Defect and Diffusion Forum Vols. 226-228 (2004) pp. 79-89
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Anisotropy of the Elastic Properties of Wurtzite InN Epitaxial Films

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Keywords: Elastic Anisotropy, Point Defects, Strain, Wurtzite Nitrides, X-Ray Diffraction

Abstract. The anisotropy of elastic bulk constants of wurtzite InN is analyzed theoretically on the basis of available data for elastic constants. A considerable anisotropy is evaluated both for Young's modulus and Poisson ratio of highly textured InN epitaxial films deposited on the basal plane. A comparative analysis of elastic properties is conducted for wurtzite InN, GaN and AlN. An approach is suggested for estimating vacancy concentrations on the basis of SIMS and x-ray diffraction measurements.

1. Introduction

Wide bandgap wurtzite semiconductors such as indium nitride (InN), galium nitride (GaN), and aluminium nitride (AlN) are promising materials for their potential use in optoelectronic, high power/temperature electronic [1] and surface acoustic wave devices [2]. Epitaxial films of these materials are highly strained (due to a large lattice mismatch and a difference in thermal expansion coefficients with the most extensively used substrate material, sapphire) and contain large amounts of structural defects: misfit and threading dislocations, point defects, stacking faults, grain and inversion domain boundaries, etc. [1, 3]. Both strain (i.e. elastic properties) and structural defects of epitaxial films substantially control its electronic, optical, diffusive, and other important physical properties. By this reason, controlling the strains (stresses) in epitaxially grown thin films is one of the most important requirements in modern technology. Because of restrictions in the choice of a substrate material, reliable strain control may be realized due to proper choice of the buffer layer material and its thickness. As it follows from numerous experimental results, through manipulation of the buffer layer thickness the substantial variations in morphology (see e.g. [4, 5]) and electronic properties [5] of III-V nitride epitaxial films may be achieved. Thus, for any deposition technique, along with main technological parameters (e.g., deposition temperature and rate), strain should be qualified as parameter playing crucial role in formation of the epitaxial film morphology and defect structure. Therefore, investigations of elastic properties of these materials are important both, from scientific and technological standpoints.

The wurtzite nitrides exhibit a significant elastic anisotropy [6 - 8], which may be ignored in those cases where only rough estimates of strains and stresses are needed. However, this anisotropy has to be taken into account for many other problems involving a precise strain-stress analysis, such as determination of the Peierls stress of a single dislocation [9], dislocation line and tension energies, dislocation interaction stresses at the network of basal dislocations, energy of the stacking fault formation [10 - 12], and activation energy of the dislocation easy-glide system [12]. In consideration of those and many other problems the theory of anisotropic elastic media [9] should be applied, since the concept of an elastically isotropic crystalline medium is an idealization. Detailed reviews and analysis of experimental and theoretical data on the elastic constants [6 – 8, 13] and elastic moduli [6, 7] of GaN and AlN are available. In [7] the anisotropy of the compressibility parameter of GaN and AlN is analyzed as well. However, in comparison to GaN and AlN, in general much less attention has been paid to the analysis of elastic properties of InN [6,14 -17] and the evaluation of its elastic moduli and parameters characterizing the elastic anisotropy.

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In this paper we derived analytical expressions connecting elastic moduli of single crystal wurtzite InN with its elastic constants. A comparative analysis of anisotropic elastic properties of InN with GaN and AlN is conducted on the bases of the obtained theoretical results. The approach developed in [18, 19] for the analysis of point defects in epitaxial films is extended to the case of anisotropic elastic theory and applied for an estimate of the vacancy concentration in InN heteroepitaxial films grown by molecular beam epitaxy..

2. Hook's generalized law in the case of wurtzite films deposited on the basal plane

A single crystal of a wurtzite structure is described by crystallographic hexagonal symmetry. At the (0001) basal planes all directions are equivalent with respect to the elastic properties, and the material is isotropic in these planes. The crystallographic *c*-axis coincides with the axis of elastic symmetry. As a rule, a wurtzite III-V nitride epitaxial film deposited on the (0001) sapphire substrate forms a *strong texture about the* [0001] *growth direction* with an effective out-of-plane misorientation angle of columnar coherent domains of the order of a few arcminutes. Besides, these coherent domains exhibit small in-plane misorientations (twists at the basal plane), which vary within a few arcdegrees [20]. In terms of elastic properties, the epitaxial film with the described morphology should be considered as a single crystal rather than a polycrystalline structure. It means that we attribute to the film the single-crystal elastic moduli. Choosing the *z*-axis of a coordinate system along the [0001] growth direction ($x\,y$ coordinate plane coincides with a basal plane), in terms of elastic moduli the equations of the Hook's generalized law for a (0001) wurtzite epitaxial film can be expressed as [21, 22]:

$$\varepsilon_{xx} = \frac{1}{E_x}\sigma_{xx} - \frac{\nu_{xy}}{E_x}\sigma_{yy} - \frac{\nu_{zx}}{E_z}\sigma_{zz} \tag{1}$$

$$\varepsilon_{yy} = -\frac{\nu_{xy}}{E_x}\sigma_{xx} + \frac{1}{E_x}\sigma_{yy} - \frac{\nu_{zx}}{E_z}\sigma_{zz} \tag{2}$$

$$\varepsilon_{zz} = -\frac{\nu_{xz}}{E_x}\sigma_{xx} - \frac{\nu_{xz}}{E_x}\sigma_{yy} + \frac{1}{E_z}\sigma_{zz} \tag{3}$$

$$\varepsilon_{xz} = \frac{1}{2G_{xz}}\sigma_{xz} \tag{4}$$

$$\varepsilon_{yz} = \frac{1}{2G_{xz}}\sigma_{yz} \tag{5}$$

$$\varepsilon_{xy} = \frac{1}{2G_{xy}}\sigma_{xy} \tag{6}$$

where ε_{ii} and σ_{ii} are the normal strain and stress components in i direction (i = x, y or z), respectively, ε_{ij} and σ_{ij} are the shear strain and stress components for (i, j) combination of directions ($i, j = x, y$ or z, $i \neq j$), respectively, E_x and E_z are the Young's moduli at the basal plane and in z direction, respectively, G_{xz} and G_{xy} are the shear moduli for the shear deformation planes normal and parallel to the plane of isotropy (i.e., to basal plane), respectively, and ν_{ij} is the Poisson ratio for the (i, j) combination of directions ($i, j = x, y$ or z, $i \neq j$), respectively. A "body" possessing the elastic properties described by Eqs. (1) - (6) is referred to as a *transversely isotropic material*. It is obvious that due to elastic symmetry, for a transversely isotropic material the following equations are fulfilled:

$$\nu_{yx} = \nu_{xy}\,, \qquad \nu_{yz} = \nu_{xz}\,, \qquad \nu_{zy} = \nu_{zx}\,, \qquad E_x = E_y\,, \qquad G_{yz} = G_{xz} \tag{7}$$

where E_y is the Young's modulus at the basal plane in y direction. The equations given by (7) are taken into account in derivation of Eqs. (1) – (6) [21, 22]. . Thus, in terms of elastic moduli, an epitaxial wurtzite film should be characterized at least by seven parameters E_x, E_z, G_{xz}, G_{xy}, ν_{xz}, ν_{zx} and ν_{xy}.

3. Relationships between elastic moduli and elastic constants

It is important from the experimental standpoint to establish the relationships between elastic moduli and elastic constants of wurtzite nitrides. The elastic constants can be measured by different *non-destructive* techniques (optical, acoustic, x-ray diffraction, etc.) [6 – 8, 13], and then from these relationships the elastic moduli can be calculated.

For the hexagonal crystal system and in particular for the wurtzite structure the relationships between elastic compliances and elastic constants (stiffnesses) are given as follows (see e.g. [23]):

$$s_{11} = \frac{1}{2}\left(\frac{c_{33}}{c} + \frac{1}{c_{11} - c_{12}}\right), \qquad s_{12} = \frac{1}{2}\left(\frac{c_{33}}{c} - \frac{1}{c_{11} - c_{12}}\right) \tag{8}$$

$$s_{13} = -\frac{c_{13}}{c}\,, \qquad s_{33} = \frac{c_{11} + c_{12}}{c}\,, \qquad s_{44} = \frac{1}{c_{44}} \tag{9}$$

$$c \equiv c_{33}(c_{11} + c_{12}) - 2c_{13}^2 \tag{10}$$

where s_{ij} and c_{ij} (i, j = 1, 2, 3 or 4) are the compliances and elastic constants, respectively, and c is auxiliary notation. From the other side, the equations connecting the compliances with the elastic moduli, Young's moduli and Poisson ratios, are written as follows [23] :

$$s_{ii} = \frac{1}{E_i} \tag{11}$$

$$s_{ij} = -\frac{\nu_{ji}}{E_j} = -\frac{\nu_{ij}}{E_i} \tag{12}$$

In (11) the indices i =1, 2, or 3 of Young's modulus correspond to coordinate directions x, y, and z, respectively (for hexagonal crystal system $s_{11} = s_{22}$). In (12) i, j =1, 2, or 3, $i \neq j$, and for parameters E_i and ν_{ij} the indices i, j =1, 2, and 3 correspond to x, y and z coordinate directions, respectively.

From Eqs. (7) – (12) after some transformations the following relationships between elastic moduli and elastic constants are obtained:

$$E_x = \frac{(c_{11}-c_{12})[c_{33}(c_{11}+c_{12})-2c_{13}^2]}{c_{33}c_{11}-c_{13}^2} \tag{13}$$

$$E_z = \frac{c_{33}(c_{11}+c_{12})-2c_{13}^2}{c_{11}+c_{12}} \tag{14}$$

$$\nu_{xy} = \frac{c_{33}c_{12}-c_{13}^2}{c_{33}c_{11}-c_{13}^2} \tag{15}$$

$$\nu_{zx} = \frac{c_{13}}{c_{11}+c_{12}} \tag{16}$$

$$\nu_{xz} = \frac{c_{13}(c_{11}-c_{12})}{c_{33}c_{11}-c_{13}^2} \tag{17}$$

Shear moduli, G_{xz} and G_{xy}, are found as follows [23]:

$$G_{xz} = c_{44} \tag{18}$$

$$G_{xy} = \frac{1}{2}(c_{11}-c_{12}) \tag{19}$$

In our further estimates we need also the bulk modulus B, which is determined from the following expression [6]:

$$B = \frac{c_{33}(c_{11}+c_{12})-2c_{13}^2}{c_{11}+c_{12}+2c_{33}-4c_{13}} \tag{20}$$

4. Anisotropy of elastic properties of wurtzite InN

In comparison to GaN and AlN, much less work has been devoted to measurements and calculations of elastic constants of wurtzite InN [6,14 -17]. To our knowledge, there is only one experimental result of InN elastic constants [17] (x-ray diffraction analysis). The data of InN c_{ij} parameters determined in [6,14 -17] are given in Table 1. For comparative analysis the elastic moduli and Poisson ratios are calculated from Eqs. (13) to (20) for all c_{ij} sets from Table 1. The results are listed in Table 2. In spite of a large scatter in their values depending on the c_{ij} data, in each case the elastic moduli and Poisson ratio exhibit a considerable elasticity anisotropy. The best agreement between data in Table 2 is achieved for theoretical c_{ij} parameters obtained by Wright [6] and Davydov [16]. A value of 0.52 calculated for ν_{xz} Poisson ratio in case of elastic constants measured by Sheleg and Savastenko [17] does not seem realistic from the physical standpoint and, unfortunately, makes their c_{ij} data unreliable.

Table 1: Wurtzite InN elastic constants in [GPa]

Ref.	Method	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}
[17]	exper.	190	104	121	182	10
[6]	calcul.	223	115	92	224	48
[14, 15]	calcul.	271	124	94	200	46
[16]	calcul.	204	85	72	217	50

Table 2: Elastic moduli (in [GPa]) and Poisson ratios of wurtzite InN calculated for the sets of c_{ij} elastic constants from Table 1

Ref. for c_{ij}	E_x	E_z	G_{xz}	G_{xy}	B	ν_{xz}	ν_{zx}	ν_{xy}
[17]	104	82	10	43	139	0.52	0.41	0.22
[6]	153	174	48	54	141	0.24	0.27	0.42
[14,15]	199	155	46	74	146	0.30	0.24	0.35
[16]	159	181	50	60	120	0.22	0.25	0.34

It is interesting to compare bulk elastic parameters of InN with those of GaN and AlN. In this comparative analysis we use from Table 2 the elastic parameters of InN calculated for the Wright's set of c_{ij} [6]. The bulk elastic parameters of GaN and AlN are also calculated from Eqs. (13) to (20) both from experimental and theoretical sets of elastic constants. For GaN we have used elastic constants $c_{11} = 390 \pm 15$ GPa, $c_{12} = 145 \pm 20$ GPa, $c_{13} = 106 \pm 20$ GPa, $c_{33} = 398 \pm 20$ GPa, and $c_{44} = 105 \pm 10$ GPa determined by Polian et al. on the basis of Brillouin scattering measurements [24] and theoretical parameters $c_{11} = 367$ GPa, $c_{12} = 135$ GPa, $c_{13} = 103$ GPa, $c_{33} = 405$ GPa, $c_{44} = 95$ GPa evaluated by Wright [6]. In calculations of the AlN bulk constants again the set of experimental data of Brillouin scattering measurements $c_{11} = 411 \pm 10$ GPa, $c_{12} = 149 \pm 10$ GPa, $c_{13} = 99 \pm 4$ GPa, $c_{33} = 389 \pm 10$ GPa, and $c_{44} = 125 \pm 5$ GPa [26] and constants $c_{11} = 396$ GPa, $c_{12} = 137$ GPa, $c_{13} = 108$ GPa, $c_{33} = 373$ GPa, and $c_{44} = 116$ GPa calculated by Wright [6] have been used. The results are presented in Table 3. Also the uncertainty in values of bulk elastic constants due to errors in c_{ij} (see above) measurements is evaluated for GaN and AlN (see in Table 3 the rows for Refs. [24] and [26], respectively). It should be mentioned that the data for c_{ij} parameters obtained in [6, 24] are qualified in review article by Vurgaftman and Meyer [8] as "recommended" values. Indeed, for GaN the results calculated from experimental [24] and theoretical [6] c_{ij} constants show excellent agreement within experimental errors (see Table 3). Our bulk elastic parameters determined for AlN again from the set of c_{ij} data calculated by Wright [6] also exhibit a satisfactory agreement with those determined from experimental c_{ij} data [26] (see Table 3).

Table 3: Elastic moduli (in [GPa]) and Poisson ratios of wurtzite InN, GaN, and AlN. The first row of data is from Table 2.

Mat.	Ref. for c_{ij}	E_x	E_z	G_{xz}	G_{xy}	B	ν_{xz}	ν_{zx}	ν_{xy}
InN	calc. [6]	153	174	48	54	141	0.24	0.27	0.42
GaN	exp. [24]	324 ± 20	356 ± 30	105 ± 10	123 ± 17	210	0.18 ± 0.06	0.20 ± 0.04	0.32 ± 0.06
GaN	calc. [6]	306	363	95	116	202	0.17	0.21	0.32
AlN	exp. [26]	346 ± 17	354 ± 14	125 ± 5	131 ± 10	210	0.17 ± 0.02	0.18 ± 0.02	0.32 ± 0.04
AlN	calc. [6]	334	329	116	130	207	0.21	0.20	0.29

The data in Table 3 show that due to experimental errors, both for GaN and AlN the anisotropy of Young's modulus and shear modulus calculated from experimental c_{ij} cannot be established in a reliable way. The same is true with respect to ν_{xz} and ν_{zx} Poisson ratios. However, the precision in measurements of c_{ij} constants enabled to reveal the anisotropy of the ν_{xy} Poisson ratio with respect to ν_{xz} and ν_{zx} parameters.

It follows from the data in Table 3 that the elastic moduli of InN are considerably smaller and Poisson ratios are larger in comparison to similar parameters of GaN and AlN.

For hexagonal crystals, two parameters are needed to describe crystal anisotropy: anisotropies of compressibility, A_c, and shear, A_s. These parameters are defined as follows [25]:

$$A_c = \frac{c_{11} + c_{12} - 2c_{13}}{c_{33} - c_{13}} \tag{21}$$

$$A_s = \frac{2c_{44}}{c_{11} - c_{12}} \tag{22}$$

Anisotropy parameters given by (21) and (22) are calculated for InN, GaN, and AlN using the same c_{ij} sets from Table 3. The results are presented in Table 4. As it follows from these data, the shear anisotropy of these materials is almost the same. In terms of the compressibility the InN is more anisotropic than GaN, but exhibits slightly less anisotropy in comparison to AlN.

The anisotropy of the compressibility for GaN and AlN is in detailed discussed in [7].

Table 4

Material	Ref. for c_{ij} data	A_c	A_s
InN	calc. [6]	1.17	0.89
GaN	exp. [24]	1.11 ± 0.10	0.86 ± 0.10
GaN	calc. [6]	0.98	0.82
AlN	exp. [26]	1.25 ± 0.12	0.95 ± 0.10
AlN	calc. [6]	1.20	0.90

5. Considering of elastic anisotropy in separation of biaxial and hydrostatic strain components

After the deposition process, all epitaxial GaN, InN, and AlN films are expected to contain a residual homogeneous strain (i.e., so-called "macrostrain") due to the residual crystal lattice mismatch between film and substrate and the presence both of native point defects and contaminations. Contributions to the total homogeneous strain from linear and planar defects (dislocations, stacking faults, and twin boundaries), which are also typical defects in epilayers, *in general* is negligibly small in comparison to contribution by lattice misfit and point defects. For instance, it is known that the inhomogeneous character of the dislocation elastic field does not lead to any observable macroscopic volumetric strain in a crystal [27].

The residual lattice misfit at the film-substrate interface leads to biaxial deformation of epitaxial films at the growth plane [28], whereas native point defects and impurities cause crystal lattice hydrostatic expansion or contraction depending on their type and relative concentrations [1]. These deformations are characterizes by *biaxial* and *hydrostatic* strains, respectively. By obvious reason, there is a special scientific interest in the development of approaches for extraction of the biaxial and hydrostatic strain components from the measured (total) strain. In some specific cases, when the type of point defects in an epilayer is known a priori, it may be possible to estimate their concentration from the extracted hydrostatic strain component applying Vegard's law. Amongst known techniques, the high resolution x-ray diffraction analysis is a powerful tool for precise strain measurements and has been applied in a series of reports for the analysis [18, 29] and estimation [19, 20] of biaxial and hydrostatic strain components in GaN epitaxial films. In average, a compressive hydrostatic strain of about -5×10^{-4} was determined even in undoped epilayers grown both by molecular beam epitaxy [19] and metal-organic chemical vapor deposition [20]. This indicates on a large amount of native point defects in those samples, most probably vacancies.

The theoretical approach suggested by Kisielowski et al. [18] for the extraction of biaxial and hydrostatic strain components is based on an isotropic approximation of elasticity theory. However, as it follows from the parameters of the compressibility anisotropy of InN and AlN (see data for parameter A_c in Table 4), we may anticipate that taking into account the elastic anisotropy of these materials can introduce a considerable correction to the extracted hydrostatic strain and, hence, to the concentration of point defects evaluated from strain.

For a linear superposition of biaxial and hydrostatic strain components in an epitaxial film the following relationships are fulfilled:

$$\varepsilon_{xx} = \varepsilon_{xx}^{(b)} + \varepsilon_{xx}^{(h)} \qquad (23)$$

$$\varepsilon_{zz} = \varepsilon_{zz}^{(b)} + \varepsilon_{zz}^{(h)} \tag{24}$$

$$\frac{\varepsilon_{zz}^{(b)}}{\varepsilon_{xx}^{(b)}} = -2\frac{c_{13}}{c_{33}} \tag{25}$$

$$A_c = \frac{\varepsilon_{zz}^{(h)}}{\varepsilon_{xx}^{(h)}} = \frac{c_{11} + c_{12} - 2c_{13}}{c_{33} - c_{13}} \tag{26}$$

where $\varepsilon_{xx}^{(b)}$ and $\varepsilon_{zz}^{(b)}$ are the in-plane and out-of-plane biaxial strain components, $\varepsilon_{xx}^{(h)}$ and $\varepsilon_{zz}^{(h)}$ are the similar components of the hydrostatic strain caused by point defects, and ε_{xx} and ε_{zz} are the total strain components. Equations (25) and (26) describe pure biaxial and pure hydrostatic deformation of a hexagonal (in particular wurtzite) crystal lattice, respectively [6]. Note that in (26) the ratio of hydrostatic strain components by itself is the anisotropy parameter of the compressibility defined by (21). Assuming that the total strain components, ε_{xx} and ε_{zz}, are found experimentally and the c_{ij} elastic constants are known, the strain components $\varepsilon_{xx}^{(b)}$, $\varepsilon_{zz}^{(b)}$, $\varepsilon_{xx}^{(h)}$, and $\varepsilon_{zz}^{(h)}$ can be determined from the set of simultaneous equations (23) – (26).

6. Estimation of vacancy concentrations in InN films on the basis of x-ray diffraction and SIMS measurements

The approach suggested in the previous section for strain analysis was applied by us to InN epitaxial layers. A series of InN epitaxial films were deposited on (0001) oriented sapphire substrates by molecular beam epitaxy with a deposition rate of 0.2 μm/hour. Deposition was conducted using In-rich conditions at a substrate temperature of 500° C. For sample No. 901 the buffer layer is GaN with a thickness of 30 nm. For three other samples, No. 920, J7, and J10, a buffer layer of AlN with a thickness about 3nm was deposited. For all samples the thickness of the InN epitaxial film was about 1 μm. No intentional doping of the films was introduced. Typical growth parameters are described in detail elsewhere [30].

The a and c –lattice parameters have been determined from high resolution x-ray diffraction measurements on the basis of an approach suggested in [19]. Further, the data of the determined lattice parameters were used for an evaluation of the hydrostatic strain components from the set of equations (23)-(26). In this procedure, for compressibility anisotropy, A_c, a value 1.17 from Table 4 was substituted in (26). From the measured x-ray diffraction spectra it was concluded that InN films form a strong texture about the [0001] growth direction. The crystallographic out-of-plane coherence length, l_z, was estimated from broadenings of (0002), (0004), and (0006) diffraction peaks applying a Williamson-Hall plot [31]. The data of a and c-lattice parameters, hydrostatic strain components and coherence length are listed in Table 5. In strain calculations, $a_0 = 3.545$ Å and $c_0 = 5.703$ Å unstrained lattice parameters [8] were used. The accuracy of measurements of lattice parameters is about ± 0.001 Å.

All samples exhibit n-type conductivity. The carrier concentration, n, and the Hall mobility, μ, have been measured. We also applied secondary ion mass spectroscopy (SIMS) to determine the concentration of oxygen contamination in samples, N_V. The data of electronic and SIMS measurements are given in Table 5. The details of above described measurements and relevant data are presented in [30].

Table 5: Parameters determined by x-ray diffraction , electronic and SIMS measurements

Samp.	Latt.pars. [Å]	$\varepsilon_{xx}^{(h)}$ $\varepsilon_{zz}^{(h)}$	N_0 [cm^{-3}]	N_V [cm^{-3}]	n [cm^{-3}]	μ [$\frac{cm^2}{Vs}$]	l_z [nm]
901	$a = 3.522$ $c = 5.727$	-6×10^{-4} -7×10^{-4}	4×10^{20}	5×10^{19}	5×10^{20}	50	41
920	$a = 3.526$ $c = 5.696$	-2.8×10^{-3} -3.3×10^{-3}	1×10^{20}	2×10^{20}	1.8×10^{20}	155	84
J 7	$a = 3.539$ $c = 5.708$	-2.6×10^{-4} -3.0×10^{-4}	1×10^{19}	2×10^{19}	7.8×10^{19}	360	113
J10	$a = 3.544$ $c = 5.698$	-6×10^{-4} -7×10^{-4}	2×10^{19}	4×10^{19}	2.8×10^{19}	67	97

As-grown InN is mostly *n*-type with a high carrier concentration as was also observed in the case of the films grown here. In the literature there is general agreement that oxygen can act as a donor in InN [3]. Oxygen donates only one electron into the conductivity band. The data in Table 5 show that for all samples the carrier concentration considerably exceeds the oxygen concentration. A second donor that may be considered is the nitrogen vacancy. This correlates with the negative sign of the hydrostatic strain (see Table 5) and a high probability of nitrogen vacancies formation under In-rich growth conditions. Considering an In-rich deposition process, the additional formation of In_N anti-site defects and In interstitials is also possible. However, the latter types of point defects should lead to crystal lattice expansion since the tetrahedral covalent atomic radius of In is much more than of N. This means, that in the samples under consideration here the concentration of In_N anti-site defects and In interstitials can be expected to be comparatively low. It is reasonable to assume that oxygen prefers nitrogen sites since their chemistry and covalent atomic radii are rather close. In comparison to nitrogen, the oxygen atomic radius is slightly less, so some contribution to the negative hydrostatic strain can be expected. It is interesting to note that except the effects of native defects and impurities, the conduction band electrons also affect the lattice parameters: they introduce a positive strain into the crystal lattice [1]. Thus, supposing that the observed, negative hydrostatic strain in the InN films considered here is mainly due to O_N substitutions, nitrogen vacancies, and conduction electrons, the following relationship may be suggested between their concentrations and the total hydrostatic strain:

$$\varepsilon_h = \beta_V N_V + \beta_0 N_0 + \beta_e n \qquad (27)$$

where

$$\beta_V \approx -\frac{1}{N_s} \qquad (28)$$

$$\beta_0 = \frac{1}{3}[(\frac{r_s}{r_h})^3 - 1]\, N_s^{-1} \tag{29}$$

$$\beta_c = -\frac{a_c}{3B} \tag{30}$$

$$\varepsilon_h = \frac{1}{3}(2\varepsilon_{xx}^{(h)} + \varepsilon_{zz}^{(h)}) \tag{31}$$

In Eqs. (27) – (31) N_V, N_0, and n are concentrations of nitrogen vacancies, oxygen substitutions at nitrogen sites, and electrons in conductivity band, respectively; N_s is the total atomic sites per unit volume in InN, r_s and r_h are the tetrahedral covalent atomic radii of solute (oxygen) and host (nitrogen) atoms, respectively; a_c is the conduction-band-energy deformation potential [32], B is the elastic bulk modulus, and $\varepsilon_{xx}^{(h)}$ and $\varepsilon_{zz}^{(h)}$ are the hydrostatic strain components introduced in Eqs. (23) – (26). It is obvious that the coefficients β_V [33] and β_0 [4] given in (28) and (29) are negative defining a negative contribution into the strain. In (31) ε_h is the *effective* strain introduced through the volumetric hydrostatic strain. Substituting into the set of Eqs. (27)-(31) the data $N_s = 6.44\times10^{22}$ cm^{-3}, r_s= 0.0678 nm [34], r_h = 0.0719 nm, a_c= – 2.8 eV [15], B =141 GPa (from Table 3) and relevant data from Table 5 for parameters $\varepsilon_{xx}^{(h)}, \varepsilon_{zz}^{(h)}$, N_0, and n, we may estimate the nitrogen vacancy concentration, N_V. The results for these concentrations are listed in Table 5.

7. Discussion

The data in Table 3 show that in wurtzite InN the Young's modulus and Poisson ratio exhibit considerable anisotropy. Especially a high anisotropy is predicted for ν_{xy} Poisson ratio with respect to ν_{xz} and ν_{zx} parameters for all considered compounds, InN, GaN and AlN. To our knowledge, there is no report yet in the literature of reliable experimental data of elastic constants of wurtzite InN. Therefore we are forced in the analysis of InN elastic properties to restrict ourselves to a theoretical consideration only. In this context, for GaN and AlN the situation is better: as it follows from the data in Table 3, rather good agreement is achieved for bulk elastic constants evaluated from experimental and theoretical data . However, a further improvement of the accuracy is needed in the measurements of elastic constants in order to reveal in a more reliable way the anisotropy of bulk constants from Eqs. (13)-(19). As it follows from the data for anisotropy parameters, in terms of compressibility the InN is more anisotropic than GaN, but exhibits slightly less anisotropy in comparison to AlN. In terms of shear deformations, InN is less anisotropic than GaN, but more anisotropic than AlN.

The approach suggested in the previous section for the analysis of vacancy concentrations in as-grown InN epilayers seems to be realistic. From the results obtained here (Table 5) it follows that at higher concentrations of oxygen and vacancies the smaller coherence length is formed. Most probably, the point defects stimulate the formation of planar defects (e.g. stacking faults) at basal planes, and the coherence length is inversely proportional to defects density. Besides, there is an obvious correlation between the Hall mobility and coherence length. Apparently, the conduction electrons are effectively scattered at planar defect.

Acknowledgement

V.H. gratefully acknowledges the support of a Fulbright Foundation fellowship, This work was supported by the Director, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering of the US Department of Energy under contract No. DE-AC03-76F00098.

References

[1] H. Morcos: Mat. Sci. and Engineering R Vol. 33 (2001), p. 135.

[2] M.T. Duffy, C.C. Wang, G.D. O'Clock, S.H. McFalne III, P.J. Zanzucchi: J. Electron. Mater. Vol. 2 (1973), p. 359.

[3] A.G. Bhuiyan, A. Hashimoto and A. Yamamoto: J. Appl. Phys. Vol. 94 (2003), p. 2779.

[4] C. Kisielowski: Semicond. Semimet. Vol. 57 (1999), p. 275.

[5] H. Lu, W.L. Schaff, J. Hwang, H. Wu, G. Koley and L.F. Eastman: Appl. Phys. Lett. Vol. 79 (2001), p. 1489.

[6] A.F. Wright: J. Appl. Phys. Vol. 82 (1997), p. 2833.

[7] J.-M. Wagner and F. Bechstedt: Phys. Rev. B Vol. 66 (2002), p. 115202.

[8] I. Vurgaftman and J.R. Meyer: J. Appl. Phys. Vol. 94 (2003), p. 3675.

[9] J.P. Hirth and J. Lothe: *Theory of Dislocations* (A Wiley-Intersci. Publ., New York 1982).

[10] K. Suzuki, M. Ichihara and S. Takeuchi: Jap. J. Appl. Phys, Part 1 Vol. 33 (1994), p. 1114.

[11] A.F. Wright: J. Appl. Phys. Vol. 82 (1997), p. 5259

[12] V. Audurier, J.L. Dement and J. Rabier: Phil. Mag. A Vol. 77 (1998), p. 843.

[13] K. Shimada, T. Sota and K. Suzuki: J. Appl. Phys. Vol. 84 (1998), p. 4951.

[14] K. Kim, W.R.L. Lambrecht and B. Segall: Phys.Rev. B Vol. 50 (1994), p.1502.

[15] K. Kim, W.R.L. Lambrecht and B. Segall: Phys.Rev. B Vol. 53 (1996), p. 16310.

[16] S.Yu.Davydov: Semiconductors Vol. 36 (2002), p. 41.

[17] A.U. Sheleg and V.A. Savastenko: Izv. Akad. Nauk SSSR, Neorg. Mater. Vol. 15 (1979), p. 1598.

[18] C. Kisielowski, J. Kruger, S. Ruvimov, T. Suski, J.W. Ager III, E. Jones, Z. Liliental-Weber, M. Rubin and E.R. Weber: Phys. Rev. B Vol. 54 (1996), p. 17745.

[19] V.S. Harutyunyan, A.P. Aivazyan, E.R. Weber, Y. Kim, Y. Park and S.G. Subramanya S.G: J. Phys. D: Appl.Phys. Vol. 34 (2001), p. A1.

[20] E. Zieliñska-Rohoziñska, M. Regulska, V.S. Harutyunyan, K. Pakula and J. Borowski: Mater. Sci. and Engineering B Vol. 91-92 (2002), p. 441.

[21] S.G. Lekhnitskii: *Theory of Elasticity of an Anisotropic Elastic Body* (Holden-Day, Inc., San Francisco 1963).

[22] S.A. Ambartsumyan: *Theory of Anisotropic Plates* (Hemish. Publ. Corp., New York 1991).

[23] R.F.S. Hearmon: *An Introduction to Applied Anisotropic Elasticity* (Oxford Univ. Press., London 1961).

[24] A. Polian, M. Grimsditch and I.G. Grzegory: J. Appl. Phys. Vol. 79 (1996), p. 3343.

[25] D.H. Chung and W.R. Buessem: in *Anisotropy in Single-Crystal Refractory Compounds*, edited by F.W. Vahldiek and S.A. Mersol (Plenum, New York 1968), Vol. 2.

[26] L.E. McNail, M. Grmsditch and R.H. French: J. Am. Ceram. Soc. Vol. 76 (1993), p. 1132.

[27] A.H. Cottrell: *Dislocations and Plastic Flow in Crystals* (Oxford University Press, Amen House, London 1953).

[28] W.D. Nix: Metall. Trans. A Vol. 20 (1989), p. 2217.

[29] A. Usikov, V.V. Ratnikov, R. Kyutt, W.V. Lundin, B. Pushnyi, N.M. Shmidt and M.P. Scheglov: MRS Internet J. Nitride Semicond. Res. 3, 42 (1998).

[30] P. Specht, R. Armitage, J. Ho, E. Gunawan, Q. Yang and E.R. Weber: J. Cryst. Growth, in press.

[31] G.K. Williamson and W.H. Hall: Acta Metall. Vol. 1 (1953), p. 22.

[32] G.S. Cargill, III, J. Angilello and K.L. Kavanagh: Phys. Rev. Lett. Vol. 61 (1988), p.1748.

[33] O. Lagerstedt and B. Monemar: Phys. Rev. B Vol. 19 (1979), p. 3064.

[34] J.A. Van Vechten and J.C. Phillips: Phys. Rev. B Vol. 2 (1970), p. 2160.

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Key Engineering Materials Vol. 237
2003, 274 pp, paperback, 2-vols. set
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