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Stability of the wurtzite-type structure under high pressure: GaN and InN

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High-pressure *in situ* x-ray-diffraction studies on GaN and InN have been carried out using an imaging-plate technique and a diamond-anvil cell up to about 60 GPa. The two compounds crystallize in the wurtzite-type structure at ambient conditions. The axial ratio c/a of GaN remains unchanged from the ambient value of 1.626 whereas c/a of InN is considerably decreased from 1.613 to 1.597 with increasing pressure to about 15 GPa. Equation-of-state data obtained for the wurtzite phase have yielded the bulk modulus of GaN to be 237(31) GPa and that of InN to be 125.5(4.6) GPa. Structural phase transition into the rocksalt-type structure takes place in GaN at 52.2 GPa and in InN at 12.1 GPa. The trend in the transition pressures of the III-V nitrides is discussed in terms of various ionicity scales.

I. INTRODUCTION

The crystal structures formed by binary octet $A^N B^{8-N}$ compounds at ambient conditions are in a great majority of cases the rocksalt and zinc-blende types.[1] The wurtzite structure appears in fewer compounds, and some of them can also crystallize into the zinc-blende structure.[1,2] Lawaetz[2] discussed the stability of the wurtzite structure relative to the zinc-blende structure in terms of a critical parameter $\Delta(c/a)$, defined as $\Delta(c/a)=c/a-1.633$, where c/a is the axial ratio. The wurtzite structure prevails when $\Delta(c/a)$ is negative for a given compound. The axial ratio can in turn be related to the ionicity charge parameter,[2] ionic radius ratio,[3] or the Bloch-Simons coordinate.[4] Compounds with relatively large negative values of $\Delta(c/a)$ are III-V nitrides: AlN, GaN, and InN.[2] The axial ratios of the nitrides deviate considerably from an ideal value for hexagonal packing, and hence each lattice is distorted from the ideal geometry to some extent.

A question arises as to whether the distortion be enhanced or redeemed with an application of pressure. An answer was given by us in a previous paper,[5] which shows a decrease in the axial ratio of AlN with pressure, deviating further from the ideal value. The decrease was subsequently demonstrated to be in qualitative agreement with first-principles calculations.[6,7]

AlN thus exhibiting a pressure-induced decrease in the axial ratio is not simply stabilized in the wurtzite structure, but it is converted into the rocksalt structure at about 23 GPa. Then another question arises if there is any critical extent in the distortion of the wurtzite structure so as to undergo a phase transition.

To answer these questions is quite important for a better understanding of the structural properties of the nitrides at high pressure. This work was undertaken to study the effect of pressure on the axial ratio of the wurtzite structure and further to examine the phase transition from this structure. We extended our study[5] on AlN toward GaN and InN. The pressure coefficients of the axial ratio were found to be different from each other. The phase transition into the rocksalt structure was observed in both GaN and InN, a description of which was given earlier very briefly.[8,9] Discussion is made of the change in the axial ratio, of the elastic as well as the transition parameters, and also of the trend in the transition pressures of the three nitrides.

II. EXPERIMENT

Samples of GaN and InN (each with stated purity >99%) were obtained from Furuuchi Chemical Co. X-ray-diffraction analysis on the samples prior to compression yielded lattice parameters and intensities for the wurtzite-type structure in good agreement with earlier reports.[10,11] The InN sample contained In_2O_3, the amount of which being less than 1% as estimated from the x-ray-diffraction pattern.

High pressure was generated in a gasketed diamond-anvil cell.[12] A Ni-based alloy or stainless steel was used for the gasket. A 0.14–0.18-mm-diam hole for a sample chamber was drilled at the center of the gasket. Powdered samples were placed into the gasket hole together with fine powders of ruby to monitor the pressure.[13] A mixture of methanol, ethanol, and water was used as a pressure-transmitting medium.

X-ray-powder-diffraction experiments *in situ* under high pressure were carried out using Mo $K\alpha$ radiation from either a rotating anode (50 kV, 250 mA) or a conventional target (55 kV, 30 mA). Pyrolytic graphite was employed for a monochromator of the x rays from the rotating Mo anode. X rays from the conventional Mo tube were filtered with Zr metal. The beam size was reduced by a double-pin-hole collimator to a diameter of 60–120 μm. Diffracted x rays were exposed on an imaging plate[14] (IP) or an x-ray film. The exposure time was typically 9 h for the IP and 48 h for the film.

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III. RESULTS

A. X-ray-diffraction data

Figure 1 shows x-ray-diffraction patterns of GaN. In the pattern taken before the pressurization [Fig. 1(a)], eight diffraction peaks are observed which can be completely assigned to the wurtzite-type structure. Upon application of pressure, the wurtzite phase persisted up to about 50 GPa. Above 52.2 GPa, all the peaks from the wurtzite-type phase were very much weakened and some new peaks appeared, suggesting that a phase transition took place. This is exemplified by Fig. 1(b) recorded at 60.6 GPa. In Fig. 1(b), all the peaks from the wurtzite phase have disappeared and instead three new peaks appear. These new peaks can unambiguously be assigned to the (111), (200), and (220) reflections of the rocksalt-type structure. Therefore the transition in GaN is found to be from the wurtzite to the rocksalt structure.

The x-ray-diffraction pattern taken upon release of pressure was broadened and weakened as shown in Fig. 1(c). Although the relative intensities between the (002) and (101) reflections are reversed from those before compression, the pattern of Fig. 1(c) can be essentially interpreted on the basis of the wurtzite-type structure. This indicates that the pressure-induced transition in GaN is reversible.

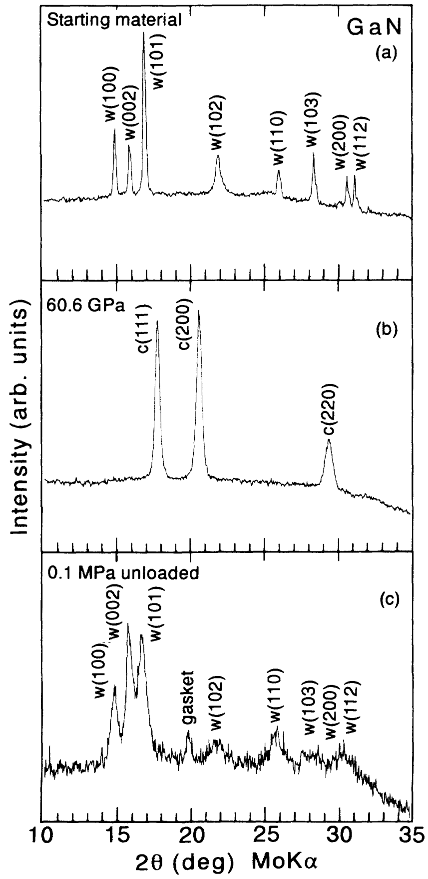

FIG. 1. X-ray-diffraction patterns of GaN at (a) ambient pressure before pressurization, (b) 60.6 GPa, and (c) ambient pressure after depressurization. The lower case *w*'s stand for the wurtzite phase and *c*'s for the rocksalt phase.

The interplanar spacings of GaN are plotted in Fig. 2 as a function of pressure. A discontinuity occurs in the *d* values at about 52 GPa, and this corresponds to the wurtzite-to-rocksalt phase transition.

Figure 3 shows representative x-ray-diffraction patterns of InN. At 6.2 GPa, 12 peaks of InN are observed and they can be completely assigned to the hexagonal wurtzite-lattice indices. Two peaks of In_2O_3 contained in the InN starting material are also observable at angles indicated by the arrows. At 9.5 GPa, two new peaks, shown by solid circles, appear between the (101) and (102) reflections of the wurtzite phase. The two peaks, however, show no further growth in intensity upon increments of pressure to 12.1 or even to 18.2 GPa. Also, these could not be interpreted by any known structure. At 12.1 GPa four new peaks appear. These four peaks are strengthened at 18.2 GPa, whereas the wurtzite phase reflections have disappeared. There is one other peak that appears at the same position as the wurtzite (101) reflection. It grows at the expense of the wurtzite (101) reflection. Consequently, five new peaks are available and they can be indexed as the (111), (200), (220), (311), and (222) reflections of the cubic lattice. Then the pressure-induced transition in InN is from the wurtzite to the rocksalt structure.

The transition of InN was also reversible as evidenced by the reappearance of the wurtzite phase in the x-ray-diffraction pattern shown at top of Fig. 3. This was taken at ambient pressure after being unloaded from 18.2 GPa.

Figure 4 shows the change of *d* values of InN as a function of pressure. The wurtzite-to-rocksalt transition takes place at a discontinuity in the *d* values. The *d* values for both the wurtzite and rocksalt type structures have very similar slopes, while the two unidentified peaks have steeper slopes. This suggests that the unidentified

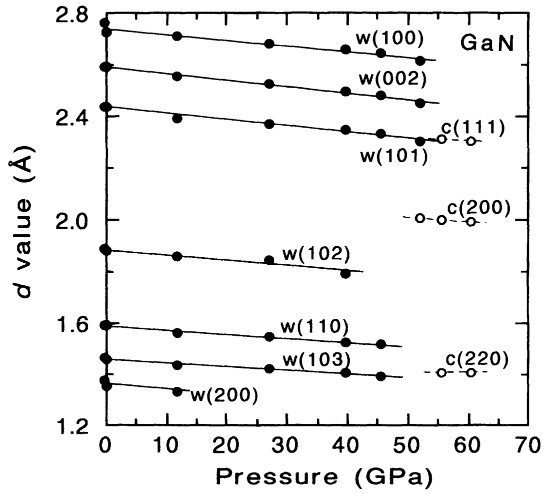

FIG. 2. Change of *d* values with increasing pressure for GaN. The solid, dashed, and dot-dashed lines are to guide the reader's eye. The solid circles are for the wurtzite phase, and the open circles are for the rocksalt phase. The lower case *w*'s denote the wurtzite phase and *c*'s the rocksalt phase.

peaks are from origins other than the wurtzite or rocksalt phase.

B. Lattice parameters

The lattice constants a and c and the axial ratio c/a for the wurtzite phase of GaN and InN are plotted in Fig. 5 as a function of pressure. In GaN, both the lattice constants a and c exhibit a monotonic decrease with increasing pressure. The axial ratio of GaN remains virtually unchanged with pressure way up to 52 GPa. In InN, the decrease of the lattice constants are also monotonous below 12 GPa. The axial ratio, however, exhibits an obvious decrease with increasing pressure.

Also, for InN but above 12 GPa, the a-axis length shows a curve and the decrease of the c-axis length becomes much faster. These changes cause a rapid fall of the axial ratio of InN as the pressure is increased past the transition (12 GPa). Actually, the two data points of the axial ratio above 12 GPa for InN were obtained from the persistent wurtzite phase after the transition.

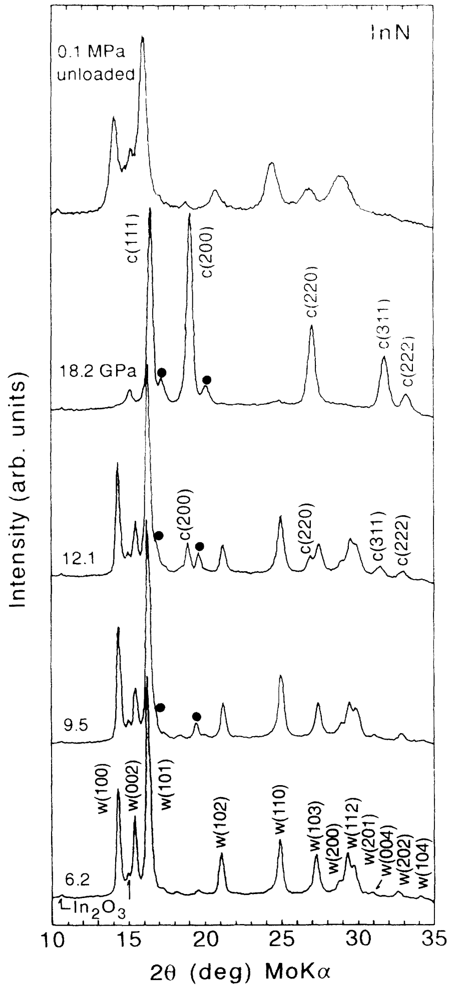

FIG. 3. X-ray-diffraction patterns of InN at ambient pressure and high pressure. The peaks indicated by solid circles are unidentified. The lower case w's are for the wurtzite phase and c's for the rocksalt phase.

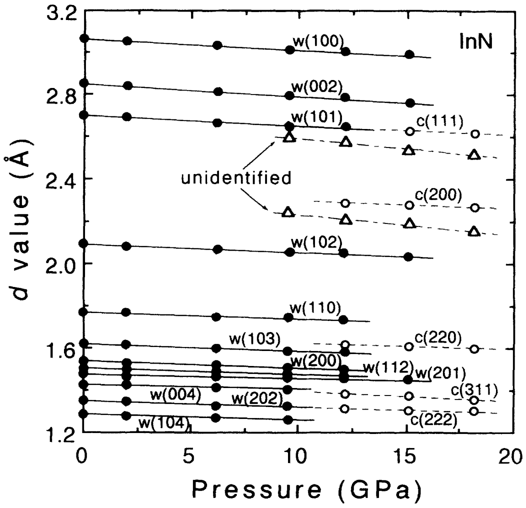

FIG. 4. Change of d values with increasing pressure for InN. The solid, dashed, and dot-dashed lines are to guide the reader's eye. The solid circles are for the wurtzite phase, and the open circles are for the rocksalt phase. The lower case w's denote the wurtzite phase and c's the rocksalt phase.

C. High-pressure phase

Table I compares the observation for d values and integrated intensities of GaN at 60.6 GPa with a calculation based on the rocksalt-type structure. The observed d values and intensities agree well with the calculations within 0.1% and 6.8%, respectively. The present finding of the phase transition supports a Raman-scattering and x-ray-absorption spectroscopic (XAS) study.[15] Also, the assignment of the high-pressure phase to the rocksalt structure is in agreement with a recent x-ray-diffraction

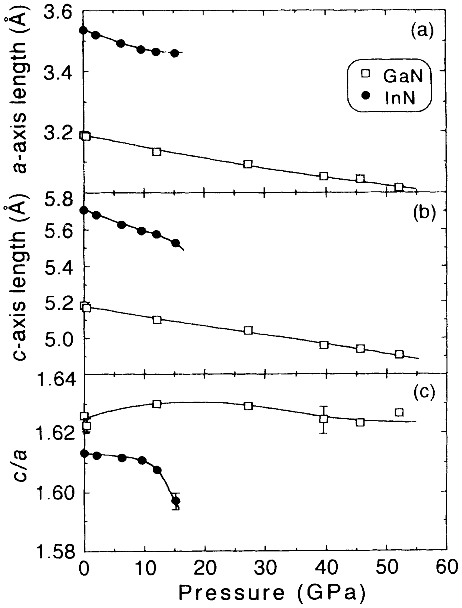

FIG. 5. Change of the lattice parameters of the wurtzite phase of GaN and InN with increasing pressure: (a) a axis, (b) c axis, and (c) axial ratio c/a.

TABLE I. Observed and calculated d values and integrated intensities for GaN at 60.6±5.9 GPa.

	Observed		Calculated[a]	
$h\,k\,l$	d_{obs} (Å)	$I/I_{0\,\text{obs}}$	d_{cal} (Å)	$I/I_{0\,\text{obs}}$
1 1 1	2.307(5)	92.2	2.305	99.0
2 0 0	1.995(1)	100.0	1.997	100.0
2 2 0	1.411(5)	66.6	1.412	66.1

[a] Calculated for the rocksalt-type structure of a cubic lattice with $a = 3.985$ Å.

experiment[16] and, furthermore, with all recent theoretical predictions.[17–19] The NiAs-type structure suggested in Ref. 18 can be excluded.

In Table II the d values and integrated intensities of InN observed at 18.2 GPa are compared with a calculation based on the rocksalt-type structure. The d values and intensities observed are in agreement with the calculation within 0.6% and 19%, respectively.

D. Equation of state

Figure 6 shows the relative volume change of GaN with increasing pressure. The volume exhibits a monotonous decrease with increasing pressure to 50 GPa and is reduced dramatically at 52.2 GPa owing to the phase transition from the wurtzite to rocksalt type. The volume reduction at 52.2 GPa is 17.9%. The pressure-volume data for the wurtzite phase are fitted with the Birch-Murnaghan equation of state.[20] The bulk modulus and its pressure derivative obtained are 237±31 GPa and 4.3±2.0, respectively.

Figure 7 shows the relative volume of InN as a function of pressure. Up to 12.1 GPa, the volume decreases monotonically. There is a drastic reduction in the volume at 12.1 GPa accompanied by the phase transition from the wurtzite to rocksalt type. The volume reduction at the transition is 17.6%.[21] The pressure-volume data for the wurtzite phase fitted to Birch-Murnaghan equation of state[29] yield a bulk modulus of 125.5±4.6 GPa and a pressure derivative of 12.7±1.4.

IV. DISCUSSION

A. Axial ratio

Figure 8 shows the axial ratio of the wurtzite structure AlN,[5] GaN, and InN plotted against pressure. The ratio is each normalized relative to the value at ambient pressure, which deviates significantly from the ideal value. The deviation is not amended by the application of pressure in each compound. In GaN, the axial ratio exhibits essentially no change with pressure. The axial ratios of AlN and InN further deviate with pressure. Consequently, the wurtzite lattices in the two nitrides are subject to further distortion from the ideal hexagonal geometry.

Eventually, at an axial ratio of about 0.995, a phase transition takes place in AlN and InN. It is likely that the wurtzite lattices at such a critical point, $(c/a)_c$, become unable to sustain strains developed by the distortion and that the wurtzite structure thus unstabilized is forced to finally collapse into the rocksalt structure. This argument is not applicable to GaN because it undergoes a phase transition without a noticeable distortion in the wurtzite lattice. Studies on other wurtzite-type compounds are required before other implications can be envisaged.

TABLE II. Observed and calculated d values and integrated intensities for InN at 18.2±0.5 GPa.

	Observed		Calculated[a]	
$h\,k\,l$	d_{obs} (Å)	$I/I_{0\,\text{obs}}$	d_{cal} (Å)	$I/I_{0\,\text{cal}}$
1 1 1	2.617(5)	100.0	2.617	100.0
2 0 0	2.267(1)	96.1	2.266	84.0
2 2 0	1.602(5)	59.7	1.602	61.9
3 1 1	1.359(5)	45.4	1.366	52.6
2 2 2	1.301(5)	16.1	1.308	19.5

[a] Calculated for the rocksalt-type structure of a cubic lattice with $a = 4.532$ Å.

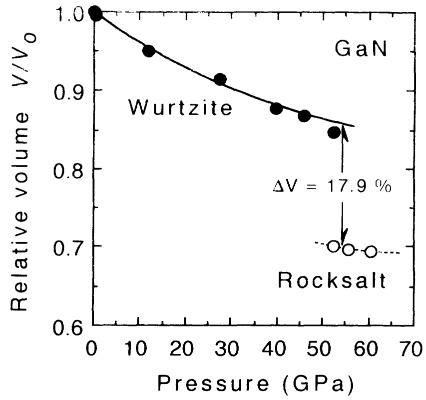

FIG. 6. Change of the relative volume of GaN with increasing pressure. The solid circles are for the wurtzite phase, and the open circles are for the rocksalt phase. The solid line is drawn by fitting the data with the Birch-Murnaghan equation of state. The dashed line is to guide the reader's eye.

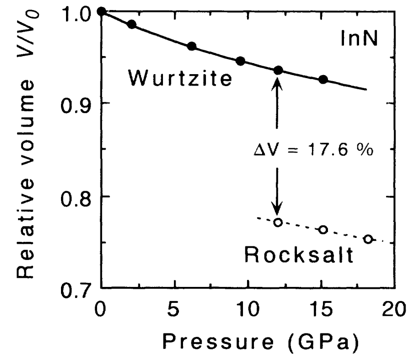

FIG. 7. Change of the relative volume of InN with increasing pressure. The solid circles are for the wurtzite phase, and the open circles are for the rocksalt phase. The solid line is drawn by fitting the data with the Birch-Murnaghan equation of state. The dashed line is to guide the reader's eye.

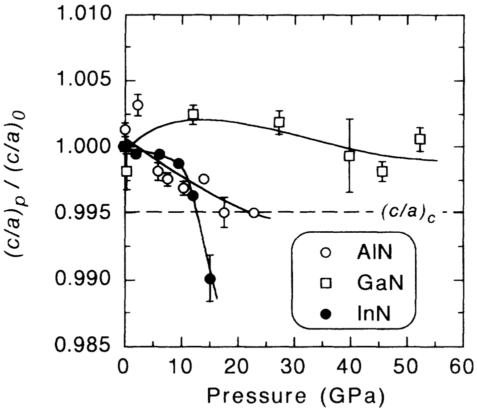

FIG. 8. Normalized axial ratio for AlN (after Ref. 5), GaN, and InN plotted against pressure. See text for $(c/a)_c$.

B. Elastic properties

The equation-of-state (EOS) data of GaN and InN are summarized in Table III. Also shown in Table III are results for wurtzite-type BN (wBN) and AlN from our previous studies.[5,8,9] We compare our data with other experimental[15,16] and theoretical studies.[6,7,17–19,22–27]

Our bulk moduli for wBN and AlN are in good agreement with some[6,7,22,25] of the calculations. In particular, the agreement is striking for wBN. For GaN, both the linear muffin-tin orbital (LMTO) calculation[17] and two[18,26] of the pseudopotential calculations yield B_0's which agree well with our experiment. There is one calculation[27] available for InN, presenting B_0 much higher than our experimental value. In addition, there are significant differences between our experiment and the calculations in the pressure derivatives of the bulk moduli (B_0') for all the nitrides.

Three sets of experimental B_0 data are available for GaN. Our B_0 is quite close to that derived from the XAS study.[15] The x-ray-diffraction experiment[16] gives a B_0 that is the smallest among the experiments and even smaller than the smallest of the calculations.

C. Transition parameters

In Table III, we also show transition parameters for AlN, GaN, and InN. Some discrepancies between the experiments and calculations occur in the transition pressure (P_t) of each nitride. It appears that the theories[6,7,23,24] underestimate the transition pressure of AlN. As noted earlier,[5] it is rational that the theoretical equilibrium pressure is always lower than the transition pressure obtained from upstroke experiments. The authors of Ref. 6 agree with this point, which is pertinent to the AlN case.

For GaN, pseudopotential calculations[18,19] predict transition pressures somewhat higher than our experimental value. The LMTO calculation[17] shows a value (65 GPa) that is significantly higher than the experiments. In the light of the above discussion on equilibrium vs experimental transition pressure, all the theories[17–19] for GaN seem to overestimate the transition pressure.

A large discrepancy by a factor of about 2 exists in the transition pressure of InN between our experiment and the calculation.[27] The calculation[27] assumes an ideal value of 1.633 for the axial ratio of the wurtzite lattice in

TABLE III. Equation-of-state data and parameters for the transition from the wurtzite-to-rocksalt phase for III-V nitrides.

	B_0 (GPa)	B_0'	P_t (GPa)	ΔV (%)	Method	Reference
wBN	**390±3**	**3.5±0.8**	no transition to 106 GPa		x-ray diffraction	8,9
	390	6.3			LCAO[b]	22
AlN	**207.9±6.3**	**6.3±0.9**	**22.9±0.2**	**19.5**[a]	x-ray diffraction	5
	204	3.10	7	21	pseudopotential	7
	195	3.74	12.9	22.5	pseudopotential	23
	221		16.6	18.1	LMTO-ASA[c]	24
	205		12.5	19	LMTO-FP[d]	6
	207	3.98			LCAO[b]	25
GaN	**237±31**	**4.3±2.0**	**52.2±3.0**	**17.9**	x-ray diffraction	this work
	245		47	14	x-ray absorption spectroscopy	15
	188	3.2	37	17	x-ray diffraction	16
	239		65	10	LMTO[e]	17
	244		55	11	pseudopotential	18
	190	2.92	55.1	14	pseudopotential	19
	240				pseudopotential	26
InN	**125.5±4.6**	**12.7±1.4**	**12.1±0.2**	**17.6**[a]	x-ray diffraction	this work
	165		25.4		LMTO[e]	27

[a] Reference 21.

[b] Linear combination of atomic orbitals.

[c] Linear muffin-tin orbital with atomic-spheres approximation.

[d] Full-potential linear muffin-tin orbital.

[e] Linear muffin-tin orbital.

spite of a significant deviation from it as verified by our experiment ($c/a = 1.613$ at ambient pressure). Since the total energy can vary with the axial ratio,[6] any refinement involving a change of the axial ratio may be needed.

No transition has been observed in wBN up to 106 GPa at room temperature. Although the wurtzite-to-rocksalt transition can be expected to occur in wBN at higher pressure, a theoretical calculation predicts a zinc-blende–to–wurtzite phase transition (133 GPa).[22]

Among the experiments undertaken on GaN, there is only a small difference in P_t between our x-ray-diffraction and the XAS (Ref. 15) experiments, whereas a big difference exists between the two x-ray-diffraction experiments (this study and Ref. 16). A difference in location of P_t arising from the difference in probing techniques has been noted in the pressure-induced transition of AlN (Ref. 5) and GaAs.[28] When a change in color of AlN was visually observed at 18–20 GPa, there was still no indication of the transition in the x-ray-diffraction pattern. In this case, the x-ray diffraction detected the onset of the transition at 22.9 GPa. Quite a similar situation can occur between the XAS (Ref. 15) and our x-ray-diffraction studies in detecting the transition of GaN. Basically, the XAS probes atomic-scale environments and hence is much more sensitive than our x-ray diffractometry. In addition, the XAS study[15] also detected a transition from blackening of the sample. Therefore the difference in P_t by 5 GPa between the XAS (Ref. 15) and our x-ray-diffraction experiments appears to be rather reasonable.

A much larger difference in P_t between the two x-ray-diffraction studies (this study and Ref. 16) may also be ascribed to the difference in the sensitivities inherent in the x-ray-diffraction techniques. In Ref. 16, a synchrotron radiation was employed for the x-ray source. This technique permits discriminating reflections that are very weak or cannot be recorded otherwise. A very simple conclusion derived from this fact would be that the synchrotron x-ray-diffraction study[16] can detect the transition of GaN most sensitively. In fact, the onset of the transition was observed at 37 GPa.

There remains, however, the question addressed to the very low value of B_0 obtained from that study, as discussed in the preceding section. The determination of B_0 primarily depends on the accuracy in determining the lattice parameters and the pressure. The IP technique[14] employed in this study is the most accurate among the three experiments undertaken for GaN. Monitoring of the pressure was made by ruby fluorescence[13] in the XAS (Ref. 15) and these experiments, while it was by the EOS of Au or GaN in the synchrotron x-ray-diffraction experiment.[16] We have at present no answer as to whether or not the difference in the pressure monitors can give rise to the difference in B_0's.

Despite the difference in B_0 and P_t between the two x-ray-diffraction experiments (this study and Ref. 16), the volume reductions (ΔV) at the transition of GaN are very close to each other. The three calculations[17–19] for GaN give values which are considerably smaller than our ΔV. In AlN, better agreement in ΔV is achieved between our experiment[5] and the calculations.[6,7,23,24]

D. Ionic character and trends in the transition

Although the first-principles calculations cited in the preceding discussions interpret the elastic properties and transition parameters reasonably well, the interpretation is limited to particular substances. No general trend or systematization is given for any series of compounds. Such information can be derived from a much more intuitive approach.

Ionicity can most successfully interpret the general trends in the pressure-induced phase transitions of $A^N B^{8-N}$ compounds. First, the pressure for the transition from the fourfold-coordinated structures into sixfold-coordinated structures decreases with increasing ionicity.[29–33] Second, the preference of the sixfold-coordinated phase, β-Sn or rocksalt structure, is governed by ionicity[30,32,34] and the ionicity separating the two structures lies between 0.3 and 0.5.[30,34]

In the nitrides, the P_t's predicted on the basis of quantum dielectric theory[29] are 90 GPa for AlN, 87 GPa for GaN, and 26 GPa for InN.[31] The predicted trend in these P_t's agree with that in Phillips ionicity (f_i), along the line of the general trend.[19,30,32,33] The fact we have obtained is that the experimental values for P_t of the nitrides do not fit this trend; P_t decreases in an order GaN (52.2 GPa)→AlN (22.9 GPa) →InN (12.1 GPa). Such a situation is also met when the anion is replaced by phosphorus. The trends in the nitrides and phosphides obviously arise from the high values of P_t in the Ga compounds and the small values of f_i for the Al compounds.

Attempts were made to plot the P_t of the III-V compounds against some ionicity scales other than f_i. The ionicity derived from the first-principles calculation (f_i^*), put forth by Christensen, Satpathy, and Pawlowska,[33] exhibits nearly the same chemical trends as f_i, but shows common drops at the Ga compounds. For the phosphides, the change of P_t becomes in harmony with the change in f_i^*. This is shown in Fig. 9. Unfortunately, there is no f_i^* available for the nitrides from the calcula-

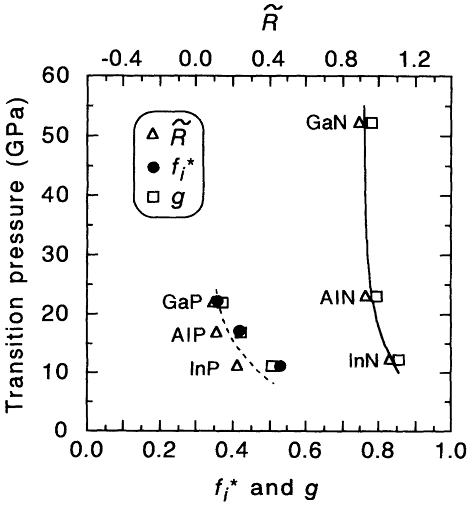

FIG. 9. Plots of the transition pressure vs f_i^* (Ref. 33), g (Ref. 35), or $\tilde{R}$ (Ref. 36). See text for f_i^*, g, and $\tilde{R}$.

tion.[33] As an alternative, we take the charge asymmetry coefficient (g) presented by García and Cohen.[35] In Fig. 9, we plot the P_t of the nitrides against g, despite the fact that the calculation is made for the zinc-blende-type structure.[35] Here, again, P_t changes smoothly relative to the change in g of the nitrides. For reference we show, in Fig. 9, P_t-vs-g plots for the phosphides. These plots are very similar to the P_t-vs-f_i^* plot, ensuring a good correspondence between f_i^* and g. A plotting is also made in Fig. 9 by another *ab initio* ionicity scale, the effective orbital ionicity ($\tilde{R}$).[36] The plot of P_t against $\tilde{R}$ for the nitrides, after $\tilde{R}$ from -0.6 to 1.4 is adjusted to between zero and unity in the g scale, exhibits a trend quite similar to the P_t-vs-g plot. For the phosphides, P_t-vs-$\tilde{R}$ plots come near to both P_t-vs-f_i^* and P_t-vs-g plots.

A significant feature exhibited by the three ionicity scales f_i, f_i^*, and g is that the scales derived from first-principles calculations (f_i^* and g) give ionicities larger than that derived from empirical dielectric theory (f_i) for the phosphides and nitrides.[33,35] Another feature is that the ionicities in f_i^* and g exhibit, respectively, minima at Ga when we move Al→Ga→In in a series of the III-V nitrides, phosphides, arsenides, or antimonides.[33,35] The effective orbital ionicity $\tilde{R}$ shows similar trends.[36] Such minima are not found in f_i.[29] Apparently, this second feature makes it possible to interpret the trends in the transition pressures of the nitrides and phosphides.

V. CONCLUSION

The present and the previous[5,8,9] x-ray-diffraction studies performed on the III-V nitrides have provided us with a very comprehensive picture of the structural properties of the wurtzite-type nitrides at high pressure.

Changes in the axial ratio (c/a) in the wurtzite phase are not unanimous; the ratio decreases with pressure in AlN and InN, deviating further from the ideal value, whereas it remains virtually unchanged in GaN. The application of pressure does not redeem the distorted wurtzite lattice back to the ideal geometry. In AlN and InN, a critical extent exists in the distortion at which the wurtzite lattice collapses and undergoes a transition.

A structural phase transition occurs at 22.9 GPa in AlN, at 52.2 GPa in GaN, and at 12.1 GPa in InN, each into the rocksalt-type structure. The existing first-principles calculations appear to overestimate the transition pressures in GaN (Refs. 17–19) and in InN (Ref. 27) and underestimate those of AlN.[6,7,23,24] The trend in the transition pressures for AlN, GaN, and InN does not fit the trend in Phillips ionicity,[29] but is instead in harmony with the ionicity scales of García and Cohen[35] and of Yeh *et al.*,[36] respectively, derived from first-principles calculations.

The bulk modulus for the wurtzite phase (390 GPa for wBN, 207.9 GPa for AlN, and 237 GPa for GaN) each agrees with first-principles calculations,[6,7,17,18,25,26] but that of 125.5 GPa for InN disagrees with the calculation.[27]

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