

Article Effects of Internal Relaxation of Biaxial Strain on Structural and Electronic Properties of In_{0.5}Al_{0.5}N Thin Film

Guanglei Zhang ^{1,2}, Guoqiang Qin ^{1,2,*} and Feipeng Zhang ³

- School of Materials Science and Engineering, Shijiazhuang Tiedao University, Shijiazhuang 050043, China; zhgl@stdu.edu.cn
- ² Hebei Provincial Engineering Research Center of Metamaterials and Micro-Device, Shijiazhuang 050043, China
- ³ Institute of Sciences, Henan University of Urban Construction, Pingdingshan 467036, China; zhfp@emails.bjut.edu.cn
- * Correspondence: qgq@stdu.edu.cn

Abstract: Ternary wurtzite $In_{0.5}Al_{0.5}N$ films and coatings are promising candidates for microelectronic or optoelectronic devices due to their excellent physical and chemical properties. However, as a universal and non-negligible phenomenon, in-plane strain and its effects on the structure and properties of $In_{0.5}Al_{0.5}N$ still need systematic research. In particular, the deformation mechanism of $In_{0.5}Al_{0.5}N$ under biaxial strain is not clearly understood currently. To reveal the role of the internal relaxation effect in lattice deformation, the lattice variation, thermal stability, and the electronic properties of ternary wurtzite compound $In_{0.5}Al_{0.5}N$ under different biaxial strains are systematically investigated, using first-principles calculations based on density functional theory. The results indicate that, compared with the classic elastic deformation mechanism with constrained atomic coordinates, atom relaxation results in a much smaller Poisson ratio. Moreover, the plastic relaxation $In_{0.5}Al_{0.5}N$ phase, generated by free atom relaxation, exhibits higher thermal stability than the elastic relaxation phase, so it is the most likely phase in reality when biaxial strain is imposed. Meanwhile, the biaxial strain has a remarkable influence on the electronic structure of $In_{0.5}Al_{0.5}N$ films, where a non-linear variety of energy band gaps can be seen between the valance band and conduction band.

Keywords: InAlN thin film; biaxial strain; electronic properties; internal relaxation

1. Introduction

Boron group elements and their nitrides, such as AlGaN and InGaN, have been extensively used in UV lasers, light-emitting diodes or high-electron-mobility transistors, and other fields [1–3], owing to their excellent physical and chemical properties, such as wide bandgap, superior luminous and quantum efficiency, as well as extraordinary resistance from high temperature, acid, alkali, and radiation. The wurtzite (WZ) compound $In_xAl_{1-x}N$, as a promising representative of these materials, has attracted extensive attention in recent years within the field because of its unique performance. For example, the adjustable bandgap with a wide range (0.7~6.2 eV) allows for the realization of emission and detection from ultraviolet to infrared in the wavelength range. Moreover, the refractive index makes it a suitable candidate for microelectronic or optoelectronic devices [4–6].

On the other hand, InAlN ternary alloy, instead of a conventional AlGaN barrier layer, is the best way to solve the problems caused by the strain of the barrier layer. In lattice-matched InAlN/GaN heterostructures, the InAlN barrier layer is in a strain-free state, which effectively eliminates the strain-related inverse piezoelectric effect and reliability problems. In fact, depending on the change of In composition, InAlN can form lattice-matched heterostructures of different channel materials, such as InAlN/AlGaN, InAlN/GaN and InAlN/InGaN, respectively, to meet different application requirements. Therefore, InAlN alloy materials bring more choices and degrees of freedom to the design of nitride-based



Citation: Zhang, G.; Qin, G.; Zhang, F. Effects of Internal Relaxation of Biaxial Strain on Structural and Electronic Properties of $In_{0.5}Al_{0.5}N$ Thin Film. *Coatings* 2022, 12, 598. https://doi.org/ 10.3390/coatings12050598

Academic Editors: Cecilia Mortalò, Valentina Zin, Silvia Maria Deambrosis and Alicia de Andrés

Received: 20 February 2022 Accepted: 27 April 2022 Published: 28 April 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). heterostructures and devices, provide opportunities for the further improvement of device performance, greatly expand the research scope, solve the device problems based on conventional AlGaN and InGaN ternary alloys, and can realize many theoretical predictions and expand the application space of nitride devices.

Compared with AlGaN, InGaN, or other Boron group element nitrides, it is more complex and challenging to obtain high-quality epitaxial thin films for $In_xAl_{1-x}N$, which is mainly due to the difference between two basic binary nitrides, i.e., AlN and InN. Specifically, the growth of AlN requires a high temperature and low III-V element ratio, while low temperature and high III-V ratio are needed for the growth of InN [7]. In addition, the lattice constant mismatch of AlN and InN in *a* and *c* are 12.3% and 13.5%, respectively, thereafter introducing tremendous strain in epitaxial $In_x Al_{1-x}N$ film. The biaxial strain is also quite universal in these thin films, and it is essential to determine the physical properties of such materials. Until now, considerable efforts have been made to address this issue, for example, introducing an AlN intermediate layer at the $In_xAl_{1-x}N/GaN$ interface [8]. However, the mechanism between biaxial strain and physical properties is not clear for $In_xAl_{1-x}N$ thin films so far, especially WZ $In_xAl_{1-x}N$. Fortunately, our previous study showed that internal relaxation plays a crucial role in the deformation of crystalline materials under biaxial strain [9]. In this study, the effects of strain on the geometry structure, stability, electronic structure, and other physical properties of this nitride are systematically investigated by applying the in-plane strains on WZ In0.5Al_{0.5}N within the framework of the first-principles analyzing method.

2. Modeling and Computational Details

The equilibrium phase of AlN and InN is a wurtzite-type structure at room temperature and atmospheric pressure. The experimental values for a and c of the crystallographic cells are 3.112 Å (3.548 Å) and 4.982 Å (5.760 Å), respectively [10,11]. It has been proved that AlN and InN could form continuous compounds in the whole compositional range with the formula $In_xAl_{1-x}N$, deviating slightly from Vegard's rule [12]. In this study, the cell of $In_{0.5}Al_{0.5}N$ was set up by replacing half of the Al atoms in the cell model, as it can be reasonably chosen as a typical representative of $In_xAl_{1-x}N$ compounds.

In this work, the CASTEP coded package was employed for computation and analysis of the structural, mechanical, stability, and electronic properties of In_{0.5}Al_{0.5}N based on a plane wave basis, set within the density functional theory framework [13,14]. The lattice structure and atomic configuration of the initial $In_{0.5}Al_{0.5}N$ cell were optimized through a ground state energy calculation, using the Perdew–Burke–Ernzerhof function within the generalized gradient approximations (GGA) to describe the electron-electron exchange and correlation effects [15]. The ultrasoft pseudopotentials method was employed, in which the atomic core, as well as the near-core electrons, were treated as Coulomb cores, and the valance electrons are N ($2s^22p^3$), Al ($3s^23p^1$), and In ($5s^25p^1$), respectively [16]. During the computation, the cut-off energy and Brillouin zone k-point mesh of 1020 eV, $11 \times 11 \times 6$, 1090 eV, $12 \times 12 \times 6$, and 1190 eV, $11 \times 11 \times 6$ were used for the AlN, InN, and In_{0.5}Al_{0.5}N, respectively. It has been examined and proved to be reason enough for the convergence of the computation. The deviation in parameters from the experimental one is lower than 5%, so the whole calculation is reasonably reliable. The method used in this work to apply biaxial strain has been reported previously. Compared with the classic elastic deformation model with fixed atomic coordinates, the effects of internal relaxation on the structure and other physical properties of $In_{0.5}Al_{0.5}N$ are investigated in detail in this research. After the structural computation, the B3LYP hybrid function [17] was employed to compute the band structures and density of states. The cut-off energy and K-point meshes were 450 eV and 3 \times 3 \times 6, respectively. The obtained lattice parameters and elastic constants for these three nitrides are summarized in Table 1. The lattice parameters obtained in this work are in considerable agreement with the previously reported experimental and theoretical values [18]. The evident deviations between the results in this work and the

Name	Method	$a = b/\text{\AA}$	c/Å	C ₁₁ /GPa	C ₁₂ /GPa	<i>C</i> ₁₃ /GPa	C ₃₃ /GPa	C ₄₄ /GPa
AlN	Experimental [19]	3.112	4.982	396	137	108	373	116
	This work	3.126	5.002	428.8	93.2	64.1	418.3	125.0
	HSE [20]	3.103	4.970	410.2	142.4	110.1	385.0	122.9
InN	Experimental [21]	3.548	5.760	225	109	108	265	55
	This work	3.593	5.835	246.0	67.6	45.7	264.8	59.6
	HSE [20]	3.542	5.711	233.8	110.0	91	238.3	55.4
In _{0.5} Al _{0.5} N	This work Others	3.348 3.35 [18]	5.527 5.37 [18]	256.5 293 [<mark>22</mark>]	89.3 128.3 [22]	84.1 105.3 [22]	321.0 298.25 [22]	69.2 73.75 [22]

experimental and theoretical values reported in the literature originate from the settings of the exchange-correlation functional in the calculations.

Table 1. Lattice parameters and elastic constants of AlN, InN, and In_{0.5}Al_{0.5}N.

GGA functionals in this work are believed to provide a better overall description of the electronic subsystem than the classic local exchange-correlation functionals, which tend to overbind atoms, so that the bond lengths and the cell volume are usually underestimated by a few percent, and the bulk modulus is correspondingly overestimated. GGA corrects this error but may underbind instead, leading to slightly long bond lengths and deviations in the elastic constants. On the other hand, despite standard Kohn–Sham approaches, the Heyd–Scuseria–Ernzerhof (HSE) screened exchange hybrid functionals scheme offers a high degree of accuracy in lattice parameters and bulk moduli, for a wide range of semiconductors, but with an additional cost.

3. Results and Discussion

It is well recognized that the Poisson phenomenon is the effect that a solid-state tends to transfer the lattice deformation to other directions. Through this effect, the solid-state system will reduce the strain energy and make the lattice more stable. Figure 1 shows the out-of-plane strain ε_{zz} as a function of in-plane strain ε_{xx} of In_{0.5}Al_{0.5}N, where the out-of-plane strain ε_{zz} decreases linearly with the increase in in-plane strain ε_{xx} . The slope of the L2 line is the Poisson ratio (-0.5228), which can be obtained using the equation $\nu = -2C_{13}/C_{33}$ for this WZ type of symmetry, where ν denotes the Poisson ratio, and C_{13} and C_{33} are elastic constants (Table 1). It is worth noting that the slope of L1 is much smaller than that of L2, illustrating that internal relaxation reduces out-of-plane train and, thus, Poisson ratio. This phenomenon has also been verified experimentally for other WZ compounds [23], and the results of this work are reliable.



Figure 1. Deviations of out-of-plane strain ε_{zz} of In_{0.5}Al_{0.5}N after different deformations of biaxial strain.

The cohesive energy (E_{coh}) of a solid refers to the energy required to separate the constituent atoms apart from each other to form an assembly of neutral free atoms [24], which can be used to evaluate of thermal stability of crystal materials. Figure 2 shows the E_{coh} of In_{0.5}Al_{0.5}N versus different deformations of biaxial strain. The same parabolic-type relationship can be found for the deformed phases, with and without internal relaxation. It is evident that under the same biaxial strain, the cohesive energy after internal relaxation is more negative than the elastically deformed phase, indicating higher thermal stability of In_{0.5}Al_{0.5}N after internal relaxation than that caused by classic elastic deformation without internal relaxation, so it is the most likely phase in reality when biaxial strain is imposed. The same phenomenon can also be found in WZ ZnO [9]; although there is still work to do yet, these results indicate that the WZ-type compounds after internal relaxation are the most likely phases.



Figure 2. Cohesive energy E_{coh} of In_{0.5}Al_{0.5}N after different deformations of biaxial strain.

The electronic properties of a material primarily depend on the type of elements that make up the material and the topology of these elements. The latter determines its electronic structure by defining the overall distribution of various fields, such as electric charge (electric field) in the material. The atomic relaxation of $In_{0.5}Al_{0.5}N$ involves adjusting atomic position, which inevitably affects its electronic structure. Figure 3 presents the results of the most stable phase (i.e., after freely atomic relaxation) under biaxial strain.



Figure 3. Energy band gaps E_g of In_{0.5}Al_{0.5}N under different biaxial strains.

From Figure 3, we can see that the band gap (E_g) of In_{0.5}Al_{0.5}N under no in-plane strain is 2.55 eV, which is in good accordance with the experimental results of optical absorption [25], verifying the reliability of our calculation method. Moreover, we noticed

To shed light on the mechanism of biaxial strain on the electronic structures, we carried out the calculations of energy-band structure and electronic density of states (DOS), as depicted in Figures 4 and 5, respectively. Many works have confirmed that the equilibrium state of $In_{0.5}Al_{0.5}N$ exhibits typical direct band-gap semiconductor characteristics, with valence band maximum (VBM) and conduction band minimum (CBM) appearing at the Γ point of the Brillouin zone. We first focus our attention on the energy band structure. The results show that the main outline of the band structure of $In_{0.5}Al_{0.5}N$ is very close to those of InN and AlN, with a relatively smooth VBM, mainly composed of N2*p* orbitals [26]. The bottom of the conduction band (CB) primarily consists of *s* orbital electrons, with a free-electron-like distribution, which leads to the lower effective mass of the charge carrier at the bottom of the conduction band (electron) than that at the top of the valence band (hole, VB). That is to say, the mobility of electron charge is higher than that of the hole in $In_{0.5}Al_{0.5}N$, thus, resulting in an n-type semiconductor at normal conditions.



Figure 4. Band structures of WZ $In_{0.5}Al_{0.5}N$ at (**a**) equilibrium, (**b**) biaxial compressive strain of -5%, (**c**) biaxial tensile strain of 1%, and (**d**) biaxial tensile strain of 5% in (0001) plane after free relaxation.

The band structure changes significantly with the application of the biaxial strain. Concerning CB, an apparent monotonic decrease can be seen for CBM under compressive strain, while CBM rises first and then decreases under tensile strain, leading to a maximum band gap between VBM and CBM, occurring at a tension strain of 1%. Furthermore, the locations of bands in VB also vary with the biaxial strain. As reported by Yang [27], the VBM consists of the near degenerate heavy hole (HH) and crystal-field-split hole (CH) bands. As can be seen from Figure 4, the HH band of WZ In_{0.5}Al_{0.5}N is consistently above CH, regardless of biaxial strain, which is different from Yang's research on other II-V and III-V WZ semiconductors, such as GaN and CdSe, where the CH band shifts upward and becomes the VBM under tensile strain. On the other hand, the positions of HH and CH and the gaps have changed remarkably, especially in our study, as the HH bands become non-degenerate.



Figure 5. Partial density of states of freely relaxed In_{0.5}Al_{0.5}N under different biaxial strains for (**A**) N2*s*, (**B**) N2*p*, (**C**) In5*p*, (**E**) Al3*s*, (**F**) Al3*p* electrons.

Beyond that, the biaxial strain also shows an apparent influence on the density of states. As revealed in Figure 5, the variety of VB is quite simple, where the peaks from every species move downward to the lower energy region under compressive strain and upward to the higher energy region under tensile strain. In contrast, a relatively complicated change can be identified for CB in Figures 4 and 5, in which the peak positions firstly undergo an upward shifting in the tiny tensile strain region ($\leq 1\%$) and then rapidly move downward, as the tensile strain continues to increase, although the peaks of CB show similar trends to that of the valence band in the compressive strain region. Moreover, the magnitude of effects of biaxial strain on the valence band and conduction band is different. In general, the shift range of the peak in the conduction band is more significant than that of the valence band. It is believed that the change in electronic structure will cause a variety of related optical behavior, which will be investigated in further work.

The above theoretical results have a particular significance for the preparation and practical application of optoelectronic devices based on $Al_xIn_{1-x}N$ materials. For example, they can be used to assist in formulating the preparation process and parameters to shift the electronic structure of $Al_xIn_{1-x}N$, to realize accurate regulation of device characteristics. They can also be used to evaluate the influence of temperature and its changes, matrix

materials, and other practical factors on the performance of the $Al_x In_{1-x}N$ -based device, to determine the best service conditions for specific performance requirements.

4. Conclusions

In summary, the influence of biaxial strain on the structure, thermal stability, as well as electronic properties, of wurtzite-type $In_{0.5}Al_{0.5}N$ was investigated based on the first-principles computations. Compared with the classical linear elastic deformation mechanism with fixed atomic coordinates, the internal relaxation, involving free atom and lattice adjustment, will lead to plastic relaxation, along with a similar linear dependence in the out-of-plane strain on the in-plane strain, although the Poisson ratio of the plastic relaxation phase is much smaller than that of its elastic relaxation counterpart under the same biaxial strain. In addition, the change in the cohesive energy of this compound after plastic relaxation, under the same strain, is also smaller than that of the elastic-deformed one, indicating that the internal relaxation will improve the thermal stability of $In_{0.5}Al_{0.5}N$, relative to elastic relaxation under biaxial strain. The electronic structure of wurtzite $In_{0.5}Al_{0.5}N$ is also significantly affected and modulated by internal relaxation.

Author Contributions: Conceptualization, G.Q.; Writing—original draft, G.Z.; Writing—review & editing, F.Z. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by Natural Science Foundation of China, Grant No. 51502179. And Hebei Natural Science Foundation, Grant No. E2020210076.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest: The authors declare no conflict of interest.

References

- 1. Arifin, P.; Sutanto, H.; Subagio, A. Plasma-Assisted MOCVD Growth of Non-Polar GaN and AlGaN on Si(111) Substrates Utilizing GaN-AlN Buffer Layer. *Coatings* **2022**, *12*, 94. [CrossRef]
- Hu, H.; Tang, B.; Wan, H.; Sun, H.; Zhou, S.; Dai, J.; Chen, C.; Liu, S.; Guo, L.J. Boosted ultraviolet electroluminescence of InGaN/AlGaN quantum structures grown on high-index contrast patterned sapphire with silica array. *Nano Energy* 2020, 69, 104427. [CrossRef]
- Khan, M.A.K.; Alim, M.A.; Gaquiere, C. 2DEG transport properties over temperature for AlGaN/GaN HEMT and Al-GaN/InGaN/GaN pHEMT. *Microelectron. Eng.* 2021, 238, 111508. [CrossRef]
- 4. Song, W.; Li, T.; Zhang, L.; Zhu, W.; Wang, L. Influence of growth parameters on microstructures and electrical properties of In_xAl_{1-x}N thin films using sputtering. *J. Alloys Compd.* **2021**, *885*, 160977. [CrossRef]
- 5. Zhou, Y.; Peng, W.; Li, J.; Liu, Y.; Zhu, X.; Wei, J.; Wang, H.; Zhao, Y. Substrate temperature induced physical property variation of In_xAl_{1-x}N alloys prepared on Al₂O₃ by magnetron sputtering. *Vacuum* **2020**, *179*, 109512. [CrossRef]
- 6. Taylor, E.; Smith, M.D.; Sadler, T.C.; Lorenz, K.; Li, H.N.; Alves, E.; Parbrook, P.J.; Martin, R.W. Structural and optical properties of Ga auto-incorporated InAlN epilayers. *J. Cryst. Growth* **2014**, *408*, 97–101. [CrossRef]
- 7. Gonschorek, M.; Carlin, J.F.; Feltin, E.; Py, M.A.; Grandjean, N.; Darakchieva, V.; Monemar, B.; Lorenz, M.; Ramm, G. Two-dimensional electron gas density in Al_{1-x} $In_xN/AIN/GaN$ heterostructures (0.03 $\leq x \leq$ 0.23). J. Appl. Phys. **2008**, 103, 93714. [CrossRef]
- Xie, J.; Ni, X.; Wu, M.; Leach, J.H.; Özgür, Ü.; Morkoç, H. High electron mobility in nearly lattice-matched AlInN/AlN/GaN heterostructure field effect transistors. *Appl. Phys. Lett.* 2007, 91, 132116. [CrossRef]
- Guoqiang, Q.; Guanglei, Z.; Dongchun, L.; Shimin, L. Lattice and internal relaxation of ZnO thin film under in-plane strain. *Thin Solid Film.* 2010, 519, 378–384. [CrossRef]
- 10. Paszkowicz, W.; Černý, R.; Krukowski, S. Rietveld refinement for indium nitride in the 105–295 K range. *Powder Diffr.* 2012, 18, 114–121. [CrossRef]
- Angerer, H.; Brunner, D.; Freudenberg, F.; Ambacher, O.; Stutzmann, M.; Höpler, R.; Metzger, T.; Born, E.; Dollinger, G.; Bergmaier, A.; et al. Determination of the Al mole fraction and the band gap bowing of epitaxial Al_xGa_{1-x}N films. *Appl. Phys. Lett.* **1997**, *71*, 1504–1506. [CrossRef]
- 12. Sapa, L.; Bożek, B.; Danielewski, M. Remarks on Parabolicity in a One-Dimensional Interdiffusion Model with the Vegard Rule. *Iran. J. Sci. Technol. Trans. A Sci.* **2021**, 45, 2135–2147. [CrossRef]

- 13. Fan, Q.; Li, C.; Yang, R.; Yu, X.; Zhang, W.; Yun, S. Stability, mechanical, anisotropic and electronic properties of oP8 carbon: A superhard carbon allotrope in orthorhombic phase. *J. Solid State Chem.* **2021**, 294, 121894. [CrossRef]
- 14. Kilic, M.E.; Lee, K.-R. First-Principles Study of Fluorinated Tetrahexcarbon: Stable Configurations, Thermal, Mechanical, and Electronic Properties. J. Phys. Chem. C 2020, 124, 8225–8235. [CrossRef]
- 15. Perdew, J.P.; Wang, Y. Accurate and simple analytic representation of the electron-gas correlation energy. *Phys. Rev. B* **1992**, 45, 13244–13249. [CrossRef] [PubMed]
- 16. Vanderbilt, D. Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. Phys. Rev. B 1990, 41, 7892–7895. [CrossRef]
- 17. Toma, M.; Kuvek, T.; Vrček, V. Ionization Energy and Reduction Potential in Ferrocene Derivatives: Comparison of Hybrid and Pure DFT Functionals. *J. Phys. Chem. A* 2020, 124, 8029–8039. [CrossRef]
- Darakchieva, V.; Xie, M.Y.; Tasnádi, F.; Abrikosov, I.A.; Hultman, L.; Monemar, B.; Kamimura, J.; Kishino, K. Lattice parameters, deviations from Vegard's rule, and E2 phonons in InAlN. *Appl. Phys. Lett.* 2008, 93, 261908. [CrossRef]
- 19. Polian, A.; Grimsditch, M.; Grzegory, I. Elastic constants of gallium nitride. J. Appl. Phys. 1996, 79, 3343–3344. [CrossRef]
- Caro, M.A.; Schulz, S.; O'Reilly, E.P. Hybrid functional study of the elastic and structural properties of wurtzite and zinc-blende group-III nitrides. *Phys. Rev. B* 2012, *86*, 14117. [CrossRef]
- Serrano, J.; Bosak, A.; Krisch, M.; Manjón, F.J.; Romero, A.H.; Garro, N.; Wang, X.; Yoshikawa, A.; Kuball, M. InN Thin Film Lattice Dynamics by Grazing Incidence Inelastic X-Ray Scattering. *Phys. Rev. Lett.* 2011, 106, 205501. [CrossRef] [PubMed]
- 22. Łepkowski, S.P.; Gorczyca, I. Elastic properties of InGaN and InAlN from first-principles calculations. AIP Conf. Proc. 2013, 1566, 83–84.
- Ashrafi, A.B.M.A.; Binh, N.T.; Zhang, B.P.; Segawa, Y. Strain relaxation and its effect in exciton resonance energies of epitaxial ZnO layers grown on 6H-SiC substrates. *Appl. Phys. Lett.* 2004, *84*, 2814–2816. [CrossRef]
- Ahmed, H.; Hashim, A. Geometry Optimization, Optical and Electronic Characteristics of Novel PVA/PEO/SiC Structure for Electronics Applications. *Silicon* 2021, 13, 2639–2644. [CrossRef]
- Alam, S.N.; Zubialevich, V.Z.; Ghafary, B.; Parbrook, P.J. Bandgap and refractive index estimates of InAlN and related nitrides across their full composition ranges. *Nature* 2020, 10, 16205. [CrossRef]
- Xie, M. Structural and elastic properties of InN and InAlN with different surface orientations and doping. Ph.D. Thesis, Linköping University Electronic Press, Linköping, Sweden, 2012; p. 79.
- 27. Yang, S.; Prendergast, D.; Neaton, J.B. Nonlinear variations in the electronic structure of II–VI and III–V wurtzite semiconductors with biaxial strain. *Appl. Phys. Lett.* 2011, *98*, 152108. [CrossRef]