitrogen vacancies are *not* responsible for unintentional *n*-type conductivity; (ii) Si and O donors can be incorporated in large concentrations, likely causing unintentional *n*-type doping; (iii) oxygen (but not silicon) behaves as a DX center in GaN under pressure and in AlGaIn alloys; and (iv) gallium vacancies are the likely source of the yellow luminescence. For *p*-type GaN we found that (i) Mg is still the acceptor of choice; (ii) the resulting hole concentration is limited due to Mg solubility; (iii) incorporation of Mg on interstitial sites or antisites is not a problem; (iv) hydrogen has a beneficial effect on *p*-type doping

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because it suppresses compensation and enhances acceptor incorporation; and (v) compensation by nitrogen vacancies may occur, likely causing the observed persistent photoconductivity.

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