

Pinning of energy transitions of defects, complexes, and surface states in AlGaN alloys

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ABSTRACT

In this work, we determine the dependence of the defect transition energies, electronic bands, and surface charge neutrality levels in AlGaIn. With Vacuum level as reference, we show that energy transitions of localized defects and the surface Fermi level are independent of the alloy composition as electronic bands diverge with the increase in the bandgap as a function of alloy composition. The invariance of localized states on the alloy composition creates a convenient internal reference energy with respect to which other energy states may be measured. We demonstrate a higher generality to the universality rule with the independence of deep transition states of otherwise shallow donor type defects [(+1/+3) transition for V_N] and defect complexes (C_N+Si_{III}) in addition to the earlier predicted independent nature of mid-gap states when they are either the antibonding state between cationic impurities and host anion or acceptors at anion sites.

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The development of AlGaIn-based deep-UV optoelectronics and high-power devices faces limitations due to their large compensating or absorbing defect concentrations, relatively poor Ohmic contacts, and high dopant activation energies due to DX formation.^{1–11} These limitations may be overcome by effective point defect identification and control. Typically, the defect control involves determining the growth regimes that ensure reduced defect incorporation and associated adverse effects.^{12–14} However, targeted reduction of point defects by increasing the defect formation energy by controlling the defect constituents' chemical potential or defect quasi Fermi level has been demonstrated as well.^{15–18} Furthermore, altering the defect configuration such as for the case of C_N in AlN to form complexes with Si that do not absorb in the technologically important UV region has also been shown.¹⁹ For the targeted reduction by controlling the defect formation energy or changing the configuration of the defect, identification of the defects, their complexes, energies of formation, and optical properties are necessary. While some of the defect properties have been calculated for pure materials (GaN and AlN),^{20–23} extending them to the alloy system AlGaIn has been limited. Consequently, an understanding of the relative energies of the defect transitions and electronic bands (conduction and valence bands) is essential to understanding the defects and their properties in the alloy. Similarly, extensive theoretical and experimental works on the surface states and the

corresponding Fermi level position have been reported.^{24–29} The surface Fermi level is likely more influential in defect formation or incorporation due to them mostly forming or incorporating at the surface as bulk diffusion is limited at typical epitaxial growth temperatures.^{15,21} Consequently, a better understanding of the energy shifts of the defect states, surface Fermi level, and electronic bands in alloys is important. Furthermore, the experimentally determined energy shifts may provide insights into the impact of alloying or strain on the Hamiltonians and their solutions employed in density functional theory (DFT) calculations. Accordingly, in this work, we describe the relationship between the point defect thermodynamic transition energies, Fermi level pinning energies or charge neutrality levels, and the electronic bands as a function of Al composition. Notably, we provide their energy shifts with the vacuum level as a reference and hence we describe the “absolute” energies and shifts of the bands and states as a function of alloy composition. The term “absolute” is used here to imply a common reference energy (vacuum level) between different materials or alloys, resulting in energy levels that may be easily compared across systems. We note that potential energy is always relative. We also demonstrate the invariance of the “absolute” defect energy with the change in the alloy composition.

AlGaIn layers were grown on either AlN single crystal substrates or AlN templates grown on c-plane α -Al₂O₃ in a vertical, rf-heated,

low-pressure Metal organic chemical vapor deposition (MOCVD) reactor. The AlN substrates were processed from AlN boules grown by physical vapor transport (PVT).^{30–32} Pre-epitaxy, acid-based AlN surface preparation is described elsewhere.³³ AlN and sapphire substrate treatment before growth included annealing in H₂ ambience at 1100 °C for 7 min and nitridation at 950 °C for 4 min. On sapphire, this was followed by a 20 nm low temperature AlN nucleation layer deposited at 650 °C and then annealed at 1050 °C for 15 min to obtain Al-polarity. A 300 nm thick AlN layer was grown to serve as a template for doped AlGaIn growth on both AlN and sapphire substrates. The reactor total pressure was kept constant at 20 Torr throughout the growth. Trimethylaluminum (TMA), triethylgallium (TEG), and NH₃ were used as Al, Ga, and N precursors, respectively. SiH₄ and Cp₂Mg were used as the Si and Mg dopant sources, respectively. The AlGaIn composition was determined by x-ray diffraction (XRD) measurements carried out using a Philips X'Pert materials research diffractometer with a Cu x-ray source. AlGaIn and AlN 2θ - ω scans in symmetric (00.2) and asymmetric (10.5) and (−10.5) reflections were conducted in a double-axis configuration with a four-bounce Ge [220] crystal monochromator. The Al molar fraction in strained AlGaIn layers on an AlN/sapphire template was determined by the relative measurement between AlN and AlGaIn peaks. The details of the measurement technique have been described elsewhere.³⁴ Photoluminescence (PL) spectra were acquired using a pulsed ArF excimer laser ($\lambda = 193$ nm) along with a Princeton Instruments Acton SP2750 0.75 m high-resolution monochromator and a PIXIS: 2KBUV cooled charge-coupled device camera.

Previously, we had determined the changes in the energy of the conduction band, valence band, and surface Fermi level with respect to the vacuum level as a function of Al composition via x-ray photoelectron spectroscopy studies.³⁵ Interestingly, the surface Fermi level is a constant with respect to the vacuum level and the alloy exhibits a constant surface work function independent of composition. Hence, there is a strong correlation between Fermi level stabilization energy and surface defects and reconstructions pinning the Fermi level. The identity of these defects and reconstructions have been discussed in the literature^{24,26–29,35–38} with a recent work describing the surface oxide structure via TEM and DFT.³⁹ Nevertheless, the surface Fermi pinning energy behaves as a reference energy independent of electronic bands and hence the alloy composition. In contrast, the conduction and valence bands diverge as³⁵

$$\Delta E_C = x^2 + 0.8x + 0.7 \text{ eV}, \quad (1)$$

and

$$\Delta E_V = -(0.8x + 2.7 \text{ eV}), \quad (2)$$

measured with respect to the surface charge neutrality level (surface Fermi level) with the bowing factor shown to be entirely incorporated as the quadratic component in the conduction band dependence.

For this work, as case studies, we have characterized technologically important defects (a) C_N and its complexes with O_N, which determine the low doping limit in Si doped AlGaIn and 265 nm absorption in AlN,^{1,4,5,10,11,40–42} (b) C_N–Si_{III} complexes that are a potential solution to absorption by C_N in AlN and AlGaIn,¹⁹ and finally (c) Mg_{III}, and (d) V_N, which determine p-type conductivity and compensation in AlGaIn.^{43–56} It has to be noted that in many of these cases, the exact identity of the defect is under debate and we label

them with the most commonly ascribed labels. Furthermore, the exact identity is not important for the conclusions of this work. For this work, the defects were identified through correlation between DFT models and experimental methods such as secondary ion mass spectroscopy (SIMS), photoluminescence and absorption studies in GaN and AlN. The corresponding Stokes shift for each of the defects was estimated from published DFT analysis and photoluminescence excitation studies.^{1,5,7,10,17,19,20,22,23,41,42,46,51–60} The Stokes shift in pure materials was obtained by a comparison of the tentatively identified defects transition energies obtained from the DFT model and luminescence/absorption measurements in AlN or GaN and the corresponding emissions in AlN or GaN, respectively. The Stokes shift for any alloy composition was assumed as the linear interpolation of the corresponding values for the pure materials. The error due to such linear interpolation is negligible since the change in the magnitude of the Stokes shift with alloy composition was negligible compared to that of the bandgap. Finally, we include the defect energy levels associated with shallow defects from the ionization energies of donor Si. Note that Si is shallow for Al compositions <85% beyond which it undergoes a DX transition.^{9,61}

Photoluminescence (PL) studies of various defects in AlGaIn with different Al compositions were performed. The identity of each defect was determined by tracking evolution of known peaks from GaN or AlN as the Al composition changed from GaN to AlN. The growth and doping conditions necessary for the dominant emission corresponding to each of the studied defects are known from our prior studies and studies by various groups.^{22,23,42,46,51–53,55,56,62–64} In particular, we have demonstrated that employing chemical potential control (CPC) allows for controlling the concentration of individual defects such as C_N, vacancy silicon complexes, etc., whose properties can then be studied individually allowing us to present this study.^{15,18} C_N or its complex with O_N^{1,4,5,7,10,11} was controlled by CPC in AlGaIn for different Al molar fractions employing ammonia partial pressure and supersaturation¹⁵ and its emission peak was characterized as a function of Al composition from 2.2 eV in GaN to 3.9 eV in AlN. The formation of the C_N + Si_{III} complex has been hypothesized to be responsible for the absence of absorption at 265 nm in PVT-grown (physical vapor transport) AlN when co-doped with Si.¹⁹ This results in a shift in the emission from 3.9 eV (C_N) to 4.3 eV (C_N+Si_{III}) in AlN. The evolution of the new emission was then studied as a function of Al composition in AlGaIn. The blue emission at 2.8 eV in GaN appeared with high Mg doping $>2 \times 10^{19} \text{ cm}^{-3}$ in MOCVD grown GaN. The emergence of the blue luminescence also corresponds to an increased resistivity, implying self-compensation. The defect associated with self-compensation has been identified as V_N (+1/+3) although the luminescence itself has also been related to Mg undergoing a large local lattice relaxation.^{43–46,54,56} This blue emission in GaN evolves from 2.8 eV in GaN to 4.8 eV in AlN with an increase in the Al molar fraction in Mg ($>2 \times 10^{19} \text{ cm}^{-3}$) doped AlGaIn. Interestingly, the emission at 4.8 eV was also related to V_N in a photoluminescence excitation and power dependent photoluminescence studies in AlN not doped with Mg, indicating that the blue luminescence is likely related to V_N rather than Mg undergoing a large local lattice relaxation. Finally, in Mg ($<2 \times 10^{19} \text{ cm}^{-3}$)-doped AlN, an emission peak at 5.5 eV was observed, and is likely related to Mg_{Al} acceptor (0/−1) transition.⁴⁶ The evolution of the Mg emission was then studied as a function of Al composition to the 3.25 eV transition observed in Mg

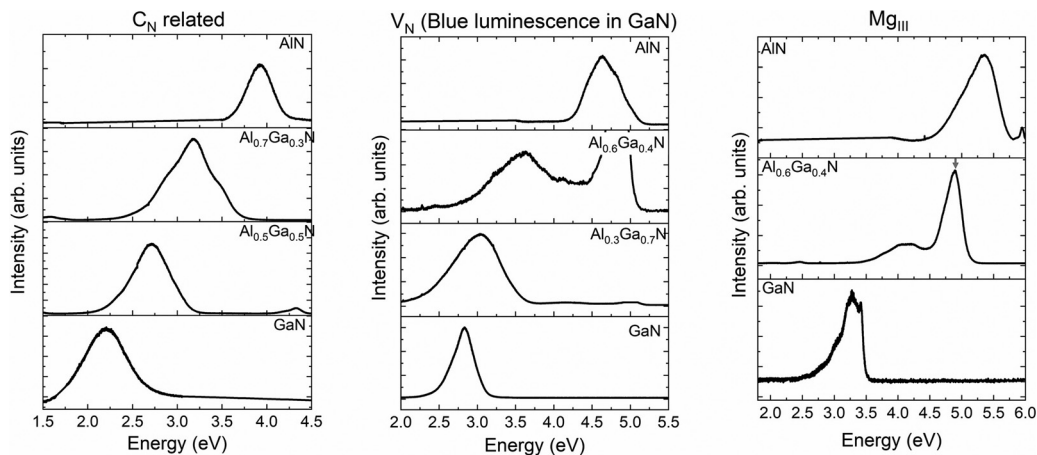


FIG. 1. Photoluminescence studies showing the dependence of the luminescence energies of various defects on the composition of AlGaIn ranging from GaN to AlN.

($< 2 \times 10^{19} \text{ cm}^{-3}$) doped GaN. This Mg emission peak is observed in highly conductive p-type GaN without self-compensation due to V_N . Interestingly, the luminescence energy associated with Mg agrees with reported electrical ionization energies and hence the associated Stokes shift is assumed to be small.^{44,46,52} Figure 1 shows the evolution of the photoluminescence peaks associated with some of the studied defects in AlGaIn. The thermodynamic transition levels associated with the defects were then obtained by a comparison between measured emission energy and Stokes shift, which provides the energy difference between a luminescence peak and thermodynamic transition energy.

Finally, the surface Fermi level and electronic bands that were previously measured with respect to the reference vacuum level were used to determine the point defect thermodynamic transitions corresponding to various defects as a function of Al molar fraction with respect to the vacuum level, as shown in Fig. 2. We observe an invariance of localized defect transitions in AlGaIn, with the localized deep states (mid-gap energies) found to be at a constant energy relative to the vacuum level, independent of Al composition. This strongly suggests that the point defect thermodynamic transition energies and the charge neutrality level are constant reference energies, independent of cations (Al or Ga molar fractions) and may be used as reference energies instead of the vacuum level, which cannot be directly measured. This is in agreement with the universality rule^{65,66} predicting independent nature of mid-gap states if they are the antibonding state between the cationic impurities and host anion and Lyons *et al.* predicting hole localization for acceptors at anion sites such as C_N , resulting in atomic-like states.⁶⁷ However, interestingly, we also demonstrate the independence of deep transition states of otherwise shallow donor type defects [(+1/+3) transition for V_N] and defect complexes ($C_N + Si_{III}$) indicating a more generality to the universality rule. Mg employed as a p-type dopant in nitrides exhibits an interesting behavior. Mg was theorized as being “accidentally” a shallow defect in GaN as described by Lyons *et al.*⁵⁶ However, while other defects show little variation with respect to the vacuum level across the alloy composition ($\leq 0.2 \text{ eV}$), Mg shifts by $\sim 0.45 \text{ eV}$ with respect to the vacuum level toward the valence band from GaN to AlN as shown in Fig. 2 hinting at a possible hydrogenic contribution with higher activation energy in AlN influenced by higher effective mass of holes in AlN and not

necessarily behaving as a localized acceptor. Furthermore, recently reported low activation energies for Mg in Al rich AlGaIn⁶⁸ clearly indicate an incomplete understanding of Mg in AlGaIn and a need for further theoretical and DFT investigation. Finally, for comparison, a resonantly shallow donor Si is included in Fig. 2 with the transition energy determined by the donor activation energy.⁹ The Si impurity remains mostly resonant with the conduction band with a minor deviation only observed after the transition to a DX state⁶¹ in AlN. To conclude, we have experimentally demonstrated and extended the universality rule by studying alloys where the band movement and defect states are studied by inducing perturbations, i.e., slowly changing the alloy composition.

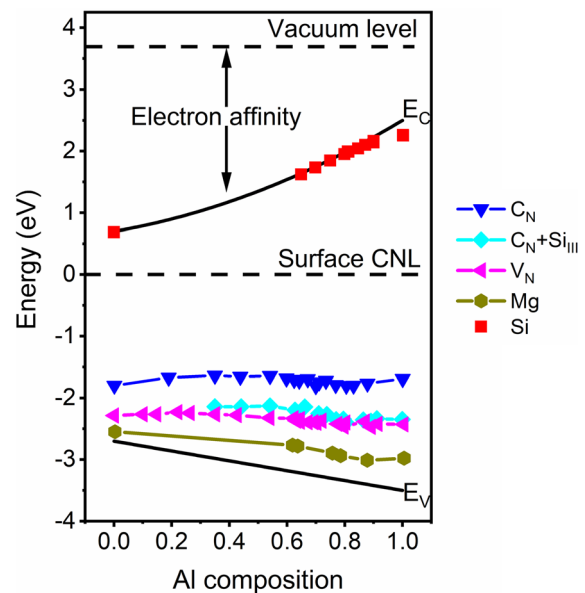


FIG. 2. The thermodynamic transition energies of different defects along, the surface charge neutrality level, and electronic bands as a function of Al composition along with the vacuum level.

In conclusion, we studied the composition dependence of the defect transition energies, electronic bands, and surface charge neutrality levels in AlGa_N as a function of the Al composition. We demonstrated that energy transitions of localized defects are independent of the alloy composition as electronic bands diverge with an increase in the bandgap where the energies were measured with respect to the vacuum level. We conclude an invariance of localized defect transitions in AlGa_N, and an easily measurable reference energy with respect to which other energy states may be measured by techniques such as photoluminescence in place of the vacuum level that cannot be easily measured. Finally, we also demonstrated a higher generality to the universality rule with the independence of deep transition states of otherwise shallow donor type defects [(+1/+3) transition for V_N] and defect complexes (C_N + Si_{III}) in addition to the earlier predicted independent nature of mid-gap states when they are either the antibonding state between the cationic impurities and host anion or acceptors at anion sites.

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REFERENCES

- ¹D. Alden, J. S. Harris, Z. Bryan, J. N. Baker, P. Reddy, S. Mita, G. Callsen, A. Hoffmann, D. L. Irving, R. Collazo, and Z. Sitar, *Phys. Rev. Appl.* **9**, 054036 (2018).
- ²J. Buckeridge, C. R. A. Catlow, D. O. Scanlon, T. W. Keal, P. Sherwood, M. Miskufova, A. Walsh, S. M. Woodley, and A. A. Sokol, *Phys. Rev. Lett.* **114**, 016405 (2015).
- ³S. F. Chichibu, H. Miyake, K. Hiramatsu, and A. Uedono, *III-Nitride Ultraviolet Emitters* (Springer, Cham, 2016), pp. 115–136.
- ⁴S. G. Christenson, W. Xie, Y. Y. Sun, and S. B. Zhang, *J. Appl. Phys.* **118**, 135708 (2015).
- ⁵D. O. Demchenko, I. C. Diallo, and M. A. Reshchikov, *Phys. Rev. Lett.* **110**, 087404 (2013).
- ⁶M. Lamprecht, C. Grund, B. Neuschl, K. Thonke, Z. Bryan, R. Collazo, and Z. Sitar, *J. Appl. Phys.* **119**, 155701 (2016).
- ⁷J. L. Lyons, A. Janotti, and C. G. V. de Walle, *Appl. Phys. Lett.* **97**, 152108 (2010).
- ⁸B. B. Haidet, B. Sarkar, P. Reddy, I. Bryan, Z. Bryan, R. Kirste, R. Collazo, and Z. Sitar, *Jpn. J. Appl. Phys., Part 1* **56**, 100302 (2017).
- ⁹R. Collazo, S. Mita, J. Xie, A. Rice, J. Tweedie, R. Dalmau, and Z. Sitar, *Phys. Status Solidi C* **8**, 2031 (2011).
- ¹⁰R. Collazo, J. Xie, B. E. Gaddy, Z. Bryan, R. Kirste, M. Hoffmann, R. Dalmau, B. Moody, Y. Kumagai, T. Nagashima, Y. Kubota, T. Kinoshita, A. Koukitu, D. L. Irving, and Z. Sitar, *Appl. Phys. Lett.* **100**, 191914 (2012).
- ¹¹F. Kaess, S. Mita, J. Xie, P. Reddy, A. Klump, L. H. Hernandez-Balderrama, S. Washiyama, A. Franke, R. Kirste, A. Hoffmann, R. Collazo, and Z. Sitar, *J. Appl. Phys.* **120**, 105701 (2016).
- ¹²A. M. Armstrong, M. W. Moseley, A. A. Allerman, M. H. Crawford, and J. J. Wierer, *J. Appl. Phys.* **117**, 185704 (2015).
- ¹³D. Koleske, A. E. Wickenden, R. L. Henry, and M. E. Twigg, *J. Cryst. Growth* **242**, 55 (2002).
- ¹⁴S. Mita, R. Collazo, A. Rice, R. F. Dalmau, and Z. Sitar, *J. Appl. Phys.* **104**, 013521 (2008).
- ¹⁵P. Reddy, S. Washiyama, F. Kaess, R. Kirste, S. Mita, R. Collazo, and Z. Sitar, *J. Appl. Phys.* **122**, 245702 (2017).
- ¹⁶P. Reddy, M. P. Hoffmann, F. Kaess, Z. Bryan, I. Bryan, M. Bobea, A. Klump, J. Tweedie, R. Kirste, S. Mita, M. Gerhold, R. Collazo, and Z. Sitar, *J. Appl. Phys.* **120**, 185704 (2016).
- ¹⁷Z. Bryan, I. Bryan, B. E. Gaddy, P. Reddy, L. Hussey, M. Bobea, W. Guo, M. Hoffmann, R. Kirste, J. Tweedie, M. Gerhold, D. L. Irving, Z. Sitar, and R. Collazo, *Appl. Phys. Lett.* **105**, 222101 (2014).
- ¹⁸P. Reddy, Q. Guo, J. Tweedie, S. Washiyama, F. Kaess, S. Mita, M. H. Breckenridge, R. Kirste, R. Collazo, A. Klump, B. Sarkar, and Z. Sitar, in 2018 IEEE Conference on Research and Applications of Photonics in Defense, RAPID (2018), pp. 1–4.
- ¹⁹B. E. Gaddy, Z. Bryan, I. Bryan, J. Xie, R. Dalmau, B. Moody, Y. Kumagai, T. Nagashima, Y. Kubota, T. Kinoshita, A. Koukitu, R. Kirste, Z. Sitar, R. Collazo, and D. L. Irving, *Appl. Phys. Lett.* **104**, 202106 (2014).
- ²⁰C. G. V. de Walle and J. Neugebauer, *J. Appl. Phys.* **95**, 3851 (2004).
- ²¹P. Kempisty, Y. Kangawa, A. Kusaba, K. Shiraishi, S. Krukowski, M. Bockowski, K. Kakimoto, and H. Amano, *Appl. Phys. Lett.* **111**, 141602 (2017).
- ²²M. A. Reshchikov and H. Morkoç, *J. Appl. Phys.* **97**, 061301 (2005).
- ²³J. S. Harris, J. N. Baker, B. E. Gaddy, I. Bryan, Z. Bryan, K. J. Mirrieles, P. Reddy, R. Collazo, Z. Sitar, and D. L. Irving, *Appl. Phys. Lett.* **112**, 152101 (2018).
- ²⁴M. Himmerlich, L. Lympirakis, R. Gutt, P. Lorenz, J. Neugebauer, and S. Krischok, *Phys. Rev. B* **88**, 125304 (2013).
- ²⁵J. P. Long and V. M. Bermudez, *Phys. Rev. B* **66**, 121308 (2002).
- ²⁶M. S. Miao, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **80**, 155319 (2009).
- ²⁷P. Reddy, I. Bryan, Z. Bryan, W. Guo, L. Hussey, R. Collazo, and Z. Sitar, *J. Appl. Phys.* **116**, 123701 (2014).
- ²⁸C. G. V. de Walle and D. Segev, *J. Appl. Phys.* **101**, 081704 (2007).
- ²⁹L. Lympirakis, P. H. Weidlich, H. Eisele, M. Schnedler, J. P. Nys, B. Grandidier, D. Stiévenard, R. E. Dunin-Borkowski, J. Neugebauer, and P. Ebert, *Appl. Phys. Lett.* **103**, 152101 (2013).
- ³⁰Z. G. Herro, D. Zhuang, R. Schlessner, R. Collazo, and Z. Sitar, *J. Cryst. Growth* **286**, 205 (2006).
- ³¹D. Zhuang, Z. G. Herro, R. Schlessner, and Z. Sitar, *J. Cryst. Growth* **287**, 372 (2006).
- ³²P. Lu, R. Collazo, R. F. Dalmau, G. Durkaya, N. Dietz, B. Raghothamachar, M. Dudley, and Z. Sitar, *J. Cryst. Growth* **312**, 58 (2009).
- ³³A. Rice, R. Collazo, J. Tweedie, R. Dalmau, S. Mita, J. Xie, and Z. Sitar, *J. Appl. Phys.* **108**, 043510 (2010).
- ³⁴J. Tweedie, R. Collazo, A. Rice, J. Xie, S. Mita, R. Dalmau, and Z. Sitar, *J. Appl. Phys.* **108**, 043526 (2010).
- ³⁵P. Reddy, I. Bryan, Z. Bryan, J. Tweedie, S. Washiyama, R. Kirste, S. Mita, R. Collazo, and Z. Sitar, *Appl. Phys. Lett.* **107**, 091603 (2015).
- ³⁶C. I. Wu and A. Kahn, *Appl. Phys. Lett.* **74**, 546 (1999).
- ³⁷C. D. Lee, Y. Dong, R. M. Feenstra, J. E. Northrup, and J. Neugebauer, *Phys. Rev. B* **68**, 205317 (2003).
- ³⁸J. E. Northrup, R. D. Felice, and J. Neugebauer, *Phys. Rev. B* **55**, 13878 (1997).
- ³⁹J. H. Dycus, K. J. Mirrieles, E. D. Grimley, R. Kirste, S. Mita, Z. Sitar, R. Collazo, D. L. Irving, and J. M. LeBeau, *ACS Appl. Mater. Interfaces* **10**, 10607 (2018).
- ⁴⁰Y. Cao, R. Chu, R. Li, M. Chen, R. Chang, and B. Hughes, *Appl. Phys. Lett.* **108**, 062103 (2016).
- ⁴¹M. A. Reshchikov, D. O. Demchenko, A. Usikov, H. Helava, and Y. Makarov, *Phys. Rev. B* **90**, 235203 (2014).
- ⁴²I. Bryan, Z. Bryan, S. Washiyama, P. Reddy, B. Gaddy, B. Sarkar, M. H. Breckenridge, Q. Guo, M. Bobea, J. Tweedie, S. Mita, D. Irving, R. Collazo, and Z. Sitar, *Appl. Phys. Lett.* **112**, 062102 (2018).
- ⁴³M. A. Reshchikov, G.-C. Yi, and B. W. Wessels, *Phys. Rev. B* **59**, 13176 (1999).
- ⁴⁴M. L. Nakarmi, N. Nepal, J. Y. Lin, and H. X. Jiang, *Appl. Phys. Lett.* **94**, 091903 (2009).
- ⁴⁵U. Kaufmann, M. Kunzer, M. Maier, H. Obloh, A. Ramakrishnan, B. Santic, and P. Schlotter, *Appl. Phys. Lett.* **72**, 1326 (1998).
- ⁴⁶M. L. Nakarmi, N. Nepal, C. Ugolini, T. M. Altahtamouni, J. Y. Lin, and H. X. Jiang, *Appl. Phys. Lett.* **89**, 152120 (2006).
- ⁴⁷P. Kozodoy, H. Xing, S. P. DenBaars, U. K. Mishra, A. Saxler, R. Perrin, S. Elhamri, and W. C. Mitchel, *J. Appl. Phys.* **87**, 1832 (2000).
- ⁴⁸S. Nakamura, T. Mukai, M. Senoh, and N. Iwasa, *Jpn. J. Appl. Phys., Part 2* **31**, L139 (1992).
- ⁴⁹D. J. Kim, D. Y. Ryu, N. A. Bojarczuk, J. Karasinski, S. Guha, S. H. Lee, and J. H. Lee, *J. Appl. Phys.* **88**, 2564 (2000).

- ⁵⁰W. Götz, N. M. Johnson, J. Walker, D. P. Bour, and R. A. Street, *Appl. Phys. Lett.* **68**, 667 (1996).
- ⁵¹Q. Yan, A. Janotti, M. Scheffler, and C. G. Van de Walle, *Appl. Phys. Lett.* **100**, 142110 (2012).
- ⁵²J. Li, T. N. Oder, M. L. Nakarmi, J. Y. Lin, and H. X. Jiang, *Appl. Phys. Lett.* **80**, 1210 (2002).
- ⁵³G. Miceli and A. Pasquarello, *Phys. Rev. B* **93**, 165207 (2016).
- ⁵⁴Z. Bryan, M. Hoffmann, J. Tweedie, R. Kirste, G. Callsen, I. Bryan, A. Rice, M. Bobea, S. Mita, J. Xie, Z. Sitar, and R. Collazo, *J. Electron. Mater.* **42**, 815 (2013).
- ⁵⁵T. Tanaka, A. Watanabe, H. Amano, Y. Kobayashi, I. Akasaki, S. Yamazaki, and M. Koike, *Appl. Phys. Lett.* **65**, 593 (1994).
- ⁵⁶J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Phys. Rev. Lett.* **108**, 156403 (2012).
- ⁵⁷J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **89**, 035204 (2014).
- ⁵⁸J. L. Lyons and C. G. V. de Walle, *npj Comput. Mater.* **3**, 12 (2017).
- ⁵⁹Q. Yan, A. Janotti, M. Scheffler, and C. G. Van de Walle, *Appl. Phys. Lett.* **105**, 111104 (2014).
- ⁶⁰M. Suzuki, J. Nishio, M. Onomura, and C. Hongo, *J. Cryst. Growth* **189–190**, 511 (1998).
- ⁶¹L. Gordon, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **89**, 085204 (2014).
- ⁶²S. F. Chichibu, H. Miyake, Y. Ishikawa, M. Tashiro, T. Ohtomo, K. Furusawa, K. Hazu, K. Hiramatsu, and A. Uedono, *J. Appl. Phys.* **113**, 213506 (2013).
- ⁶³M. P. Hoffmann, J. Tweedie, R. Kirste, Z. Bryan, I. Bryan, M. Gerhold, Z. Sitar, and R. Collazo, *Proc. SPIE* **8986**, 89860T (2014).
- ⁶⁴H. Obloh, K. H. Bachem, U. Kaufmann, M. Kunzer, M. Maier, A. Ramakrishnan, and P. Schlotter, *J. Cryst. Growth* **195**, 270 (1998).
- ⁶⁵A. Zunger, *Phys. Rev. Lett.* **54**, 849 (1985).
- ⁶⁶M. J. Caldas, A. Fazzio, and A. Zunger, *Appl. Phys. Lett.* **45**, 671 (1984).
- ⁶⁷J. L. Lyons, A. Janotti, and C. G. Van de Walle, *J. Appl. Phys.* **115**, 012014 (2014).
- ⁶⁸T. Kinoshita, T. Obata, H. Yanagi, and S. Inoue, *Appl. Phys. Lett.* **102**, 012105 (2013).