

Band parameters for nitrogen-containing semiconductors

I. Vurgaftman and J. R. Meyer

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APPLIED PHYSICS REVIEWS—FOCUSED REVIEW

Band parameters for nitrogen-containing semiconductors

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We present a comprehensive and up-to-date compilation of band parameters for all of the nitrogen-containing III–V semiconductors that have been investigated to date. The two main classes are: (1) “conventional” nitrides (wurtzite and zinc-blende GaN, InN, and AlN, along with their alloys) and (2) “dilute” nitrides (zinc-blende ternaries and quaternaries in which a relatively small fraction of N is added to a host III–V material, e.g., GaAsN and GaInAsN). As in our more general review of III–V semiconductor band parameters [I. Vurgaftman *et al.*, J. Appl. Phys. **89**, 5815 (2001)], complete and consistent parameter sets are recommended on the basis of a thorough and critical review of the existing literature. We tabulate the direct and indirect energy gaps, spin-orbit and crystal-field splittings, alloy bowing parameters, electron and hole effective masses, deformation potentials, elastic constants, piezoelectric and spontaneous polarization coefficients, as well as heterostructure band offsets. Temperature and alloy-composition dependences are also recommended wherever they are available. The “band anticrossing” model is employed to parameterize the fundamental band gap and conduction band properties of the dilute nitride materials. [DOI: 10.1063/1.1600519]

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I. INTRODUCTION

The second half of the 1990s witnessed an explosive expansion of research on nitrogen-containing semiconductors, which has continued unabated to the present. Early studies^{1,2} of GaN and related compounds and alloys tended to generate skepticism concerning whether devices based on materials with such high defect densities could ever be practical. However, by now most of those doubts have been dispelled by improvements in the epitaxial growth technology, coupled with a better appreciation of the relationship between defects and device performance. Most of the interest in the nitrides has hinged on their unique advantages in two fundamental application areas: short-wavelength light emitters and high-power/high-temperature electronics. Although the large band gaps of GaN and AlN are key to both applications, another critical factor is that they are III–V semiconductors. Whereas the reliability of related wide-gap II–VI devices remains problematic despite a great deal of research, nitride lasers and light-emitting diodes (LEDs) have by now attained commercially attractive lifetimes (e.g., $\approx 10\,000$ h).³

In response to this intensive research and commercial interest in nitride semiconductors, several recent works have reviewed their material and physical properties.^{3–9} Nonetheless, rapid ongoing developments have already led to obsolescence of much of the reported quantitative data, especially regarding the band parameters. In an earlier publication, we comprehensively reviewed the literature and recommended consistent, up-to-date band parameters for all of the common

III–V semiconductors and their alloys, including the nitrides.¹⁰ While most of the tabulations presented in that work (assembled early-to-mid 2000) remain current apart from a few minor adjustments based on new information, it is striking how many of the nitride properties have already been superseded, not only quantitatively but qualitatively.

The present review was written to remedy that obsolescence, by providing a completely revised and updated description of the band parameters for nitride-containing semiconductors. We cover both to the “conventional” nitrides (GaN, AlN, InN, and their alloys), and also to the “dilute” nitride ternaries and quaternaries, in which at most a few percent of N is introduced to a more common III–V semiconductor (e.g., to form GaAsN or GaInAsN). Although in many ways these two classes of nitrogen-containing III–V materials are not closely related, they share the common attribute that what is known about their band properties has evolved quite rapidly in a very short period of time. In the case of the conventional nitrides, a prime example is the energy gap of InN, which was recently revised downward to less than 50% of its consensus value from a few years ago. Similarly, just recently it has become unequivocally clear that the band anticrossing (BAC) model provides the most useful parameterization of the dilute nitride alloys, even though the physical meaning of that model is not yet resolved.

As in the earlier review,¹⁰ we provide values of the energy gaps, spin-orbit and crystal-field splittings, electron and hole effective-mass parameters, conduction and valence band deformation potentials, and band offsets on an absolute scale. In treating the base materials for the dilute nitride alloys (e.g., GaAs as the basis for GaAsN), parameters should be taken from our earlier review.¹⁰ Once again, we maintain full internal consistency, e.g., between expressions for the alloy composition and temperature dependences and their end points. For completeness, lattice constants and elastic moduli are also listed for GaN, AlN, and InN.

For each parameter, the text briefly discusses the most salient results from the literature, followed by the specification of a recommended value. While in many cases it was again impractical to cite every published work that ever treated a given parameter, we have endeavored to include enough references to provide a nearly complete picture of the available knowledge base.

Although one must naturally be concerned that the present review may be doomed to the same early obsolescence that befell its predecessors, we believe that with regard to the most important nitride material properties the field is now displaying a trend towards convergence. Since our focus is strictly on band parameters, the reader should consult other sources such as the article by Jain *et al.*³ for a comprehensive recent review of the growth, characterization, and various other properties. The book by Nakamura and Fasol¹¹ provides an excellent overview of nitride light emitters.

II. “CONVENTIONAL” NITRIDE BAND PARAMETERS

A. Methodology

GaN, InN, AlN, and their alloys can crystallize in both wurtzite and zinc-blende lattice forms, and the corresponding

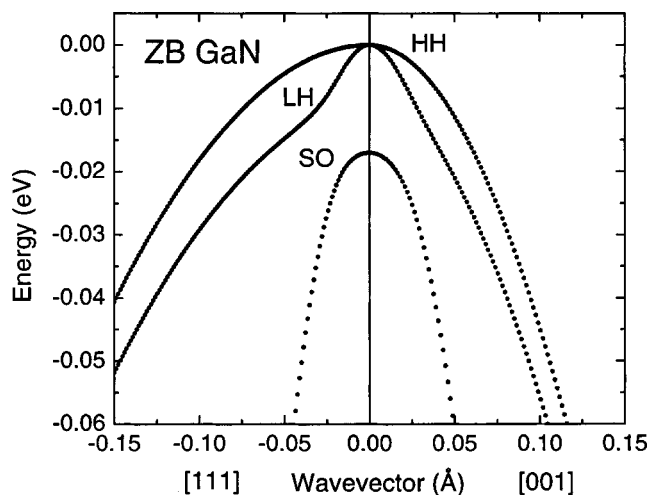


FIG. 1. Valence band structure of zinc-blende GaN, using the parameters from our earlier review (Ref. 10).

band structures are quite distinct due to differences in the underlying symmetries. For the zinc-blende case, our earlier review¹⁰ sketched how three Luttinger parameters and the spin-orbit splitting provide a minimal description of the valence band structure, while the energy gap and interband coupling strength are also needed to parameterize both conduction and valence bands. The split-off hole mass can be treated as an independent parameter, even though it does not appear as such within the commonly used 8-band $\mathbf{k}\cdot\mathbf{p}$ model. The increase of the electron effective mass due to interactions with higher conduction bands may be included via the so-called F parameter. The well-known relevant expressions may be obtained either from our earlier review¹⁰ or from a large number of other works.^{12–16}

The set of band parameters for the wurtzite lattice must be augmented due to its lower symmetry. Since GaN and AlN have a wide energy gap, and InN is now believed to have a moderate gap, it may be assumed that interband coupling effects on the hole masses are secondary. Therefore, in light of the existing uncertainties there is no pressing need to parameterize the effects of either the valence bands or the higher conduction bands on the electron effective mass, i.e., we omit the interband matrix element and the F parameter and just list an electron mass. Owing to the reduced symmetry, that mass can display some anisotropy, although it is believed to be rather weak. On the other hand, a full description of the wurtzite valence band structure requires both the spin-orbit splitting (Δ_{so}) and the crystal-field splitting (Δ_{cr}), along with the seven so-called A parameters. The latter parameterize the hole masses along the different directions, performing a similar function to that of Luttinger parameters in zinc-blende materials. For comparison, we plot the valence band structure near the Γ point for zinc-blende and wurtzite GaN in Figs. 1 and 2, respectively. The distinction between Figs. 2(a) and 2(b) will be discussed in Sec. II B.

As in our earlier review, we parameterize the temperature dependence of the energy gap using the commonly employed Varshni formula

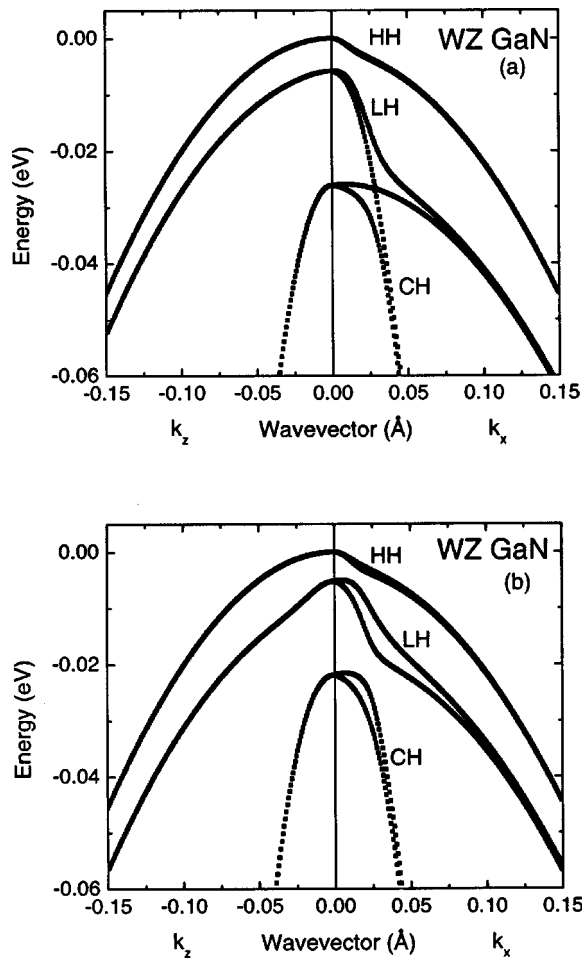


FIG. 2. Valence band structure of wurtzite GaN, using the parameters (a) recommended by Ren *et al.* (Ref. 80) and (b) recommended in this review.

$$E_g(T) = E_g(T=0) - \frac{\alpha T^2}{T + \beta}, \quad (1)$$

although results have been compiled elsewhere for other forms of the energy gap's temperature dependence.¹⁷ Since in zinc-blende materials one is also interested in the indirect gaps and masses, we have compiled best estimates (which are theoretical for the moment) for the X and L valleys.

The parameters described above are generally sufficient to describe the conduction and valence band structures of bulk nitride materials. However, since epitaxially grown heterostructures now routinely combine layers of lattice-mismatched constituents, the material properties under strain must also be specified. This is conventionally done within the deformation potential theory, which for the zinc-blende crystal symmetry requires a hydrostatic potential and three valence-band potentials (sufficient to account for epitaxial growth along an arbitrary direction).^{14,16} On the other hand, wurtzite materials generally require as many as two potentials for the shift of the energy gap, along with six valence-band deformation potentials.¹⁴ For completeness, we also list the six (three) elastic constants for the wurtzite (zinc-blende) forms of the nitride materials. Our recommendations are chosen from a rather broad spectrum of values for these parameters in the literature.

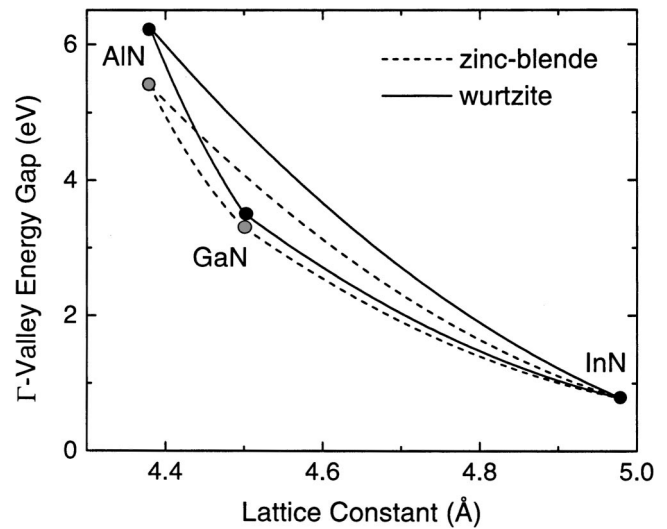


FIG. 3. Recommended energy gaps of wurtzite (solid curves) and zinc-blende (dashed) nitride semiconductor alloys and binaries (points), as a function of lattice constant for the zinc-blende form.

Wurtzite heterostructures are also strongly influenced by spontaneous polarization, which for lattice-mismatched layers must be supplemented by the piezoelectric coefficients. In describing the piezoelectric effect and spontaneous polarization, we follow the methodology of our earlier review¹⁰ with one difference: the values of d_{33} , d_{13} , and d_{15} are now listed (in units of pm/V) rather than the corresponding e_{ij} parameters (in units of C/m²). This change avoids conversions associated with differing sets of elastic constants in the original references.

The composition dependences of the energy gaps for the ternary alloys AlGa_{1-x}N, GaIn_{1-x}N, and AlIn_{1-x}N are assumed to follow the simple quadratic form

$$E_g(A_{1-x}B_x) = (1-x)E_g(A) + xE_g(B) - x(1-x)C, \quad (2)$$

where the so-called bowing parameter C accounts for the deviation from a linear interpolation (virtual-crystal approximation) between the two binaries A and B . The bowing parameter is always positive for these materials, which reflects a reduction of the alloy energy gaps. The bowing-parameter concept can be straightforwardly generalized to the other nitride alloy material parameters, as outlined in our earlier review. Linear interpolation has been assumed whenever no information on the bowing is available. We also emphasize that it is the hole masses rather than the A parameters or Luttinger parameters that should be interpolated. Recommended energy gaps (see below) for the wurtzite and zinc-blende nitride semiconductors are plotted in Fig. 3 as a function of lattice constant for the zinc-blende form. The bowing effect is clearly evident in the curves connecting the binary end points.

B. GaN

GaN is a wide-gap semiconductor that usually crystallizes in the wurtzite lattice (also known as hexagonal or α -GaN). However, under certain conditions zinc-blende GaN (sometimes referred to as cubic or β -GaN) can be grown on

a zinc-blende substrate. Under very high pressure, GaN and other nitrides experience a phase transition to the rocksalt lattice structure.¹⁸ In what follows, the wurtzite phase is implied if the crystal structure of a given nitride semiconductor is not stated, whereas the less common zinc-blende phase is always specified explicitly. Unlike all of the non-nitride wide-gap III–V semiconductors, GaN has a direct energy gap that makes it suitable for blue lasers and LEDs.

1. Wurtzite GaN

It has been known since the early 1970s that the energy gap of wurtzite GaN is about 3.5 eV.^{19,20} In order to determine the gap accurately from luminescence experiments, one must measure the energy of one of the pronounced exciton transitions and add to it the exciton binding energy. Perhaps the most reliable indicator in relatively-pure GaN is the peak associated with the free A exciton (E_A). That transition energy can be determined quite precisely, despite its typical proximity to the B exciton and also neutral–donor bound exciton transitions. Early measurements^{19,21,22} led to a value $E_A = 3.475$ eV near $T = 0$, in conjunction with an estimate of 28 meV for the binding energy. Numerous other photoluminescence (PL) and absorption studies from the 1990s^{23–35} broadened the range of reported A exciton transition energies at 0 K to 3.474–3.496 eV, where some of the spread was apparently attributable to variations in the strain conditions.³⁶ Experimental binding energies for the A exciton range from 18 to 28 meV.^{22,23,27,28,31,34,37–39} Owing to uncertainty in the hole effective mass, the corresponding theoretical⁴⁰ range for the binding energy is 23–28 meV. Based on median values for both E_A and the binding energy, we recommend a value of 3.510 eV for the zero-temperature energy gap.

While the first measured temperature dependence of the GaN energy gap²² yielded Varshni coefficients with signs opposite from those of the other III–V materials,¹⁰ subsequent investigations achieved good fits with the conventional signs for α and β . From optical absorption measurements on bulk single crystals and epitaxial layers grown on sapphire, Teisseyre *et al.*⁴¹ obtained $\alpha = 0.939$ –1.08 meV/K and $\beta = 745$ –772 K. For the temperature variation of the A exciton resonance, Shan *et al.* reported $\alpha = 0.832$ meV/K and $\beta = 836$ K,²⁴ whereas Petalas *et al.*⁴² fixed $\beta = 700$ K and found $\alpha = 0.858$ meV/K using spectroscopic ellipsometry. Salvador *et al.*⁴³ obtained $\alpha = 0.732$ meV/K and $\beta = 700$ K, based on PL results. Manasreh²⁹ reported $\alpha = 0.566$ –1.156 meV/K and $\beta = 738$ –1187 K from absorption measurements on samples grown by MBE and MOCVD. The contactless electroreflectance study of Li *et al.*³² led to $\alpha = 1.28$ meV/K and $\beta = 1190$ K for the A exciton transition energy, while Zubrilov *et al.*⁴⁴ suggested $\alpha = 0.74$ meV/K and $\beta = 600$ K based on exciton luminescence spectra. PL data from a study of free and bound excitons by Reynolds *et al.*⁴⁵ were fitted to a modified Varshni-like form. While the general trends are roughly consistent, it is not obvious how to reconcile these diverse parameter sets quantitatively. Not only do the exciton transition energies become more difficult to identify precisely at higher temperatures, but also a small temperature variation in the binding energy may limit the accuracy of the fits. Our recommended Varshni

parameters of $\alpha = 0.909$ meV/K and $\beta = 830$ K represent simple averages over the more credible reported values. These agree well with the parameters suggested by absorption measurements on AlGaIn, for which negligible composition dependence was reported.⁴⁶ Owing to the small relative change in the bandgap energy (only 72 meV between 0 and 300 K), GaN device characteristics tend to be relatively insensitive to the precise values of the Varshni parameters.

All conventional nitrides in the wurtzite phase exhibit a direct energy gap, and the next conduction valleys are at least 2 eV higher than the Γ valley.⁴⁷ Therefore, we do not specify wurtzite indirect gaps or other critical-point energies in this review, although various theoretical and experimental estimates may be found in Refs. 47–52.

The bottom of the conduction band in GaN is well approximated by a parabolic dispersion relation, although a slight anisotropy may be expected because of the reduced lattice symmetry.⁵³ In early experimental studies, Barker and Illegems⁵⁴ obtained $m_n = 0.20m_0$ from reflectivity measurements, and Rheinlander and Neumann⁵⁵ inferred 0.24–0.29 m_0 from a Faraday-rotation investigation of heavily *n*-doped GaN. Sidorov *et al.*⁵⁶ also studied heavily *n*-doped samples and derived masses of 0.1 m_0 –0.28 m_0 , depending on what primary scattering channel was assumed, from fits to the thermoelectric power. Other early values may be found in the reviews from the 1970s.^{1,2} Since then, a considerable body of work has produced more precise evaluations of the electron mass. Meyer *et al.*⁵⁷ and Witowski *et al.*⁵⁸ obtained masses of 0.236 m_0 and 0.222 m_0 , respectively, from shallow-donor transition energies. The latter result has the smallest error bounds quoted in the literature (0.2%). Pointing out the importance of the polaron correction (8%) in GaN, owing to its strong polar nature, Drechsler *et al.* derived a bare mass of 0.20 m_0 from cyclotron resonance data.⁵⁹ Perlin *et al.*⁶⁰ obtained a similar result from infrared-reflectivity and Hall-effect measurements, and also found the anisotropy to be less than 1%. A slightly higher dressed mass of 0.23 m_0 was recently obtained by Wang *et al.*⁶¹ and Knap *et al.*⁶² The former may require a small downward revision because the electrons were confined in a quantum well, whereas the latter authors apparently corrected for that effect. No appreciable correction appears to be necessary for the infrared ellipsometry measurements on bulk *n*-doped GaN reported by Kasic *et al.*,⁶³ which yielded slightly anisotropic electron masses of $0.237 \pm 0.006m_0$ and $0.228 \pm 0.008m_0$ along the two axes. Finally, Elhamri *et al.*,⁶⁴ Saxler *et al.*,⁶⁵ Wong *et al.*,⁶⁶ Wang *et al.*,⁶⁷ and Hang *et al.*⁶⁸ determined masses ranging from 0.18 m_0 to 0.23 m_0 from Shubnikov–de Haas data for two-dimensional electrons at a GaN/AlGaIn heterojunction. It was suggested⁶⁴ that strain effects might have compromised somewhat the masses obtained by some of the other studies. Our composite recommendation is to use 0.20 m_0 for the bare electron effective mass and 0.22 m_0 for the experimentally relevant dressed mass. This bare mass agrees quite well with a number of theoretical estimates, which cluster around 0.20 m_0 (see the list in Ref. 69). We do not attempt to specify an F parameter for wurtzite GaN (for definiteness, it is assumed to vanish), owing to the large uncertainty. The interband matrix element

may be obtained from the relation between the electron mass and the relevant zone-center energies.¹⁰

In wurtzite materials, both the spin-orbit and the crystal-field splittings affect the structure of the valence band.⁷⁰ In the following, we take $\Delta_2 = \Delta_3 = \Delta_{so}/3$ (although a small Δ_2/Δ_3 anisotropy has sometimes been reported^{71,72}) and $\Delta_1 = \Delta_{cr}$. Experimentally, the splitting parameters are deduced from the energies of the A, B, and C free excitons, which have nonlinear dependences⁷³ on the various splittings. An early study of Dingle *et al.* found $\Delta_{cr} = 22$ meV and $\Delta_{so} = 11$ meV.¹⁹ A recent and detailed analysis by Gil *et al.* yielded the values $\Delta_{cr} = 10$ meV and $\Delta_{so} = 18$ meV,²⁶ although Chuang and Chang rederived $\Delta_{cr} = 16$ meV and $\Delta_{so} = 12$ meV from the same data using a more precise description of strain variations of the valence band-edge energies.⁷⁴ Reynolds *et al.* obtained $\Delta_{cr} = 25$ meV and $\Delta_{so} = 17$ meV from a fit to exciton data.³⁸ Using similar approaches, Δ_{cr}/Δ_{so} values of 22 meV/15 meV were obtained by Shikanai *et al.*,³¹ 37.5 meV/12 meV by Chen *et al.*,²⁷ 9 meV/20 meV by Korona *et al.*,⁷⁵ and 9–13 meV/17–18 meV by Campo *et al.*,^{76,77} while the values 10 meV/17 meV were determined by both Yamaguchi *et al.*⁷¹ and Edwards *et al.*⁷⁸ Finally, a recent detailed experimental investigation by Rodina *et al.*³⁵ found one of the smallest reported crystal-field splittings to date, $\Delta_{cr} = 9$ meV, along with $\Delta_{so} \approx 18$ meV. One *ab initio* theoretical calculation⁷⁹ derived a spin-orbit splitting of 13 meV that agrees well with the experimental data, although the same calculation apparently overestimated the crystal-field splitting (42 meV). Other first-principles studies have also been reported.^{51,74,80–82} Since the latest experiments seem to converge on the splittings $\Delta_{cr} \approx 10$ meV and $\Delta_{so} \approx 17$ meV, we recommend those values.

While early work suggested $0.8m_0$ for the effective mass of holes in GaN,^{1,83,84} consideration of the acceptor binding energies led Orton⁸⁵ to suggest a much smaller value of $0.4m_0$. Salvador *et al.* obtained an even smaller mass of $0.3m_0$ from a fit to PL spectra.⁴³ On the other hand, the absorption measurements of Im *et al.* yielded a rather heavy m_h of $2.2m_0$.³⁰ Merz *et al.*²⁸ obtained an isotropically averaged heavy-hole bare mass of $0.54m_0$ from luminescence data. Those authors also pointed out that the polaron correction for heavy holes in GaN is nearly 13%. Fits of the exciton binding energies yielded hole masses in the range 0.9–1.2 m_0 ,^{33,86} while Kasic *et al.*⁶³ obtained 1.4 m_0 for *p*-doped GaN from an infrared ellipsometric study. A nonparabolic heavy-hole dispersion was reported by Shields *et al.*,⁸⁷ with masses in the 0.75–1.8 m_0 range. A bare heavy-hole mass of $0.52m_0$ was deduced from fits to experimental exciton-luminescence data by Chtchekine *et al.*³⁴ Perhaps the most detailed such study to date was by Rodina *et al.*,³⁵ whose fits produced bare and dressed hole masses in both directions for excitons associated with all three valence bands.

From the theoretical viewpoint, the six hole masses are readily expressible in terms of the first six *A* parameters, which may then be input to a detailed band structure calculation.^{53,88} In the quasicubic approximation, those parameters may also be recast in terms of the Luttinger param-

eters that are familiar from treatments of zinc-blende materials.⁷⁰ On the other hand, it must be emphasized that the actual valence band structure of a wurtzite nitride semiconductor is strongly non-parabolic due to the small spin-orbit and crystal-field splittings. Fits of the data to more detailed band structure calculations have produced a number of candidate *A* parameters in the literature.^{27,51,53,74,80–82} We recommend the parameter set proposed by Ren *et al.*,⁸⁰ who derived the value of 93.7 meV Å (note the unit error in the original article) for the inversion parameter *A*₇. That parameter breaks the light-hole and crystal-hole spin degeneracies in the in-plane direction. However, the reader must be cautioned that using *A* parameters from Ren *et al.*⁸⁰ carries with it the employment of their values for the spin-orbit and crystal-field splittings (21.1 and 10.8 meV, respectively), which deviate from the recommended values derived from the best experimental evidence as discussed above. Unfortunately, a more consistent set of valence-band parameters is not available at present, since that would require the availability of another *ab initio* pseudopotential calculation. Note also that whereas the experiments tend to be more sensitive to the band splittings (Δ_{so} and Δ_{cr}) than to the hole effective masses, the calculated valence band structure (even in the immediate vicinity of the Γ point) is affected significantly by the values chosen for Δ_{so} , Δ_{cr} , and all seven *A* parameters.

This sensitivity is illustrated in Fig. 2(a) and 2(b), in which the noticeable wurtzite GaN spin splitting parameterized via the *A*₇ parameter⁸⁰ is shown. Figure 2(a) was derived using the splittings and *A* parameters from Ren *et al.*,⁸⁰ while Fig. 2(b) shows the results of using the *A* parameters from that reference combined with our recommended values for the spin-orbit and crystal-field splittings. It does not appear possible to straightforwardly modify the *A* parameters so as to recover a band structure resembling Fig. 2(a) (but with the corrected values of the splitting energies). We therefore anticipate a later refinement of our suggested *A* parameter sets, following a more rigorous reparameterization using pseudopotentials or some other detailed approach.

Six distinct valence-band deformation potentials, in addition to the strain tensor and the overall hydrostatic deformation potential, are necessary to describe the band structure of GaN under strain. In the cubic approximation, these can be re-expressed in terms of the more familiar *a*_v, *b*, and *d* potentials.⁷⁰ Christensen and Gorczyca⁴⁷ reported a hydrostatic deformation potential *a* = −7.8 eV, which agrees well with a fit to the data of Gil *et al.* (−8.16 eV).²⁶ A somewhat lower value of *a* = −6.9 eV was derived from an *ab initio* calculation by Kim *et al.*⁸⁹ The hydrostatic potential is in fact anisotropic owing to the reduced symmetry of the wurtzite crystal. A recent calculation⁹⁰ yielded values of −4.09 and −8.87 eV for the two hydrostatic interband deformation potentials. Fits to mobility data implied conduction-band deformation potentials approaching −9 eV.^{91,92} Shan *et al.*⁹³ reported *a*₁ = −6.5 eV and *a*₂ = −11.8 eV for the two hydrostatic interband components. Other experimental studies obtained *a*₁ = −3.1 eV with *a*₂ = −11.2 eV⁹⁴ and *a*₁ = −5.22 eV with *a*₂ = −10.8 eV.⁹⁵ Our recommended set (*a*₁ = −4.9 eV and *a*₂ = −11.3 eV) represents an average of all the measured values.

Numerous sets of valence-band deformation potentials have been derived from both first-principles calculations^{74,88,96–98} and fits to experimental data.^{26,31,71,93–95,99,100} There are considerable discrepancies between the reported data, and further work is needed to resolve which results are the most accurate. We form our composite set of deformation potentials by averaging the most widely quoted results: $D_1 = -3.7$ eV, $D_2 = 4.5$ eV, $D_3 = 8.2$ eV, $D_4 = -4.1$ eV, $D_5 = -4.0$ eV, and $D_6 = -5.5$ eV (which satisfy the quasi-cubic approximation⁷⁴).

Elastic constants for wurtzite GaN have been obtained from a number of experiments^{101–106} and calculations.^{89,90,107–110} Overall, theory agrees best with the data of Polian *et al.*,¹⁰² who obtained the recommended values: $C_{11} = 390$ GPa, $C_{12} = 145$ GPa, $C_{13} = 106$ GPa, $C_{33} = 398$ GPa, and $C_{44} = 105$ GPa. However, the various experiments disagree to a considerable extent, and the topic remains controversial.

The piezoelectric coefficients for GaN are also somewhat controversial. Bykhovki *et al.* attempted to derive e_{31} and e_{33} from the e_{14} coefficient in zinc-blende GaN, obtaining values of $e_{31} = -0.22$ C/m² and $e_{33} = 0.43$ C/m².¹¹¹ Studies of polycrystalline GaN on zinc-blende Si and single-crystal GaN on wurtzite SiC by Guy *et al.*^{112,113} produced the results $d_{33} = 2.6$ pm/V and $d_{33} = 3.7$ pm/V, respectively. Measurements by Lueng *et al.* yielded a thin-film value (on an AlN buffer) of $d_{33} = 3.1$ pm/V.^{114,115} Since there was no way to independently determine d_{13} from those experiments, the relation $d_{13} = -d_{33}/2$ was used. A calculation of Shimada *et al.* yielded $e_{31} = -0.32$ C/m² and $e_{33} = 0.63$ C/m²,¹⁰⁷ and Bernardini *et al.* derived $e_{31} = -0.49$ C/m² and $e_{33} = 0.73$ C/m² from first principles.¹¹⁶ A recent theoretical work by Bernardini and Fiorentini¹¹⁷ discussed the reliability of the experimental results, and proposed values of $d_{33} = 2.7$ pm/V and $d_{13} = -1.4$ pm/V. Our recommended coefficients are intermediate between the most reliable theoretical and experimental values: $d_{33} = 3.1$ pm/V and $d_{13} = -1.6$ pm/V. Based on recent measurements¹¹⁸ and calculations¹¹⁷ of the shear piezoelectric coefficient, we recommend $d_{15} = 3.1$ pm/V.

Several first-principles calculations of the spontaneous polarization P_{sp} in GaN have derived very different values, ranging from -0.034 to -0.074 C/m².^{116,119–121} On the other hand, only differences in the spontaneous polarization are important in heterostructure band calculations. We recommend $P_{sp}(\text{GaN}) = -0.034$ C/m², although a full discussion is deferred until the AlN section.

A complete listing of the recommended band structure parameters for wurtzite GaN is compiled in Table I.

2. Zinc-blende GaN

A number of theoretical and experimental studies have determined energy gaps for zinc-blende GaN,^{42,122–130} some of which relied on explicit comparisons with the better-understood case of wurtzite GaN. The most accurate experiments appear to be those based on low-temperature luminescence measurements of the free-exciton peak,^{131–133} which is estimated to be 26.5 meV below the energy gap. While low-temperature gaps ranging from 3.2 to 3.5 eV have been mea-

TABLE I. Recommended band structure parameters for wurtzite nitride binaries.

Parameters	GaN	AlN	InN
a_{lc} (Å) at $T = 300$ K	3.189	3.112	3.545
c_{lc} (Å) at $T = 300$ K	5.185	4.982	5.703
E_g (eV)	3.510	6.25	0.78
α (meV/K)	0.909	1.799	0.245
β (K)	830	1462	624
Δ_{cr} (eV)	0.010	-0.169	0.040
Δ_{so} (eV)	0.017	0.019	0.005
m_e^{\parallel}	0.20	0.32	0.07
m_e^{\perp}	0.20	0.30	0.07
A_1	-7.21	-3.86	-8.21
A_2	-0.44	-0.25	-0.68
A_3	6.68	3.58	7.57
A_4	-3.46	-1.32	-5.23
A_5	-3.40	-1.47	-5.11
A_6	-4.90	-1.64	-5.96
A_7 (eV Å)	0.0937	0	0
a_1 (eV)	-4.9	-3.4	-3.5
a_2 (eV)	-11.3	-11.8	-3.5
D_1 (eV)	-3.7	-17.1	-3.7
D_2 (eV)	4.5	7.9	4.5
D_3 (eV)	8.2	8.8	8.2
D_4 (eV)	-4.1	-3.9	-4.1
D_5 (eV)	-4.0	-3.4	-4.0
D_6 (eV)	-5.5	-3.4	-5.5
c_{11} (GPa)	390	396	223
c_{12} (GPa)	145	137	115
c_{13} (GPa)	106	108	92
c_{33} (GPa)	398	373	224
c_{44} (GPa)	105	116	48
d_{13} (pm/V)	-1.6	-2.1	-3.5
d_{33} (pm/V)	3.1	5.4	7.6
d_{15} (pm/V)	3.1	3.6	5.5
P_{sp} (C/m ²)	-0.034	-0.090	-0.042

sured, the most reliable tend to fall approximately midway, between 3.29 and 3.35 eV.^{124,126,127} We recommend using the average value of the luminescence results, $E_g(T=0) = 3.299$ eV. The temperature dependence of the energy gap was studied in detail by Ramirez-Flores *et al.*¹²⁷ and Petalas *et al.*⁴² While both found $\beta = 600$ K (using the more reliable model 1 in Ref. 42), the α parameters differed so we recommend the average value of 0.593 meV/K. Although the indirect-gap energies have not been measured, a recent calculation of Fan *et al.* puts the X -valley and L -valley minima at 1.19 and 2.26 eV above the Γ valley, respectively.¹²⁸ Ramirez-Flores *et al.* measured the spin-orbit splitting in zinc-blende GaN to be 17 meV.¹²⁷

Electron spin resonance measurements on zinc-blende GaN determined an electron effective mass of $0.15m_0$.¹³⁴ Since this appears to be the only experimental result, and is similar to the Γ -valley masses derived from first-principles calculations by Chow *et al.*¹³⁵ and Fan *et al.*,¹²⁸ we adopt it as our recommendation. Effective masses of $m_l^* = 0.5m_0$ and $m_t^* = 0.3m_0$ were recently calculated for the X valleys in GaN,¹²⁹ which are similar to the theoretical results of Fan *et al.*¹²⁸ These values are recommended.

Although the hole effective masses in zinc-blende GaN have apparently not been measured, a number of theoretical sets of Luttinger parameters are available.^{128–138} The

TABLE II. Recommended band structure parameters for zinc-blende nitride binaries.

Parameters	GaN	AlN	InN
a_{lc} (Å) at $T=300$ K	4.50	4.38	4.98
E_g^Γ (eV)	3.299	5.4	0.78
$\alpha(\Gamma)$ (meV/K)	0.593	0.593	0.245
$\beta(\Gamma)$ (K)	600	600	624
E_g^X (eV)	4.52	4.9	2.51
$\alpha(X)$ (K)	0.593	0.593	0.245
$\beta(X)$ (meV/K)	600	600	624
E_g^L (eV)	5.59	9.3	5.82
$\alpha(L)$ (meV/K)	0.593	0.593	0.245
$\beta(L)$ (K)	600	600	624
Δ_{so} (eV)	0.017	0.019	0.005
m_e^* (Γ)	0.15	0.25	0.07
m_l^* (X)	0.5	0.53	0.48
m_t^* (X)	0.3	0.31	0.27
γ_1	2.70	1.92	3.72
γ_2	0.76	0.47	1.26
γ_3	1.11	0.85	1.63
m_{so}^*	0.29	0.47	0.3
E_p (eV)	25.0	27.1	17.2
F	-0.95	-1.01	-4.36
VBO (eV)	-2.64	-3.44	-2.34
a_c (eV)	-6.71	-4.5	-2.65
a_v (eV)	-0.69	-4.9	-0.7
b (eV)	-2.0	-1.7	-1.2
d (eV)	-3.7	-5.5	-9.3
c_{11} (GPa)	293	304	187
c_{12} (GPa)	159	160	125
c_{44} (GPa)	155	193	86

recommended values are based on averages of the heavy-hole and light-hole masses along [001], as well as the degree of anisotropy $\gamma_3 - \gamma_2$. This results in the parameter set: $\gamma_1 = 2.70$, $\gamma_2 = 0.76$, and $\gamma_3 = 1.11$. Averaging all the reported split-off masses^{128–130,138,139} leads to $m_{so}^* = 0.29m_0$.

An average of the two theoretical values for E_p in zinc-blende GaN^{130,139} yields $E_p = 25.0$ eV, which in turn implies $F = -0.95$. Caution is advised, since these values have not been verified experimentally.

Since various calculations put the hydrostatic deformation potential for zinc-blende GaN in the range -6.4 to -8.5 eV,^{47,79,128,129,135,140} we choose the average of $a = -7.4$ eV. The same procedure yields the recommendation of $b = -2.0$ eV (the full range is -1.6 to -3.6 eV). We adopt the Wei and Zunger¹⁴¹ value of $a_v = -0.69$ eV (-0.69 to -13.6 eV range) for the valence-band deformation potential, since it is consistent with the expectation that most of the strain shift should occur in the conduction band. The recommendation $d = -3.7$ eV is an average of the published results from Ohtoshi *et al.*,¹⁴⁰ Van de Walle and Neugebauer,¹⁴² and Binggeli *et al.*¹⁴³ No experimental confirmations of any of these deformation potentials for zinc-blende GaN appear to exist. Elastic constants of $C_{11} = 293$ GPa, $C_{12} = 159$ GPa, and $C_{44} = 155$ GPa are taken from the theoretical analysis of Wright.¹⁰⁷ Very similar sets were calculated by Kim *et al.*,¹⁴⁴ and Bechstedt *et al.*¹¹⁹

The recommended band structure parameters for zinc-blende GaN are compiled in Table II.

C. AlN

AlN is the endpoint of the AlGaN alloy, which is technologically important because it is a key ingredient in most nitride quantum wells. Experimental studies of AlN have focused almost exclusively on the wurtzite phase.

1. Wurtzite AlN

Wurtzite AlN is the only technologically significant Al-containing III–V semiconductor compound with a direct energy gap, and it in fact has the largest gap of any material still commonly considered to be a semiconductor. The absorption measurements of Yim *et al.*¹⁴⁵ and Perry and Rutz¹⁴⁶ indicated that the energy gap in wurtzite AlN varies from 6.28 eV at 5 K to 6.2 eV at room temperature. Varshni parameters of $\alpha = 1.799$ meV/K and $\beta = 1462$ K were reported by Guo and Yoshida, who also found the low-temperature gap to be 6.13 eV.¹⁴⁷ Vispute *et al.* reported a similar energy gap.¹⁴⁸ Tang *et al.* resolved what they believed to be the free or shallow-impurity-bound exciton in their cathodoluminescence data, at an energy of 6.11 eV at 300 K.¹⁴⁹ Wethkamp *et al.* used spectroscopic ellipsometry to determine that the energy gap varies from 6.20 eV at 120 K to 6.13 eV at 300 K.¹⁵⁰ Brunner *et al.* reported a variation from 6.19 eV at 7 K to 6.13 eV at 300 K.⁴⁶ Kuokstis *et al.* resolved a low-temperature free-exciton transition at 6.07 eV.¹⁵¹ Guo *et al.* reported the temperature dependence of the reflectance spectra, but fitted it to the Bose–Einstein expression.¹⁵² We recommend an intermediate value of 6.23 eV for the low-temperature bandgap, in conjunction with the Varshni parameters of Guo and Yoshida.¹⁴⁷ Although Brunner *et al.*⁴⁶ also reported Varshni parameters, their finding of no significant differences from GaN for the entire AlGaN alloy composition range may indicate that those results are somewhat less reliable.

The crystal-field splitting in AlN is believed to be negative, which implies that the topmost valence band is the crystal hole. Various calculations have yielded $\Delta_{cr} = -58$ meV by Suzuki *et al.*,⁵³ $\Delta_{cr} = -217$ meV by Wei and Zunger,⁷⁹ $\Delta_{cr} = -176$ meV by Shimada *et al.*,¹⁰⁸ $\Delta_{cr} = -244$ meV by Wagner and Bechstedt,⁹⁰ $\Delta_{cr} = -104$ meV and -169 meV from first-principles and semiempirical pseudopotential calculations, respectively, by Pugh *et al.*,¹³⁰ and $\Delta_{cr} = -215$ meV by Kim *et al.*⁸² Averaging all of the available theoretical crystal-field splittings, we obtain our recommended value of $\Delta_{cr} = -169$ meV. Spin-orbit splittings ranging from 11 (Ref. 130) to 20 meV⁵³ have been cited in the literature. We adopt the value of 19 meV suggested by Wei and Zunger.⁷⁹ Again, it is important to emphasize that our recommendations for the crystal-field and spin-orbit splittings in AlN are only provisional because little or no experimental data exist.

A number of studies have calculated the AlN electron effective mass,^{53,82,130,153,154} which is predicted to have greater anisotropy than in wurtzite GaN.⁵³ The recommended bare mass values of $m_e^\perp = 0.30m_0$ and $m_e^\parallel = 0.32m_0$ are obtained by averaging the available theoretical masses, although it is again noted that experimental studies are needed to verify the calculations. A number of theoretical sets of valence-band parameters are available.^{53,74,81,82} An apparent

disagreement in the signs for A_5 and A_6 is in fact irrelevant, since only absolute values of those parameters enter the Hamiltonian.^{82,130} We recommend the A parameters given by Kim *et al.*,⁸² since their crystal-field and spin-orbit splittings are closest to the ones recommended in this review.

The hydrostatic deformation potential for wurtzite AlN is believed to lie between -7.1 eV and -9.5 eV,^{47,89} which is consistent with the observation that the band gap pressure coefficients for AlGaIn alloys have little dependence on composition.¹⁵⁵ Our recommended set ($a_1 = -3.4$ eV and $a_2 = -11.8$ meV) is taken from the recent work of Wagner and Bechstedt.⁹⁰ Theoretical values are also available for a few of the valence-band deformation potentials ($D_3 = 9.6$ eV, $D_4 = -4.8$ eV).⁸⁹ We recommend the complete set presented by Shimada *et al.*: $D_1 = -17.1$ eV, $D_2 = 7.9$ eV, $D_3 = 8.8$ eV, $D_4 = -3.9$ eV, $D_5 = -3.4$ eV, and $D_6 = -3.4$ eV, with the last value derived using the quasicubic approximation.

The elastic constants for wurtzite AlN were measured by Tsubouchi *et al.*,¹⁵⁶ McNeil *et al.*,¹⁵⁷ and Deger *et al.*¹⁰⁶ Theoretical results are also available.^{82,108,110,158–160} We recommend the values $C_{11} = 396$ GPa, $C_{12} = 137$ GPa, $C_{13} = 108$ GPa, $C_{33} = 373$ GPa, and $C_{44} = 116$ GPa suggested by Wright, who provides a detailed discussion of their expected accuracy.¹⁰⁷

Several early piezoelectric coefficients^{161,162} for AlN are summarized in Ref. 113. The result $d_{33} = 5.6$ pm/V obtained in that reference is in reasonable agreement with the previous determinations. Lueng *et al.*¹¹⁵ measured $d_{33} = 5.1$ pm/V. Although these experiments found only d_{33} , both d_{33} and d_{13} can be calculated from first principles.^{108,116,117,163,164} We recommend the recent theoretical values of Bernardini and Fiorentini: $d_{33} = 5.4$ pm/V and $d_{13} = -2.1$ pm/V,¹¹⁷ although the elastic coefficients given in that reference are somewhat larger than the values we recommend. Based on recent measurements^{118,162} and a calculation¹¹⁷ of the shear piezoelectric coefficient, we recommend $d_{15} = 3.6$ pm/V.

The difference between the GaN and AlN spontaneous polarizations strongly influences the band profiles and energy levels in GaN/AlN quantum heterostructures. Although rigorous calculations^{116,119–121} of the spontaneous polarization P_{sp} (AlN) have produced results spanning a fairly broad range, from -0.09 to -0.12 C/m², values for the difference P_{sp} (AlN)– P_{sp} (GaN) have tended to be more consistent, with most falling between 0.046 and 0.056 C/m². Experimentally, for some time the majority of workers on the GaN/AlGaIn system reported somewhat smaller P_{sp} (AlN)– P_{sp} (GaN). For example, Leroux *et al.*^{165,166} derived $-0.051 < P_{sp} < -0.036$ C/m² for AlN. A study of the charging of GaN/AlGaIn field-effect transistors led to a similar conclusion,¹⁶⁷ and Hogg *et al.* were able to fit their luminescence data by assuming negligible spontaneous polarization.¹⁶⁸ Park and Chuang¹⁶⁹ required $P_{sp} = -0.040$ C/m² to reproduce their GaN/AlGaIn quantum-well data. On the other hand, Cingolani *et al.*¹⁷⁰ reported good agreement with experiment using a higher value derived from the original Bernardini *et al.*¹¹⁶ calculation.

A significant step toward resolving this discrepancy has been the recent realization that the AlGaIn spontaneous po-

larization cannot be linearly interpolated between the values at the binary endpoints.^{171,172} In combination with an improved nonlinear-strain treatment of the piezoelectric effect, the discrepancy between theory and experiment for GaN/AlGaIn quantum wells has been largely eliminated.¹²⁰ We adopt $P_{sp} = -0.090$ C/m² as the recommended value for AlN, in conjunction with P_{sp} (GaN) = -0.034 C/m².

The recommended band structure parameters for wurtzite AlN are compiled in Table I.

2. Zinc-blende AlN

Since very few successful growths of zinc-blende AlN have been reported,^{173,174} our recommended parameter set must rely primarily on theoretical projections. The only quantitative experimental study of the band gap is Ref. 174, which deduced a Γ -valley gap of 5.34 eV at room temperature, although it was also concluded that the lowest gap is indirect. Assuming the same Varshni parameters as for zinc-blende GaN, we obtain a low-temperature gap of 5.4 eV. Values of 4.9 and 9.3 eV are recommended for the X- and L-valley gaps, respectively.^{47,128,130} The spin-orbit splitting should be nearly the same as in wurtzite AlN (19 meV).^{79,82,138,175} Averaging theoretical results from a number of different sources,^{82,128,130,137,139} we obtain a recommended Γ -valley effective mass of $0.25m_0$. The longitudinal and transverse masses for the X valley are predicted to be $0.53m_0$ and $0.31m_0$, respectively.¹²⁸ The same procedure employed for GaN yields recommended Luttinger parameters of $\gamma_1 = 1.92$, $\gamma_2 = 0.47$, and $\gamma_3 = 0.85$ ($m_{so} = 0.47m_0$).^{82,128,130,137,139} The recommended momentum matrix element is an average of the reported values.^{130,139} $E_P = 27.1$ eV ($F = -1.01$). Hydrostatic deformation potentials of -9.0 (Ref. 47) and -9.8 eV¹²⁸ have been reported. For the deformation potentials, we recommend $a = -9.4$ eV, $a_v = -4.9$ eV,^{79,128} $b = -1.7$ eV,^{128,142,143} and $d = -5.5$ eV.^{89,142,143} The adopted elastic constants of $C_{11} = 304$ GPa, $C_{12} = 160$ GPa, and $C_{44} = 193$ GPa, from the calculations of Wright,¹⁰⁷ are similar to the sets quoted in other theoretical works.^{119,144,176}

The recommended band structure parameters for zinc-blende AlN are compiled in Table II.

D. InN

Although InN is rarely, if ever, used in devices in its binary form, when alloyed with GaN it forms a core constituent of the blue diode laser.¹¹ For that reason, and especially since some degree of segregation commonly occurs when the GaInN alloy is grown, it is important to understand the properties of bulk InN in its wurtzite phase.

1. Wurtzite InN

Early absorption studies on sputtered thin films concluded that the InN band gap is in the 1.7 – 2.2 eV range.^{177–181} Those polycrystalline or nanocrystalline thin films typically had high electron densities and low mobilities. From a subsequent investigation of epitaxially grown wurtzite InN, Guo and Yoshida¹⁴⁷ measured low-temperature and room-temperature gaps of 1.994 and 1.97 eV, respectively, along with Varshni parameters of $\alpha = 0.245$ meV/K

and $\beta = 624$ K. However, recent advances in the epitaxial growth of single-crystal InN have brought about a dramatic re-evaluation of the fundamental energy gap in this compound.^{182–185} Absorption, photoluminescence, and photoluminescence excitation experiments indicate that the bandgap is actually in the 0.7–0.8 eV range. In an interesting exchange, Nag¹⁸⁶ pointed out that this gap is unusually low in the context of trends exhibited by other semiconductor materials, whereas Davydov *et al.*¹⁸⁷ emphasized the definitive nature of the experiments determining the low value. We recommend a zero-temperature gap of 0.78 eV,¹⁸⁴ although there is one report of a value as low as 0.65 eV.¹⁸⁸ For lack of better information, we continue to recommend the Varshni parameters of Guo and Yoshida¹⁴⁷ until a careful temperature-dependent study of the newer high-quality InN becomes available.

Estimates for the crystal-field splitting in wurtzite InN range from 17 to 301 meV.^{51,79,130} We recommend a provisional value of 40 meV. Based on calculated spin-orbit splittings varying from 1 to 13 meV,^{79,130} we recommend $\Delta_{so} = 5$ meV.

Several measurements of the electron effective mass in InN produced values of $0.11m_0$,¹⁷⁹ $0.12m_0$,¹⁸⁹ and $0.14m_0$,¹⁹⁰ as well as $0.24m_0$ for the mass perpendicular to the *c* axis.¹⁹¹ The result of Kasic *et al.*¹⁹⁰ closely matches at least one theoretical projection.⁴⁹ However, the recent realization that the InN band gap is narrower than previously thought prompted a re-examination of the effective-mass issue.¹⁹² Accounting for the substantial nonparabolicity that can cause an overestimate of the mass in highly doped samples leads to a band-edge effective mass of $0.07m_0$, which is our recommended value. Valence-band mass parameters were calculated by Yeo *et al.*⁵¹ using the empirical pseudopotential method, and also by Pugh *et al.*¹³⁰ and Dugdale *et al.*⁸¹ using essentially the same technique. The results of the first two studies are quite similar, and we recommend the parameters derived by Pugh *et al.*¹³⁰ However, it should be pointed out that the lower InN energy gap may require a downward revision of the light-hole mass.

Christensen and Gorczyca predicted a hydrostatic deformation potential of -4.1 eV for wurtzite InN,⁴⁷ although a smaller value of -2.8 eV was calculated by Kim *et al.*⁸⁹ We recommend the average of the two: $a = -3.5$ eV. Since, there have been no calculations of the valence-band deformation potentials, we recommend appropriating the set specified above for GaN. While elastic constants were measured by Sheleg and Savastenko,¹⁰¹ we recommend the improved set of Wright:¹⁰⁷ $C_{11} = 223$ GPa, $C_{12} = 115$ GPa, $C_{13} = 92$ GPa, $C_{33} = 224$ GPa, and $C_{44} = 48$ GPa. Alternative sets calculated by Kim *et al.*⁸⁹ and Davydov¹¹⁰ are also available. Since the piezoelectric coefficients in InN have apparently not been measured, we recommend the theoretical values of Bernardini and Fiorentini:¹¹⁷ $d_{33} = 7.6$ pm/V, $d_{13} = -3.5$ pm/V, and $d_{15} = 5.5$ pm/V. Even though the spontaneous polarization data for GaN/GaInN structures are inconclusive at this point, most likely owing to material imperfections, the recommended value $P_{sp}(\text{InN}) = -0.042$ C/m² is consistent with the most thorough comparison of experiment and theory.¹²⁰

Recommended band structure parameters for wurtzite InN are compiled in Table I.

2. Zinc-blende InN

Although the growth of zinc-blende InN has been reported,¹⁹³ only theoretical estimates of its band parameters are available. It is projected to have a direct band alignment, with Γ -, *X*-, and *L*-valley gaps of 1.94, 2.51, and 5.82 eV, respectively.¹²⁹ However, since that calculation was performed before the true energy gap of wurtzite InN was known, we recommend revising the Γ -valley gap to be 0.78 eV. Spin-orbit splittings in the range 3–13 meV have been projected,^{79,138,175} from which 5 meV is recommended. We recommend an electron effective mass identical to that in wurtzite InN, $0.07m_0$, which is lower than the calculated values of 0.10 – $0.14m_0$ ^{129,130,139} owing to the reduction in the energy gap. The longitudinal and transverse masses for the *X* valley are predicted to be $0.48m_0$ and $0.27m_0$, respectively.¹²⁹ The recommended Luttinger parameter set ($\gamma_1 = 3.72$, $\gamma_2 = 1.26$, and $\gamma_3 = 1.63$) is derived from Pugh *et al.*,¹³⁰ and the split-off mass is chosen to be $m_{so}^* = 0.3m_0$.^{129,130} For the E_P parameter we recommend the value given by Meney *et al.*,¹³⁹ since the alternative value of Pugh *et al.*¹³⁰ implies too large a value for *F*. The resulting recommended parameter set is $E_P = 17.2$ eV and $F = -4.36$. For the hydrostatic deformation potential, we recommend an average value of -3.35 eV from the theoretical^{47,89,129} range of -2.2 to -4.85 eV. The recommended valence-band deformation potentials are a composite from the calculations of Wei and Zunger,⁷⁹ Kim *et al.*,⁸⁹ Tadjer *et al.*¹²⁹ and Van de Walle and Neugebauer:¹⁴² $a_v = -0.7$ eV, $b = -1.2$ eV, and $d = -9.3$ eV. Elastic constants of $C_{11} = 187$ GPa, $C_{12} = 125$ GPa, and $C_{44} = 86$ GPa are adopted from the calculations of Wright,¹⁰⁷ which are similar to other calculated sets.^{119,144}

The recommended band structure parameters for zinc-blende InN are compiled in Table II.

E. Alloys

1. GaInN

GaInN quantum wells represent a key constituent in the active regions of blue diode lasers and LEDs.¹¹ The reliability of early determinations of the energy-gap bowing parameter for GaInN must now be questioned in light of the considerable overestimate of the InN gap (see Sec. II D). Further complications resulted from the frequent occurrence of chemical ordering and (partial) phase decomposition effects,¹⁹⁴ with clustering of In-rich regions.¹⁹⁵ However, recent work has produced considerable progress toward a fundamental understanding of the $\text{Ga}_{1-x}\text{In}_x\text{N}$ energy gap.

A fit to the early data of Osamura *et al.*¹⁷⁷ yielded a bowing parameter *C* of ≈ 1.0 eV. That result was consistent with the theories of Wright and Nelson,¹⁹⁶ Kassali and Bouarissa,¹⁹⁷ Brandt *et al.*,¹⁹⁸ (performed for the zinc-blende form of GaInN), Goano *et al.*,⁶⁹ Ferhat *et al.*^{199,200} (for wurtzite GaInN), and other early calculations.^{201,202} For low In compositions, Nakamura found that this bowing parameter produced a good fit to PL data.²⁰³ A slightly larger

bowing was obtained by Li *et al.*,²⁰⁴ on the basis of PL from GaInN/GaN superlattices. A similar value of 1.4 eV was reported for zinc-blende GaInN, although that study employed relatively thin GaInN layers in which the strain was not fully relaxed.²⁰⁵ Bellaiche and Zunger²⁰⁶ established that a large apparent reduction in the GaInN band gap could result from the effects of short-range atomic ordering. Strain and ordering effects were also considered by Wright *et al.*²⁰⁷

A number of later works cast doubt on the picture of a small bowing parameter in GaInN alloys. For example, the experimental band gap results of McCluskey *et al.* for $\text{Ga}_{1-x}\text{In}_x\text{N}$ epilayers with $x < 0.12$ implied a bowing as large as 3.5 eV.²⁰⁸ First-principles calculations by the same authors indicated that the bowing parameter itself may be a strong function of composition, at least for small In fractions. Kent *et al.* also calculated a strong variation of C with x , and additionally determined that epitaxial layers may have a slightly smaller valence band offset than bulk materials.²⁰⁹ Similarly large bowings (in the range 2.4–4.5 eV) were reported by a large number of subsequent studies.^{210–227} PL emission consistent with fairly strong bowing was also found in an investigation of zinc-blende GaInN.²²⁸ All of these works focused on $\text{Ga}_{1-x}\text{In}_x\text{N}$ with In fractions less than 20%. However, after noticing a weak temperature dependence of the alloy PL peak, as well as a Stokes shift between the PL and photoreflectance lines, Shan *et al.*²¹² suggested that the PL may in fact be emitted primarily from material that is locally In-rich. Such ordering would naturally lead to an overestimate of the bowing parameter. Teles *et al.*²²⁹ argued that smaller bowing is appropriate once corrections are made for the lattice constant and clustering. Bellaiche *et al.*²³⁰ suggested the interesting possibility that “clustering-like” electronic effects may be produced without any actual chemical clustering, due to localization of the hole wave functions on the In sites. Stepanov *et al.*²³¹ noted that much of the scatter in the bowing parameter would be removed (to obtain $C = 2.1\text{--}2.4$ eV) were the same value of Poisson’s ratio used in all of the studies.

Naturally, since the earlier band gap data for In-rich $\text{Ga}_{1-x}\text{In}_x\text{N}$ are no longer credible, many of these conclusions must be re-evaluated. The recent growth of high-quality epitaxial samples with large x has considerably broadened the compositional range over which the bowing could be determined reliably.^{188,232} Wu *et al.*²³² attributes a strong downward shift of the PL peak energy with respect to the absorption band edge to emission primarily from localized In-rich regions. Based on their work we recommend $C = 1.4$ eV, which is also consistent with many of the theoretical estimates discussed above. The same energy-gap bowing parameter is recommended for both wurtzite and zinc-blende GaInN.

Very little information is available on the other band parameters for GaInN. Tight-binding calculations⁴⁹ provide some support for our recommended standard procedure¹⁰ of using the band-gap bowing parameter to derive the compositional variation of the electron effective mass, and then interpolating the rest of the quantities linearly. Effective-mass parameters for Ga-rich alloys were compiled by Pugh *et al.*²³³ For the X-valley gap in zinc-blende GaInN, a small

TABLE III. Nonzero bowing parameters for GaInN, AlGaIn, and AlInN.

Parameters	GaInN	AlGaIn	AlInN
E_g^Γ (eV)	1.4	0.7	2.5
E_g^X (eV)	0.69	0.61	0.61
E_g^L (eV)	1.84	0.80	0.80
P_{sp} (C/m ²)	−0.037	−0.021	−0.070

bowing of $C = 0.38$ eV was estimated from first principles.⁴⁹ Another calculation gave bowing parameters of 0.69 and 1.84 eV for the X-valley and L-valley gaps, respectively. On the basis of calculations as a function of composition,^{234,235} we take the piezoelectric coefficients for wurtzite GaInN to be unbowed. We recommend a bowing parameter of $C(P_{sp}) = -0.037$ C/m² for the spontaneous polarization in the alloy, in order to be consistent with a recent detailed comparison of theory and experiment.¹²⁰

The recommended nonzero bowing parameters for GaInN are summarized in Table III.

2. AlGaIn

AlGaIn is often used as the barrier material for nitride electronic and optoelectronic devices. Initial studies of the compositional dependence of the energy gap reported downward²³⁶ as well as upward^{237,238} bowing. Subsequent early PL²³⁹ and absorption²⁴⁰ measurements found a bowing parameter of +1.0 eV, which has often been used in band structure calculations. Since then, many studies of materials fabricated under a variety of growth conditions have been published. A good review of the results up to 1999 was presented by Lee *et al.*,²⁴¹ who divided the previous works into three general classes. They noted that the early findings of an upward bowing^{237,238} have generally not been duplicated (with the somewhat inconclusive exception of Ref. 242). The second class of materials, which were grown at high temperatures, generally exhibited a strong downward bowing of at least +1.3 eV.^{46,243–248} Often those results could not be fit with a continuous, parabolic curve, since they tended to jump to stronger bowing as the Al fraction increased.²⁴¹ It was proposed that the apparent observation of the strong bowing was actually an artifact resulting from defect- or impurity-related transitions at energies below the bandgap.²⁴⁹ Lee *et al.*²⁴¹ further suggested that only samples fabricated by first growing a GaN buffer on sapphire at low temperature, followed by high-temperature growth of the alloy layer, may be expected to yield reliable energy gaps.^{210,250–254} Residual anomalies for materials of the third class were attributed to incomplete strain relaxation. Based on these considerations, Lee *et al.* recommended the bowing parameter $C = 0.6$ eV.²⁴¹

Since then, there have been many other reports of energy gaps in $\text{Al}_x\text{Ga}_{1-x}\text{N}$. Ochalski *et al.*²⁵⁵ observed no detectable bowing for $x < 0.3$ (this work falls broadly into the third class of Lee *et al.*). A wider range of Al compositions was considered by Shan *et al.*,²⁵⁶ who deduced a bowing of +1.33 eV for alloy layers grown on AlN buffers. Meyer *et al.*²⁵⁷ reported $C = 0.7$ eV for material that again falls into the third class as defined above. A similar value of C

$=0.8$ eV was reported by Omnes *et al.*²⁵⁸ Bergman *et al.* obtained $C=1.2$ eV, and reported no evidence for x -dependent local band gap variations induced by chemical ordering.²⁵⁹ Cathodoluminescence, absorption, and reflectance measurements of epitaxial AlGaIn grown on Si(111) suggested $C=1.5$ eV.^{260–262} Ebling *et al.*²⁶³ found a large bowing parameter in AlGaIn with partial chemical ordering. Other materials representing the third class were recently investigated by Jiang *et al.*²⁶⁴ ($C=0.53$ eV), Wagner *et al.*²⁶⁵ ($C\approx 1$ eV), Zhou *et al.*²⁶⁶ ($C=0.85$ eV), Katz *et al.*²⁶⁷ ($C=1.38$ eV), and Yun *et al.*²⁶⁸ ($C=1.0$ eV). Paduano *et al.*²⁶⁹ ($C=0.70$ eV) suggested that the data are reliable only when a specific sequence of buffer layers (giving narrow x-ray diffraction features) is employed, and special efforts are taken to compensate for the strain dependence of the energy gap. Besides their own, they assigned two other studies^{241,257} to that category. Finally, there exists one report of weak bowing in zinc-blende AlGaIn with a relatively small Al fraction.²⁷⁰

Most theories project that the Γ valley in zinc-blende AlGaIn should have a small downward bowing ($C=0.05$ – 0.53 eV),^{128,196,271} except for the early work of Albanesi *et al.*²⁷² ($C=-0.4$ eV). The bowing parameters calculated for wurtzite AlGaIn fall in a similar range: 0.61 eV,²⁷³ 0.353 eV,²⁷⁴ and ≈ 0 eV.^{69,275} Based on the consistent finding of a relatively small bowing parameter by the theories, as well as by some of the most authoritative experiments, we recommend $C=0.7$ eV for both the wurtzite and zinc-blende forms of AlGaIn.

Recommended values for the X -valley (0.61 eV) and L -valley (0.80 eV) bowing parameters are taken from the empirical pseudopotential method calculations of Fan *et al.*¹²⁸ Some of the effective mass parameters for zinc-blende²⁷¹ and wurtzite²³³ AlGaIn have been calculated, but no experimental verification exists. A bowing of $C(P_{\text{sp}})=-0.021$ C/m² for the spontaneous polarization is consistent with a recent detailed comparison of theory and experiment.¹²⁰

The recommended non-zero bowing parameters for GaInN are summarized in Table III.

3. AlInN

$\text{Al}_x\text{In}_{1-x}\text{N}$ is drawing increasing attention, because at $x=0.83$ it becomes lattice-matched to GaN. The band gap bowing derived from the first experimental study of sputtered AlInN was so strong that it yielded a smaller energy gap for the lattice-matched alloy than for GaN.²⁷⁶ The standard quadratic expression did not provide a reasonable fit to the compositional variation, and it is now known that the gap for the InN binary significantly exceeded the appropriate value for single-crystalline material. Guo *et al.*²⁷⁷ presented results for InN-rich AlInN, and similarly measured an incorrect gap in the InN limit. From an investigation of the opposite limit of Al-rich alloys, Kim *et al.* found consistency with a downward bowing of at least 2.5 eV.²⁷⁸ While Peng *et al.* gave a cubic expression for the energy gap that fit results spanning the entire range of compositions,²⁷⁹ that result cannot be used in its original form since it overestimates the InN gap. Furthermore, the strong bowing implied by their mea-

surements, and also those of Yamaguchi *et al.*,^{280,281} may be artifacts of polycrystallinity and clustering, by analogy to the effects discussed in the section on GaInN alloys. For $\text{Al}_{0.32}\text{In}_{0.68}\text{N}$ Shubina *et al.*²⁸² reported a substantially higher band gap of 2.74 eV, which implies a slight upward bowing in combination with our recommended binary endpoint values. Finally, Lukitsch *et al.*²⁸³ reported strong downward bowing over a wide range of compositions, although the energy gap for InN was again too high. While the general trend is toward large C (3 – 4 eV), in view of the results for the other nitrides we conclude that the available experimental literature for AlInN may not yet provide a reliable bowing parameter.

On the theoretical side, a first-principles calculation for zinc-blende AlInN yielded a bowing parameter of 2.53 eV, which was assumed to be equal to that in the wurtzite alloy.²⁸⁴ A more recent result for cubic AlInN is 1.32 eV for the direct-gap and -0.51 eV for the indirect (Γ – X) transition.²⁸⁵ A calculation for wurtzite AlInN produced a similar bowing of 2.38 eV,⁶⁹ while other values from the literature are 1.32 eV²²⁹ and 2.20 – 4.67 eV.²⁰⁰ Unfortunately, none of those theories derived an InN energy gap as small as our recommended value. Therefore, we provisionally recommend a bowing parameter of 2.5 eV for both wurtzite and zinc-blende AlInN, and note that the uncertainty is considerably larger than for the related GaInN and AlGaIn alloys. To be consistent with a recent detailed comparison of theory and experiment,¹²⁰ we recommend a spontaneous-polarization bowing of $C(P_{\text{sp}})=-0.070$ C/m².

The recommended non-zero bowing parameters for AlInN are summarized in Table III.

4. AlGaInN

Energy gaps have also been reported for AlGaInN with rather small In fractions.^{280,286–288} Recent results indicate a nearly linear bandgap reduction when $\text{In} < 2\%$.²⁸⁹ The cut-off wavelengths of AlGaInN (lattice matched to GaN) ultraviolet photodetectors are also generally consistent with a linear interpolation.²⁹⁰ A linear variation with In concentration is therefore recommended for this quaternary with dilute In, since in view of the small parameter space studied to date it is too early to suggest any more detailed relation.

F. Band offsets

Even after strain effects are factored out, there is no *a priori* reason to expect the wurtzite and zinc-blende versions of any given nitride heterojunction to have the same band offsets. In fact, in all cases the offset of either the conduction or the valence band *must* differ somewhat, because the wurtzite and zinc-blende energy gaps are not identical. The calculations of Murayama and Nakayama²⁹¹ and Wei and Zunger,⁷⁹ which did not account for spontaneous polarization effects, found rather small differences. These results are supported by the experimental work of Lu *et al.*,²⁹² which derived a conduction band offset of 0.3 eV between zinc-blende and wurtzite GaN with a marginal type-II alignment of the conduction and valence bands in the two forms of the material [valence band offset (VBO) ≈ -0.09 eV]. However,

Bernardini and Fiorentini²⁹³ suggest that once the large electrostatic fields are included, even defining the band offset for a wurtzite system's polar interface [our discussion is confined to the (0001) orientation] becomes nontrivial.

Because there are fewer ambiguities, we first briefly examine the theoretical band offsets for zinc-blende GaN/AlN heterojunctions. Numerous calculations have yielded unstrained offsets (under the assumption of full lattice relaxation) ranging from 0.25 to 1.0 eV,^{79,121,143,294–303} with only a weak dependence on the interface's orientation axis.^{297,301} Since most of the results lie within the fairly narrow range of 0.75–0.85 eV, we recommend the value 0.8 eV. By convention, a positive offset corresponds to AlN having the lower valence-band maximum.

In the more complex wurtzite heterostructure, the electrostatic potential takes on a characteristic sawtooth profile owing to the macroscopic polarization and corresponding interface charges.^{293,304} One additional complication is that the GaN/AlN and AlN/GaN cases are inequivalent,³⁰⁵ meaning that the two must be specified separately.^{293,304} A number of first-principles calculations found offsets in the rather narrow 0.7–0.8 eV range, although polarization and strain effects were not accounted for consistently.^{79,296,301,305} From a detailed treatment of the strain-induced asymmetry at the (0001) polar heterojunction, Bernardini and Fiorentini obtained 0.2 eV for AlN/GaN and 0.85 eV for GaN/AlN.²⁹³

On the experimental side, the valence-band discontinuity at the GaN/AlN interface was first probed by Sitar *et al.*,¹²⁴ who obtained 1.4 eV from fits to optical measurements on GaN/AlN superlattices. Subsequently, Baur *et al.* extracted a VBO of 0.5 eV from the difference between iron acceptor levels in each material.³⁰⁶ A fit to the PL spectrum of GaN/AlGaIn quantum wells was consistent with a VBO of ≈ 0.9 eV.⁴³ A more recent fit by Nam *et al.*³⁰⁷ implied ≈ 0.8 eV, and much the same value was obtained from deep-acceptor level emission data.³⁰⁸ X-ray photoemission spectroscopy yielded a VBO of 0.8 ± 0.3 eV at the wurtzite GaN/AlN junction,³⁰⁹ which was revised to 0.70 ± 0.24 eV in a later article by the same authors.³¹⁰ Using the same approach, Waldrop and Grant found a considerably different value of 1.36 ± 0.07 eV.³¹¹ A related study reported a nearly linear VBO variation in the AlGaIn alloy, with a positive bowing parameter of 0.59 eV.³¹² Using X-ray and ultraviolet photoelectron spectroscopy, King *et al.* found that the GaN/AlN VBO ranged from 0.5 to 0.8 eV, depending on the growth temperature.³¹³ They surmised that the differences arose from strain, defects, and film stoichiometry effects. Rizzi *et al.*³¹⁴ reported a VBO in the 0.15–0.4 eV range for relaxed heterojunctions, and pointed out that the Ga 3*d* core level, which has been used as a reference in GaN, is in fact hybridized with other valence bands. Overall, in consideration of the numerous pitfalls that can plague the experimental investigations, we do not find a compelling reason to doubt the soundness of the theoretical evaluation by Bernardini and Fiorentini.²⁹³

Several theoretical works have studied the valence band offset at the important InN/GaN interface.^{79,142,297,298,302,303,315} Most obtain a relatively small unstrained VBO of 0.26–0.3 eV for the zinc-blende version

of the interface,^{79,142} and 0.48 eV for wurtzite.⁷⁹ Whereas the macroscopic polarization effects are smaller for this junction, they may alter the value suggested in Ref. 79. On the other hand, the x-ray photoemission spectroscopy measurements of Martin *et al.* found a large VBO of 1.05 eV,³¹⁰ and optical measurements on GaInN/GaN quantum wells were also consistent with a large value.³¹⁶ Martin *et al.*³¹⁰ employed corrections for the piezoelectric fields, and found no significant deviation from the transitivity rule when measurements of the VBO at the InN/AlN heterojunction were included. Although the value of the bandgap in InN was recently re-evaluated, we expect most of the difference to appear in the energy of the conduction band rather than the valence band. We therefore recommend a VBO of 0.3 eV for the zinc-blende InN/GaN interface and 0.5 eV for the wurtzite interface. In the wurtzite case, we recommend the same value for both InN/GaN and GaN/InN, since at present there is no compelling evidence for a significant difference. Assuming transitivity, this implies a VBO of 0.5 eV for the zinc-blende version of the InN/AlN heterointerface. We note that all three zinc-blende interfaces exhibit a type-I alignment. The matter is more complicated for the wurtzite form of the InN/AlN junction, with likely growth-sequence asymmetries arising from the very different spontaneous polarizations in the two materials. The resolution of this issue awaits further studies.

The band offsets for zinc-blende nitrides can be related tentatively to those of the non-nitride III–V compounds as collected in our earlier review.¹⁰ In this context, we consider the VBO to be an intrinsic property of a given zinc-blende semiconductor, since interface dipole contributions tend to be small and transitivity is generally a good assumption. Divergent measurements of the GaAs/GaN VBO have been reported in the literature. Martin *et al.*³¹⁷ obtained a GaAs/GaN conduction-band offset of 0.9 eV from the current–voltage characteristic of an *n*-type structure with a thin GaN barrier. The energy gap difference of ≈ 1.8 eV then implies a VBO of 0.9 eV. Similar measurements on *n*-type and *p*-type devices were carried out by Huang *et al.*,³¹⁸ who derived an approximate VBO of 0.5 eV. It is difficult to estimate the influence of the large GaAs/GaN lattice mismatch on those results. On the other hand, Ding *et al.*³¹⁹ obtained a VBO of 1.84 ± 0.1 eV from x-ray photoemission spectroscopy, which implies a nearly vanishing conduction-band discontinuity. We recommend this last result, which agrees reasonably well with the recent theoretical estimates of Wei and Zunger³¹⁵ and Agrawal *et al.*³²⁰ Employing -0.80 eV for the VBO of GaAs relative to the valence-band maximum of InSb,¹⁰ we obtain absolute offsets of -2.64 , -3.44 , and -2.34 eV for zinc-blende GaN, AlN, and InN, respectively. On the other hand, for wurtzite nitride heterointerfaces it is less clear that the VBO can be treated analogously as a bulk parameter.

At present, all of our band-offset recommendations should be considered provisional. Especially in the cases of interfaces involving InN, future developments may significantly alter the accepted values. Recommended absolute valence band offsets (relative to InSb) for the three zinc-blende binary nitrides are collected in Table II, and recommended asymmetric wurtzite offsets are listed in Table IV. For lack of other information, we ignore any bowing of the band

TABLE IV. Recommended valence-band offsets (including strain and polarization effects) for the binary wurtzite interface combinations. A positive VBO corresponds to a higher valence band maximum in the first material than in the second.

Heterojunction	VBO (eV)
AlN/GaN (0001)	-0.20
GaN/AlN (0001)	0.85
InN/GaN (0001)	0.50
GaN/InN (0001)	-0.50

offsets for the nitride alloys. The results are presented in a graphic form in Fig. 4.

III. "DILUTE" NITRIDE BAND PARAMETERS

A. Methodology

We do *not* recommend that the type of bowing discussed above in Sec. II A be used to describe the "dilute" nitride alloys, in which a small N fraction on the order of a few percent is added to a conventional III-V semiconductor such as GaAs, GaInAs, or GaP (an exception is the linear interpolation of lattice constants between the host material and zinc-blende GaN or GaInN). A single bowing parameter is in general inadequate even if the goal is only to describe the energy gap for a relatively wide range of compositions.³²¹ Here the main interest is in materials incorporating only a few percent nitrogen,³²² since it is highly questionable whether more than 10%–16% N can be incorporated stably. It is by now well established that the properties of the conduction band in these materials (a few % N usually has little effect on the valence bands) can be parameterized in terms of the band anticrossing model.³²³ While this two-parameter model can be cast formally in terms of the many-impurity Anderson model within the coherent potential approximation, it can also be thought of simply as the interaction between a single, spatially localized N level and the conduction

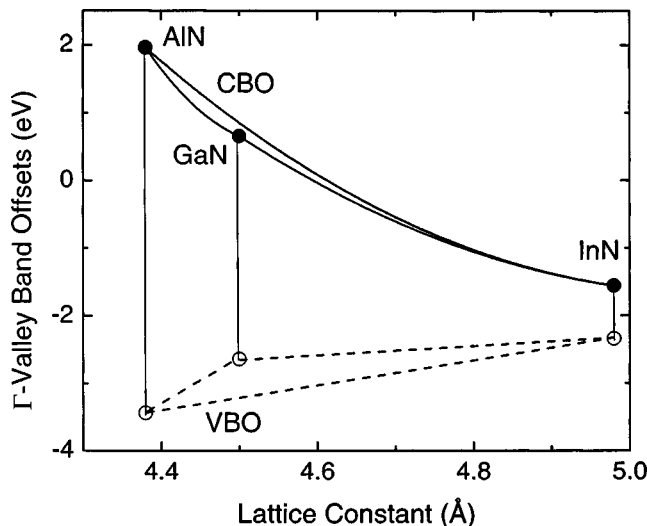


FIG. 4. Conduction (filled) and valence (open) band offsets for the binary and ternary zinc-blende nitrides as a function of lattice constant. The conduction (valence) band offset between any two materials corresponds to their energy difference on the absolute scale of the figure.

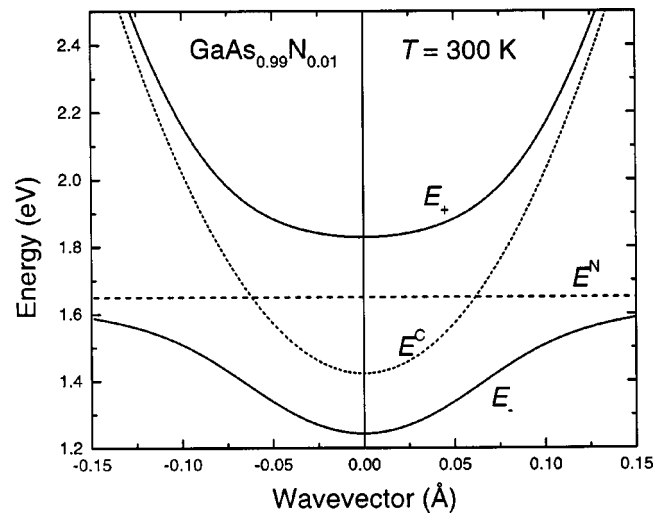


FIG. 5. Conduction-band dispersion relations for $\text{GaAs}_{0.99}\text{N}_{0.01}$ at 300 K from the BAC model (solid curves). For comparison, the unperturbed GaAs conduction band and the position of the nitrogen level are shown as the dotted and dashed curves, respectively.

band of the underlying non-nitride semiconductor. However, the recent derivation by Lindsay *et al.*³²⁴ points out that identical fundamental bandgap predictions may be obtained even if the interaction involves a weighted average of perturbed upper states rather than a single N level.

If the effect on the valence bands is completely neglected, the BAC model yields the following dispersion relations for the two coupled bands:

$$E_{\pm}(k) = \frac{1}{2} \{ [E^C(k) + E^N] \pm \sqrt{[E^C(k) - E^N]^2 + 4V^2x} \}, \quad (3)$$

where $E^C(k)$ is the conduction-band dispersion of the unperturbed non-nitride semiconductor, E^N is the position of the nitrogen isoelectronic impurity level in that semiconductor, V is the interaction potential between the two bands, and x is the N fraction. Dispersion relations for the two coupled conduction bands in $\text{GaAs}_{0.99}\text{N}_{0.01}$, with the characteristic anticrossing, are plotted in Fig. 5. Note that any temperature dependence arises from the shift of the conduction-band dispersion $E^C(k)$, which is assumed to follow the Varshni formula of Eq. (1), whereas E^N is taken to be independent of T . One consequence is a considerable weakening of the fundamental energy gap's variation with temperature, e.g., if we compare GaAsN to GaAs.³²⁵ Another is that the deformation potential theory must be applied carefully, with a view to the much weaker shift of E^N with applied pressure. Therefore, the strain dependence of the E_{\pm} transitions should be determined by substituting the appropriate deformation parameters of the host semiconductor to obtain $E^C(k)$, and then deriving $E_{\pm}(k)$ from Eq. (3) or an even more detailed $\mathbf{k} \cdot \mathbf{p}$ formalism. We suggest that elastic constants of the host material should be used, although there is no data to prefer this procedure over the alternative of linearly interpolating between the host and zinc-blende GaN.

We can straightforwardly extend the BAC model to treat ten bands (spin-doubled conduction, valence, and nitrogen impurity bands) by modifying the 8-band $\mathbf{k} \cdot \mathbf{p}$ theory.^{326–329}

Coupling of the nitrogen band to the X and L valleys may also be introduced.^{330,331} While adding further parameters can in principle afford greater flexibility in fitting the data, at this juncture we think it preferable to avoid complicating the simple two-parameter fit of Eq. (3). Note also that the fixed position of the nitrogen level with respect to vacuum implies a tandem shift with the valence band maximum of the host III–V material. If viewed as a single level, one then need specify only its alignment with respect to some well-characterized energy. However, in order to account for the experimental observation of small yet non-negligible deviations from referencing to the valence band offset, we will specify a separate nitrogen level for each host material.

It will be seen below that Eq. (3) provides a useful and reliable basis for describing a variety of dilute-nitride material properties, such as the fundamental energy gap (governed by the transition from E_- to the top of the valence band), the temperature shift of the gap, the electron effective mass, and the characteristics of the upper band E_+ (within the theory of Lindsay *et al.*,³²⁴ there is not necessarily a single well-defined E_+ band). However, the extent to which the BAC representation may be considered fundamentally realistic is still controversial at this writing.^{332,333} The BAC model does not consider anything more complicated than a single nitrogen level on a substitutional lattice site (or a narrow impurity band formed from such levels). It neglects not only mixing with the L and X valleys, but also more complex nitrogen behavior in the semiconductor matrix, e.g., the formation of nitrogen pairs and clusters. On the other hand, the more complicated modeling based on pseudopotentials^{334–336} requires a substantial computational effort. The numerical results are then difficult to use without parameterization into a form such as Eq. (3). The very recent work by Lindsay *et al.*³²⁴ points out that the most amply verified prediction of the BAC model, the dependence of the band gap on the N content, may be unaffected by generalizing to a multiplicity of higher-lying states.

The implementation of Eq. (3) requires input of the host semiconductor's band parameters. Although we do not reproduce the non-nitride parameters in this work in order to preserve space, all of the required values are tabulated in our earlier review.¹⁰ We recommend that in all cases, the valence band offset for an unstrained dilute nitride should be set equal to that of the host semiconductor. Within the BAC model the primary effects of the nitrogen are on the conduction band, and even the ten-band model influences the hole dispersion relations without shifting the valence band maximum in the absence of strain or quantum confinement. Although some experimental studies have reported a finite type-I or type-II offset in strained structures (see the next subsection on GaAsN), at present there is no evidence compelling enough to alter our recommendation of a null offset relative to the host in the absence of strain.

B. GaAsN

It has long been known that small quantities of nitrogen in GaAs and GaP form deep-level impurities.³³⁷ However, only recently has the growth of $\text{GaAs}_{1-x}\text{N}_x$ alloys with ap-

preciable ($\approx 1\%$ or more) N fractions been reported.^{338,339} (Reports³⁴⁰ of the incorporation of small amounts of As into GaN are uncommon).

PL measurements of GaAsN with N fractions up to 1.5% were used to extract the dependence of the energy gap on composition.³⁴¹ A huge bowing of 18 eV was found, which for small compositions is equivalent to a linear model with that slope.³⁴² Early theoretical studies projected bandgap bowings based primarily on calculations for large N fractions.^{206,343–350} Although the large bowing was originally expected to produce a semimetallic overlap at intermediate compositions,³⁴⁵ more detailed studies found a reduction of the bowing parameter with increasing composition.^{347,348} This result was confirmed by the experiments of Bi and Tu, who studied N compositions as large as 15%.³⁵¹

Subsequent investigations confirmed a highly nonlinear reduction in the energy gap for small N compositions.^{352–358} Another notable finding was a significant weakening of the temperature and pressure dependences of the band gap for GaAsN (and GaInAsN with small In fraction).^{355,359,360} It became clear that the simple bowing approximation could not adequately describe the GaAsN alloy in its full complexity, which motivated Shan *et al.* to propose the band-anticrossing model.³⁶¹ Those authors confirmed a weak pressure dependence for the nitrogen-band transitions (with a deduced deformation potential of -1.2 eV), although the density-functional calculation of Jones *et al.* also predicted a reduced pressure dependence without invoking the BAC model.^{362,363}

Also favoring the BAC parameterization was the finding, by Skierbiszewski *et al.* and other workers, of a significantly increased electron mass in GaInAsN.^{364–369} Note, however, that another set of measurements by Young *et al.*³⁷⁰ found a reduction in the effective mass with increasing N content, in apparent conflict with the BAC model, which predicts an increase even at the zone center. The temperature dependence of the band gap was confirmed to be substantially weaker in GaAsN than in GaAs, as predicted by the BAC model,^{325,371} and an electroreflectance study³⁷² resolved both the E_- and E_+ transitions (see the typical conduction-band structure in Fig. 5). A band gap reduction was also observed in nitrogen-implanted $\text{Al}_{0.27}\text{Ga}_{0.73}\text{As}$ samples.³⁷³ The transition between “doped” and “alloyed” materials was studied by Zhang *et al.*,^{374,375} who observed evidence for impurity banding at N concentrations as small as 0.1% N, and also by Klar *et al.*,³⁷⁶ who put the transition at 0.2%. Zhang *et al.* proposed an alternative (non-BAC) parameterization of the energy gap.³⁷⁷

Figure 6 plots the fundamental band gap, between the valence band maximum and the E_- conduction band minimum, as a function of N fraction x for $\text{GaAs}_{1-x}\text{N}_x$ at 300 K. A curve with a constant bowing parameter of 18 eV (dotted), and also a curve with the variable bowing parameter of $(20.4 - 100x)$ eV suggested in our earlier review¹⁰ (dashed) are displayed for comparison. It can be seen that the BAC model predicts a substantially higher energy gap once the N fraction exceeds 1.5%. The available experimental data (points in Fig. 6), which were compiled in Ref. 323 clearly show much better agreement with the BAC parameterization

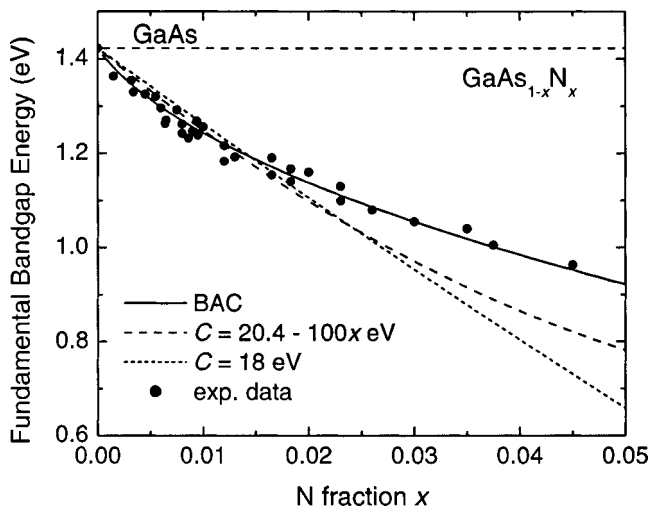


FIG. 6. Energy of the fundamental band gap transition in GaAsN as a function of nitrogen fraction x (a) from the BAC model (solid curve), (b) using the variable bowing parameter from our earlier review (Ref. 10) (dashed curve), and (c) using a constant bowing parameter (dotted curve). For comparison, the available experimental data as compiled in Ref. 323 is also plotted (circles).

than with either of the two curves based on bowing.

So far, no upper limit on the N compositions for which the BAC model remains valid has been identified. Moreover, since $\text{GaAs}_{1-x}\text{N}_x$ alloys with $x > 5\%$ become increasingly difficult to grow, such compositions may be expected to have only minor technological significance.³²² Although there is some spread in the reported values for the two primary parameters E^N (1.65–1.71 eV, referenced to the GaAs valence-band maximum) and V (2.3–2.7 eV), we follow the parameterization of Shan and co-workers and recommend: $E^N = 1.65$ eV, $V = 2.7$ eV.³⁶¹

Although the conventional BAC model assumes that the addition of N has little effect on the valence bands, two recent studies noted a larger-than-expected heavy/light-hole splitting in GaAsN with a few percent nitrogen.^{378,379} This implies a strong bowing in the valence-band shear deformation potential b , although the deformation-potential enhancements obtained by the two works did not agree. Additional study is necessary to confirm the effect, and perhaps reformulate the basic band structure model to account for it.

The nature and magnitude of the GaAs/GaAsN heterojunction's band alignment represents an interesting and technologically important question. Although a straightforward interpretation of the BAC model implies that the GaAsN conduction band minimum must lie below that in GaAs, it is

less clear whether the valence band maximum in GaAsN should exhibit any relative shift. Theoretical studies of that issue have come to differing conclusions.^{343,350} X-ray photoelectron spectroscopy data suggested a type-II band alignment,³⁸⁰ with quite large error bars on the VBO. While subsequent PL measurements found a similar result,³⁸¹ more recent optical and electrical characterizations have pointed decisively toward a type-I alignment.^{382–385} Unfortunately, it appears that the built-in strain was not (completely) relaxed in any of the heterostructures employed in the above studies. Accounting for strain effects, Egorov *et al.*³⁸⁴ deduced that the band offset for unstrained $\text{GaAs}_{0.98}\text{N}_{0.02}$ with respect to GaAs approximately vanishes. This is our general recommendation for dilute GaAsN.

The recommended BAC model parameters for GaAsN and all of the other dilute nitrides for which information is available are summarized in Table V.

C. InAsN

InAsN attracted some early theoretical interest,^{343,386} and a more recent tight-binding calculation focused on the effects of nitrogen clustering in the alloy.³⁸⁷ Several experimental investigations of this dilute nitride have been published.^{388–392}

Two measurements of the electron effective mass in InAsN showed a large increase,^{391,392} analogous to that in GaInAsN.³⁶⁴ The authors of those studies^{391,392} appeared to believe that the BAC model could not account for any increase greater than a doubling of the mass in the nitrogen-free host material. However, that view is contradicted by a closer examination of the model, and also by the results for GaInAsN,³⁶⁴ which clearly display a similarly large mass enhancement. Therefore, at this point there is no compelling reason not to accept the BAC parameterization for InAsN, although the available information is incomplete and future evidence may favor a different picture. Extracting the position of the nitrogen level (with respect to the valence-band maximum in InAs) from the valence-band offsets given in our earlier review, we recommend $E^N = 1.44$ eV. Based on the measurements of Naoi *et al.*,³⁸⁸ which are consistent with values for the potential V ranging between 1.9 and 2.3 eV, we recommend $V = 2.0$ eV.

D. GaInAsN

Having established provisional BAC parameters for $\text{GaAs}_{1-x}\text{N}_x$ and $\text{InAs}_{1-x}\text{N}_x$, it remains to specify them for the important $\text{Ga}_{1-y}\text{In}_y\text{As}_{1-x}\text{N}_x$ alloy. Most of the

TABLE V. Band anticrossing (BAC) model parameters for the dilute nitride semiconductors.

Parameters	E^N w. r. t. VBM (eV)	V (eV)
GaAsN	1.65	2.7
InAsN	1.44	2.0
$\text{Ga}_{1-x}\text{In}_x\text{AsN}$	$1.65(1-x) + 1.44x - 0.38x(1-x)$	$2.7(1-x) + 2.0x - 3.5x(1-x)$
GaPN	2.18	3.05
InPN	1.79	3.0
$\text{Ga}_{1-x}\text{In}_x\text{PN}$	$2.18(1-x) + 1.79x$	$3.05(1-x) + 3.0x - 3.3x(1-x)$
InSbN	0.65	3.0

technological interest in dilute nitrides has so far centered on this quaternary, since it provides a promising basis for long-wavelength telecommunications lasers, solar cells, and photovoltaics that can be grown on GaAs substrates rather than InP. Whereas conventional GaInAs quantum wells would have too much compressive strain to reach the desired wavelength range when grown on GaAs, the addition of N narrows the band gap for lower In concentrations, while at the same time providing tensile strain compensation.

The applicability of the BAC parameterization to the case of GaInAsN is well established.^{328,329,360,361,364,366} Since the main lines of evidence are analogous to those discussed above for GaAsN, we do not repeat them here. Studies that employed very low In compositions,^{360,361,364} on the order of 10%, generally found no significant differences from GaAsN apart from the expected decrease of the GaInAs energy gap (including bowing).¹⁰ However, for materials with larger In fractions, which have been grown on both GaAs^{393,394} and InP³⁹⁵ substrates, Zhukov *et al.*³⁹⁶ proposed an alternative parameterization. Pan *et al.*³⁶⁸ took E^N to be independent of the In concentration, and used $V=2.5$ eV. Although Choulis *et al.*^{328,329,397} employed the same assumption regarding E^N , their value for the coupling potential was considerably lower: $V=1.675$ eV. A similar value ($V=1.7$ eV) was independently deduced by Polimeni *et al.*³⁹⁴ for In compositions ranging from 25% to 41%. On the other hand, Sun *et al.*³⁹⁸ found that $V=2.8$ – 3.0 eV, depending on the particular transition between the conduction and valence subbands, was necessary to explain luminescence data for GaInAsN/GaAs quantum wells with an In content of 27.2%.

The finding of a smaller band gap reduction in GaInAsN than in GaAsN is in fact expected theoretically, due to ordering of the nitrogen atoms in the GaInAs matrix.^{399,400} There is some experimental evidence for carrier localization in the presence of both In and N in the quaternary alloy.^{401,402} One study⁴⁰² reported a series of five distinct transitions, which were attributed to five different environments for the N atom in the alloy. In order to incorporate the best available information on the GaInAsN quaternary, while maintaining consistency with the parameters recommended above for GaAsN and InAsN, we propose the following scheme. The position of the nitrogen band E^N should be determined from the shift of the valence-band offset in GaInAs,¹⁰ including the small, yet non-negligible bowing. This leads to a smooth variation of E^N , between 1.65 eV (GaAsN) and 1.44 eV (InAsN), and is also consistent with the intuitive expectation (so far not contradicted by any definitive experiments) that the nitrogen level's position should not vary with respect to vacuum. Then we propose a bowing of the coupling potential V in the $\text{Ga}_{1-y}\text{In}_y\text{AsN}$ alloy: $V=2.7(1-y)+2.0y-3.5y(1-y)$ eV. While this parameterization does not fully agree with the reported experimental results for the quaternary,^{328,329,360,361,364,368,394} it is roughly consistent with the median values, and it of course agrees with the recommended binary endpoints. As before, any strain must be added to the host-semiconductor properties in the basic BAC model before these parameters are employed.

E. GaAsSbN

Another quaternary alloy that has the potential for reaching long wavelengths on GaAs substrates is $\text{GaAs}_{1-x-y}\text{Sb}_y\text{N}_x$.^{403–405} Unfortunately, owing to the sparsity of the data for this material, and the complete lack of any reports on $\text{GaSb}_{1-x}\text{N}_x$, we can only recommend that the procedure recommended above for GaInAsN be followed. The exception is that constant $V=2.7$ eV (at least for Sb fractions $\leq 20\%$) should be assumed.

F. InPN

Two experimental studies of $\text{InP}_{1-x}\text{N}_x$ have been reported.^{406,407} Since GaAs and InP have similar energy gaps and valence-band offsets, it is natural to expect the BAC model to apply equally well to InPN. Yu *et al.*⁴⁰⁷ derived a parameterization in which the GaAs/InP VBO was assumed to be 0.35 eV. Since the consensus value recommended in our earlier review¹⁰ is 0.14 eV, for consistency we adjust the result $E^N=2.0$ eV from Yu *et al.* to the recommended value $E^N=1.79$ eV (both with respect to the valence-band maximum of InP). A rederivation of the coupling potential that is most consistent with the data of Yu *et al.*⁴⁰⁷ leads to our recommendation: $V=3.0$ eV.

G. InSbN

Since InSb is the III–V binary with the smallest energy gap, the addition of N may in principle be exploited to reach arbitrarily small band gaps and arbitrarily long emission wavelengths. Murdin *et al.*^{408–410} observed experimentally that the effective mass in $\text{InSb}_{1-x}\text{N}_x$ increases despite a considerable reduction of the band gap. Even though our simple rule for determining E^N based on the VBO would lead to an energy 0.85 eV above the top of the valence band, those authors derived $E^N=0.65$ eV, which we adopt as the recommended value. They also reported $V=2.2$ eV, and supplemented the minimal BAC parameterization of Eq. (3) with an additional shift of the nitrogen level's position with increasing N fraction.^{408,409} However, it appears that their value for V leads to an underestimate of the observed band gap decrease.⁴⁰⁸ We therefore recommend $V=3.0$ eV, which should yield better agreement with the sparse available data. We also recommend that the full ten-band $\mathbf{k}\cdot\mathbf{p}$ model be used for any calculations of the InSbN band structure, since the nitrogen band significantly affects the light-hole dispersion.

H. GaPN

$\text{GaP}_{1-x}\text{N}_x$ is distinct from the other dilute nitride semiconductors discussed in this review, in that the GaP host is an indirect-gap semiconductor with both X and L valleys lower in energy than the Γ point. Nitrogen acts as an isoelectronic impurity in GaP, and has been employed as the active material of visible LEDs.⁴¹¹ Initial studies of GaP with an alloy-like concentration of N were reported by Baillargeon *et al.*^{412,413} Miyoshi *et al.* explored the transition of the GaPN luminescence spectrum with increasing N fraction, and was able to resolve the emission from excitons bound to nitrogen pairs for $x<0.5\%$.⁴¹⁴ Bi and Tu reported $\text{GaP}_{1-x}\text{N}_x$

with x as large as 16% using gas-source molecular-beam epitaxy.⁴¹⁵ A number of theoretical works from the same period predicted that GaPN retains its indirect-gap nature up to relatively large (“nondilute”) N concentrations.^{343,348,350,416}

Shan and co-workers reexamined this view within the BAC model,^{417,418} which yields that the anticrossing between Γ -valley states and the N impurity band moves E_- below the X valley for arbitrarily small values of x . Those authors derived $V=3.05$ eV using the well-known value of $E^N=2.18$ eV (relative to the valence-band maximum, which places the nitrogen level slightly below the conduction X valley). The analogy with GaAsN is further supported by a decrease in the pressure dependence of the fundamental transition (with a deformation potential of -1.2 eV),⁴¹⁷ a reduction in its temperature dependence,^{419,420} a large increase in the electron effective mass,⁴²¹ and strong luminescence for small N fractions,^{422,423} all of which occur despite the indirect gap of the GaP host.

On the other hand, the simple BAC model is clearly incapable of describing the full complexity of such features as the evolution of transitions due to isolated N centers, N pairs, and N clusters that is observed for $x < 1\%$, as well as the mixing with X - and L -valley states.^{424–426} For example, Buyanova *et al.* observed an abrupt reduction in the fundamental transition’s radiative lifetime when $x > 0.5\%$, which was attributed to an effective indirect-to-direct crossover.⁴²⁷ It is perhaps more likely that the wealth of phenomena reported for GaPN can be explained within a more flexible theoretical framework, such as the supercell pseudopotential formulations of Kent and Zunger.^{333–335}

Although the predictive power of the BAC parameterization is perhaps more limited in GaPN than in the other dilute nitride alloys owing to the proximity of the X valley and the complex experimental observations at “intermediate” compositions, we nevertheless recommend the parameter set $E^N=2.18$ eV and $V=3.05$ eV of Shan *et al.*⁴¹⁷

I. GaInPN

One report of the energy gap in bulk $\text{Ga}_{0.46}\text{In}_{0.54}\text{PN}$ is available.⁴²⁸ That alloy represents a special case, in that we expect a close proximity of the nitrogen energy level and the host conduction band edge (within 10–20 meV, according to estimates based on the VBO dependence in GaInP).¹⁰ If we presume for the moment that the BAC parameterization remains valid in this limit, the reported energy gaps allow us to obtain a coupling potential in the 2.1–2.3 eV range. Since this is considerably smaller than the recommended values for both InPN and GaPN, by analogy with GaInAsN we postulate a bowing of the $\text{Ga}_{1-y}\text{In}_y\text{PN}$ interaction potential: $V=3.05(1-x)+3.0x-3.3x(1-x)$ eV. It is gratifying that the bowing parameters derived for the two quaternaries are quite similar, although clearly further studies are needed to confirm this provisional value.

IV. SUMMARY

We have reviewed the literature, and based on the available information offered recommended band structure parameters for all of the conventional and dilute nitride semi-

conductors that have been investigated to date. The present treatment is considerably updated, reworked, and expanded by comparison with the nitride portion of our earlier III–V semiconductor band parameter review.¹⁰ The breathtaking pace of ongoing research on these materials has necessitated what are in some cases major changes in the recommendations.

For some of the parameters, we believe that the ultimate convergence toward a consensus value is (nearly) complete. These include energy gaps for the wurtzite forms of GaN, AlN, and InN, as well as the zinc-blende form of GaN, the electron effective masses in all of these materials, and the magnitude of the energy gap reduction for GaAsN, GaInAsN, InPN, and GaPN as parameterized by the band anticrossing model. Agreement may be at hand for the spin-orbit and crystal-field splittings in these materials, as well as the bowing parameters for GaInN and AlGaIn. The understanding of piezoelectric coefficients and spontaneous polarizations in GaN, AlN, InN, and their alloys has reached a new plateau, although further research is needed to fully confirm the proposed values. A definitive GaN valence parameter set, which is fully consistent with the recommended consensus values for the spin-orbit and crystal-field splittings, also remains to be generated.

Areas which remain somewhat or highly uncertain at present include the band offsets for GaN, AlN, InN, and their alloys, the bandgap bowing parameter for AlInN, many or most of the zinc-blende GaN, AlN, and InN properties, deviations of the band offsets for the dilute nitrides from the host values, bowings of the coupling potentials for GaInAsN and GaInPN, X -valley and L -valley mixing effects in GaPN and related materials, and the accuracy of the BAC model’s effective-mass predictions when applied to the more exotic dilute nitrides. Our recommendations concerning those parameters should be considered provisional, awaiting more detailed and definitive experimental and theoretical evidence.

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