Electronic, optical, and mechanical properties of BN, AlN, and InN with zinc-blende structure under pressure

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In this work, the electronic, optical, and mechanical properties of BN, AlN, and InN under the action of pressure are calculated. For each of these compounds, the energy band structure, band gaps (E_g^L, E_g^Γ, E_g^X), refractive index (n), dielectric constants (ε_∞, ε_0), elastic constants (C_{11}, C_{12}, C_{44}), and relevant parameters such as bulk (B_u), shear (S_h), and Young's (Y_0) moduli are studied, and other important parameters such as bond-stretching (α), bond-bending (β) force constant, internal-strain parameter (ζ), effective charges (e_T^*, Z^*), anisotropy factor (I_s), Poisson's ratio (P_o), Cauchy ratio (C_a), the ductility index (μ_D), and linear compressibility (C_0) are also calculated. The effects of pressure on all studied properties are investigated. Our results are in good agreement with the available experimental and theoretical data for BN, AlN, and InN.

Keywords: electronic properties, optical properties, mechanical properties, BN, AlN, InN

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1. Introduction

Nitrides form a specific subgroup of the III–V materials described by wide energy gaps, high ionicity, strong bonds, low compressibility, and high thermal conductivity, and mechanical stability.[1] Wide energy gap nitride semiconductors such as BN, AlN, InN, and GaN have received a great deal of research interest and achieved important development due to their device applications in blue and ultraviolet wavelengths. They can be utilized in blue and ultraviolet light emitting diodes, room temperature laser diodes (LDs), solar cells, and the field-effect transistors.[2–6] Recently, the blue light III–V nitride semiconductor laser was first successfully fabricated by Nekamura.[7] The pressure dependence and temperature dependence of the electronic, optical, and mechanical properties in semiconductors have become the subjects of many studies.[8–23] These studies can supply further worthy data about the energy band structure and energetic properties of the nitride group.

In this paper, we carry out calculations to determine the electronic band structures, optical and mechanical properties of BN, AlN, InN compounds using the empirical pseudopotential method (EPM). The studied properties for each of the considered materials are the E_g, n, ε_∞, ε_0, (C_{11}, C_{12}, C_{44}), S_h, B_u, and Y_0, and other important parameters such as P_0, C_0, μ_D, C_a, I_s, α, β, ζ, and e_T^* of the studied binary compounds are also investigated under the action of pressure.

2. Theory and calculation

The calculations are carried out using the EPM. The pressure-dependent eigenvalues $E_{nk}(P)$ are found out by solving numerically the secular determinant,

$$\left\| \frac{1}{2}\left|\boldsymbol{k}+\boldsymbol{G}'\right|^2 - E_{nk}(P) + \sum_{\boldsymbol{G}\neq\boldsymbol{G}'} V\left(\left|\boldsymbol{G}-\boldsymbol{G}'\right|, P\right) \right\| = 0, \quad (1)$$

where

$$V\left(\left|\boldsymbol{G}-\boldsymbol{G}'\right|, P\right) = W^{\mathrm{s}}(\Delta\boldsymbol{G}, P)\cos(\Delta\boldsymbol{G}\cdot\boldsymbol{\tau}) + \mathrm{i}W^{\mathrm{a}}(\Delta\boldsymbol{G}, P)\sin(\Delta\boldsymbol{G}\cdot\boldsymbol{\tau}) \quad (2)$$

is the pressure-dependent pseudo-potential. W^{s} and W^{a} are the symmetric and anti-symmetric pressure-dependent form factors, respectively. The EPM involves the fitting of the atomic form factors to experimental values of energy gaps of studied semiconductors. $\boldsymbol{G}$ and $\boldsymbol{G}'$ are the reciprocal lattice vectors, with $\Delta\boldsymbol{G} = \boldsymbol{G} - \boldsymbol{G}'$ and $\boldsymbol{\tau} = \frac{a(P)}{8}(1,\ 1,\ 1)$ is the position vector of each atom in the unit cell with $a(P)$ being the pressure-dependent lattice constant.

The pressure-dependent lattice constant is calculated from the relation[22]

$$a(P) = a(0)\left[1 + \left(\frac{B'}{B_u}\right)P\right]^{-1/(3B')}, \quad (3)$$

where B_u is the bulk modulus, B' is its pressure derivative, $a(0)$ and $a(P)$ are the lattice constants at $P = 0$ and $P \neq 0$, respectively. Equation (1) is solved numerically by using our MATLAB language program, which is a 65×65 matrix based on 65 bulk reciprocal lattice vectors $\boldsymbol{G}$'s. These values are corresponding to $|\Delta\boldsymbol{G}|^2 = 3$, 4, and 11 for zinc-Blende-type structure, which satisfy the condition $|\Delta\boldsymbol{G}|^2 \leq 11$, which gives the non-zero pseudo-potential.[20]

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The valence and conduction energy band gaps of the studied compounds are obtained by arranging the obtained eigenvalues $E_{nk}(P)$ and setting the top of the valence bands to be zero energy. The calculated energy band gaps used in the fitting procedure and the adjusting form factors of BN, AlN, and InN for various pressures are recorded in Table 1.

Optical properties are of fantastic significance in the design and evaluation of optoelectronic devices. The refractive index is a completely vital parameter in the semiconductor. It represents an essential physical aspect that describes their optical and electronic properties, knowing n is crucial for devices such as photonic crystals, wave guides, solar cells, and detectors.[24] Numerous efforts have been made to relate the index of refraction to the energy band gap E_g through simple relations.[25–30] There are different methods to calculate the refractive index; our calculations are obtained by using the Moss formula.[25] The dielectric characteristic is a key optical quantity to extract all different optical properties like absorption spectrum, energy loss function, refractive index, and reflectivity. The dielectric function depicts the linear response of a system to electromagnetic radiation.[31] Knowing the refractive index of the considered materials, we calculate the high frequency ε_∞ and static ε_0 dielectric constants.[12]

The influence of strain on the electronic property requires the knowledge of the mechanical properties of materials, and precise elastic constants which characterize the response to an applied macroscopic stress.[32] The cubic crystal has only three independent elastic constants, specifically C_{11}, C_{12}, and C_{44}.[33–35] The elastic constants of the materials are calculated by knowing the polarities of the studied materials, which are derived from the adjusted symmetric $W^{\mathrm{S}}(P)$ and anti-symmetric $W^{\mathrm{A}}(P)$ form factors at $G(1,\ 1,\ 1)$ as shown in Ref. [36],

$$\alpha_p(P) = -\frac{W_3^{\mathrm{A}}(P)}{W_3^{\mathrm{S}}(P)}. \tag{4}$$

The elastic constants C_{11}, C_{12}, and C_{44} of the considered materials are calculated by following the same procedure used by Bouarissa which turned into primarily based essentially on the work of Baranowski[37,38] as shown below,

$$C_{11}(P) = \frac{\sqrt{3}}{4d^5}\left[4.37\frac{\hbar^2}{m}(5+\lambda)\left(1-\alpha_p^2(P)\right)^{3/2} - 0.60751\left(1-\alpha_p^2(P)\right)^{1/2}\frac{\hbar^2}{m}\right], \tag{5}$$

$$C_{12}(P) = \frac{\sqrt{3}}{4d^5}\left[4.37\frac{\hbar^2}{m}(3-\lambda)\left(1-\alpha_p^2(P)\right)^{3/2} + 0.60751\left(1-\alpha_p^2(P)\right)^{1/2}\frac{\hbar^2}{m}\right], \tag{6}$$

$$C_{44}(P) = \frac{3(C_{11}(P)+2C_{12}(P))(C_{11}(P)-C_{12}(P))}{(7C_{11}(P)+2C_{12}(P))}, \tag{7}$$

where d is the nearest-neighbor distance. The knowledge of these elastic constants permits us to determine the bulk (B_{u}), shear (S_{h}), and Youn's (Y_0) modulus of each of the considered materials as follows:[34,35]

$$B_{\mathrm{u}}(P) = \frac{(C_{11}(P)+2C_{12}(P))}{3}, \tag{8}$$

$$S_{\mathrm{h}} = \frac{C_{11}(P)-C_{12}(P)}{2}, \tag{9}$$

$$Y_0(P) = \frac{(C_{11}(P)+2C_{12}(P))(C_{11}(P)-C_{12}(P))}{(C_{11}(P)+C_{12}(P))}. \tag{10}$$

The bond stretching $\alpha(P)$, bond-bending $\beta(P)$ force constant, and internal-strain parameter $\zeta(P)$ of studied compounds are also determined, which are related to the elastic constants as indicated in Refs. [39]–[41],

$$\alpha(P) = \frac{d(P)}{\sqrt{3}}[C_{11}(P)+3C_{12}(P)] + \frac{d(P)}{3\sqrt{3}}[1.473S(P)C_0(P)], \tag{11}$$

$$\beta(P) = \frac{d(P)}{\sqrt{3}}[(C_{11}(P)-C_{12}(P)) - 0.053S(P)C_0(P)], \tag{12}$$

$$\zeta(P) = \frac{2C_{12}(P)-0.314S(P)C_0(P)}{C_{11}(P)+C_{12}(P)-0.314S(P)C_0(P)}, \tag{13}$$

where $C_0(P)$ is the pressure-dependent linear compressibility that is given by Ref. [22]

$$C_0(P) = \frac{1}{C_{11}(P)+2C_{12}(P)}. \tag{14}$$

The parameter $S(P)$ is given by Ref. [41]

$$S(P) = \frac{Z^{*^2}(P)}{\varepsilon(P)}, \tag{15}$$

where $\varepsilon(P)$ is the pressure-dependent static dielectric constant, $Z^*(P)$ is the pressure-dependent effective charge which was calculated according to the following relation:[42]

$$Z^*(P) = e_{\mathrm{T}}^*(P) - \frac{8}{3}(\alpha_{\mathrm{p}}(P)(1-\alpha_{\mathrm{p}}^2(P)), \tag{16}$$

where $e_{\mathrm{T}}^*(P)$ is the pressure-dependent transverse effective charge that is given from the following relation:[43]

$$2e_{\mathrm{T}}^*(P) = \left[-\Delta Z + \frac{8\alpha_{\mathrm{p}}(P)}{1+\alpha_{\mathrm{p}}^2(P)}\right], \tag{17}$$

where ΔZ is the change in valence of the studied material.

Other important constants such as Cauchy $C_{\mathrm{a}}(P)$ and Born $B_0(P)$ ratios could also be determined in terms of the elastic constants as[22]

$$C_{\mathrm{a}}(P) = \frac{C_{12}(P)}{C_{44}(P)}, \tag{18}$$

$$B_0(P) = \frac{(C_{11}(P)+C_{12}(P))^2}{4C_{44}(P)(C_{11}(P)-C_{44}(P))}. \tag{19}$$

The ductility index (μ_{d}) can be calculated according to the empirical formula of Pugh,[35]

$$\mu_{\mathrm{d}} = \frac{B_{\mathrm{u}}}{S_{\mathrm{h}}}. \tag{20}$$

3. Results and discussion

The pressure dependent eigenvalues $E_{nk}(P)$ for the considered compound are found by solving the secular equation (1) at room temperature and different pressures. The experimental value of the energy band gap as a function of pressure which is used in the fitting procedure is given from Ref. [22],

$$E_g(P) = E_g(0) + aP + bP^2, \tag{21}$$

where a and b represent the pressure coefficients.

The properties at high-pressure values may be different from those under normal conditions. The influence of pressure on the calculated energy band gap of each of BN, AlN, and InN is listed in Table 1 and displayed in Fig. 1. Our calculated results show that BN and AlN are indirect semiconductors under the normal pressure and stay indirect in the studied region of pressure (0 kbar–120 kbar, 1 bar = 10^5 Pa). In contrast, InN is a direct semiconductor till 40 kbar and becomes indirect (X) in the other region of the studied pressure (40 kbar–120 kbar). Table 1 also contains the lattice constants of the considered materials at different pressures. Our calculated results are compared with the available published data and show excellent accordance.[23,44–48]

Figure 1 shows the variations of energy band gaps of BN, AlN and InN with pressure. The behaviors of the E_g^L, E_g^Γ, and E_g^X with pressure could be described by the following polynomials:

For BN

$$E_g^L(P) = 11.479 + 0.0075P - 6\times10^{-5}P^2, \tag{22}$$
$$E_g^\Gamma(P) = 10.021 + 0.0341P - 0.0002P^2, \tag{23}$$
$$E_g^X(P) = 6.1219 - 0.0002P + 6\times10^{-6}P^2. \tag{24}$$

For AlN,

$$E_g^L(P) = 8.9013 + 0.0205P - 3\times10^{-5}P^2, \tag{25}$$
$$E_g^\Gamma(P) = 6.2748 + 0.0456P - 7\times10^{-5}P^2, \tag{26}$$
$$E_g^X(P) = 5.1788 + 0.0017P + 1\times10^{-5}P^2. \tag{27}$$

For InN

$$E_g^L(P) = 5.8141 - 0.0008P + 1\times10^{-5}P^2, \tag{28}$$
$$E_g^\Gamma(P) = 1.9 + 0.0019P + 4\times10^{-7}P^2, \tag{29}$$
$$E_g^X(P) = 2.5098 - 0.0142P + 7\times10^{-5}P^2. \tag{30}$$

Table 1. Energy band gaps for BN, AlN, and InN at various pressures.

BN							
P/kbar	0	20	40	60	80	100	120
E_g^L/eV	11.479, 11.5[a]	11.619	11.694	11.704	11.677	11.611	11.51
E_g^Γ/eV	10.021, 10.0[a]	10.678	11.146	11.44	11.616	11.691	11.674
E_g^X/eV	6.1219, 6.1[a]	6.1125, 6.112[b]	6.1242, 6.124[b]	6.1312, 6.136[b]	6.1442, 6.148[b]	6.1662, 6.16[b]	6.1764, 6.172[b]
a/Å	3.6155	3.561	3.5155	3.4766	3.4427	3.4126	3.3856
AlN							
P/kbar	0	20	40	60	80	100	120
E_g^L/eV	8.9013, 9.07[c]	9.2581	9.6779	10.02	10.349	10.63	10.894
E_g^Γ/eV	6.2748, 6.2[d]	7.0812	8.0067	8.7825	9.529	10.18	10.791
E_g^X/eV	5.1788, 5.1[e]	5.1811, 5.1826[b]	5.2687, 5.2626[b]	5.3319, 5.3398[b]	5.4125, 5.4142[b]	5.4827, 5.486[b]	5.557, 5.555[b]
a/Å	4.37	4.2604	4.1689	4.0951	4.0335	3.9806	3.9345
InN							
P/kbar	0	20	40	60	80	100	120
E_g^L/eV	5.8141, 5.82[f]	5.7812	5.7914	5.8102	5.8298	5.8443	5.8609
E_g^Γ/eV	1.90, 1.94[f]	1.9395, 1.9399[b]	1.975, 1.9797[b]	2.0193, 2.0193[b]	2.0586, 2.0587[b]	2.0989, 2.098[b]	2.1374, 2.1371[b]
E_g^X/eV	2.5098, 2.51[f]	2.1694	2.0199	1.9264	1.8613	1.8038	1.7602
a/Å	4.96	4.8297	4.7676	4.7266	4.6961	4.6718	4.6516

[a]Ref. [44], [b]Ref. [22], [c]Ref. [45], [d]Ref. [46], [e]Ref. [47], [f]Ref. [48].

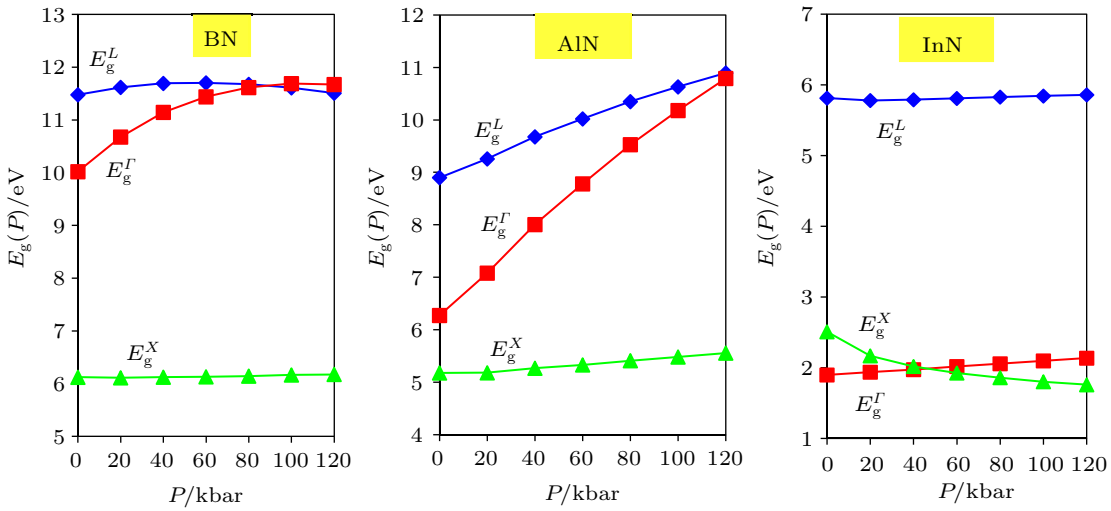


Fig. 1. (color online) Variations of energy band gaps of BN, AlN, and InN with pressures.

The final adjusted pseudo-potential form factors of BN, AlN, and InN at different values of pressure are listed in Table 2. From this table we note that the pseudo-potentials increase with pressure increasing.

Figure 2 shows the electronic energy band structures for BN, AlN, and InN for two values of pressure, $P = 0$ kbar (solid lines) and $P = 120$ kbar (dash lines). Applied hydrostatic pressure affects the electronic band structures of zinc-blende BN, AlN, and InN without changing the shapes of the bands. Note that all the bands are shifted. Each shift is not constant and depends on the k-point and energy. The figure shows that both conduction and valence energy bands are affected by pressure. It is seen that the first conduction energy band is more affected by pressure than the other bands and exhibits greater enhancement at the Γ-high point of symmetry. Also, it is noticed that the InN is less sensitive to pressure than BN and AlN.

Figure 3 shows the variations of the refractive indices of BN, AlN, and InN with pressure. The refractive indices of BN and AlN are approximately the same and less sensitive to pressure, while InN has a large refractive index that decreases almost linearly with pressure increasing.

Table 2. The adjusted form factors of BN, AlN, and InN at different values of pressure.

Form factors Ry \ P	0	20	40	60	80	100	120
BN							
$W_3^s(P)$	−0.52873	−0.52856	−0.52843	−0.52823	−0.52813	−0.52805	−0.528
W_8^s(P)	−0.01700	−0.016	−0.016	−0.016	−0.016	−0.016	−0.01609
$W_{11}^s(P)$	0.4679	0.5115	0.5531	0.5930	0.6310	0.6700	0.70
$W_3^a(P)$	0.120014	0.1200	0.1200	0.1200	0.1200	0.1201	0.1201
$W_4^a(P)$	0.3200	0.3201	0.3202	0.3205	0.3206	0.3208	0.3209
$W_{11}^a(P)$	0.1200	0.1201	0.1203	0.1204	0.1207	0.1209	0.12
AlN							
$W_3^s(P)$	−0.50300	−0.502	−0.502	−0.502	−0.502	−0.502	−0.502
W_8^s(P)	0.2309	0.2311	0.2312	0.2314	0.2317	0.2318	0.2319
$W_{11}^s(P)$	0.029951	0.05	0.0867	0.11	0.1315	0.1502	0.1676
$W_3^a(P)$	0.200013	0.2001	0.2003	0.2006	0.2007	0.2009	0.2011
$W_4^a(P)$	0.322993	0.3231	0.3232	0.3234	0.3237	0.3238	0.3240
$W_{11}^a(P)$	0.090077	0.090377	0.090477	0.090677	0.090777	0.090877	0.090977
InN							
$W_3^s(P)$	−0.35889	−0.35879	−0.35869	−0.35849	−0.35839	−0.35819	−0.35799
W_8^s(P)	0.253999	0.2542	0.2543	0.2545	0.2546	0.2549	0.2549
$W_{11}^s(P)$	0.207999	0.21	0.2165	0.2193	0.2215	0.2235	0.2253
$W_3^a(P)$	0.139967	0.1400	0.1401	0.1403	0.1406	0.1407	0.1408
$W_4^a(P)$	0.429999	0.4301	0.4302	0.4305	0.4307	0.4308	0.4309
$W_{11}^a(P)$	0.3990	0.3992	0.3993	0.3995	0.3996	0.3998	0.3999

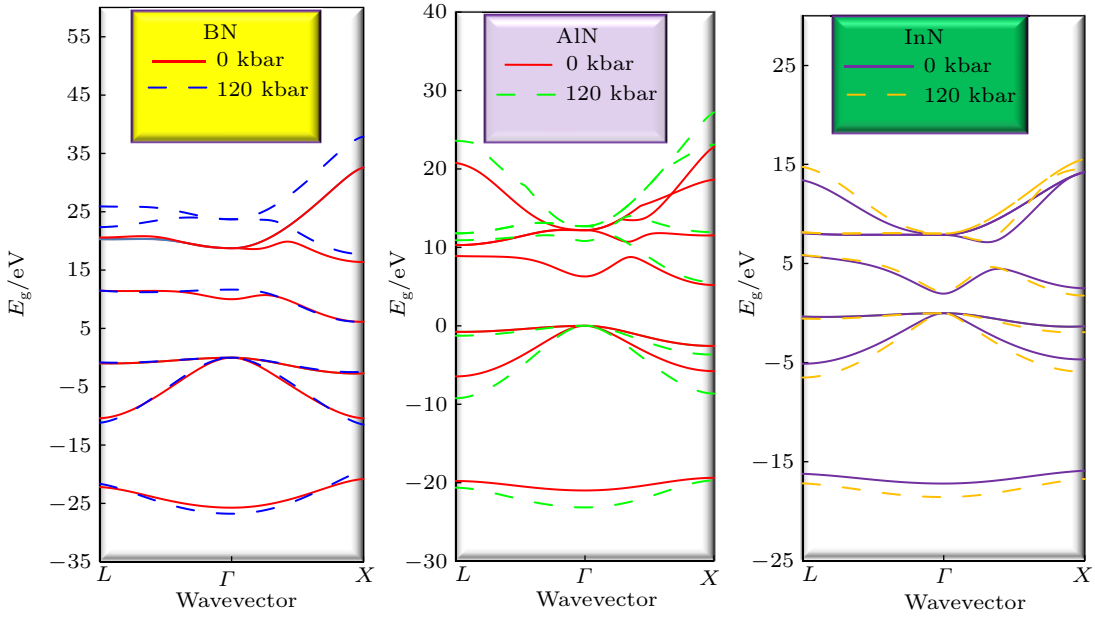


Fig. 2. (color online) Electronic energy band structures for BN, AlN, and InN for pressures $P = 0$ kbar (solid lines) and $P = 120$ kbar (dash lines).

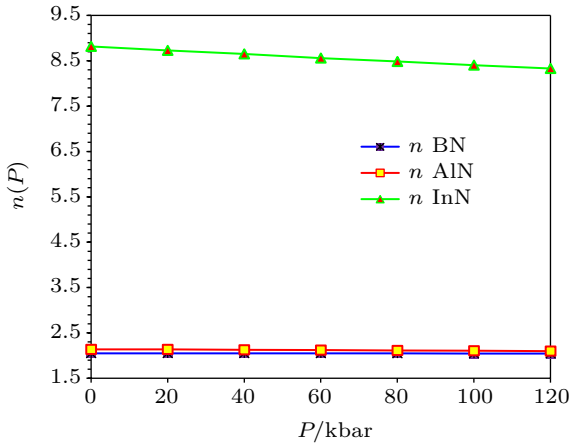


Fig. 3. (color online) Refractive indices of BN, AlN, and InN versus pressure.

The variations of high frequency and the static dielectric constants for BN, AlN, and InN with pressure are displayed in Fig. 4. The figure shows that the optical dielectric constants for BN and AlN are less sensitive to pressure than InN, which has high values and decreases linearly with pressure increasing. The variations of the static dielectric constants for the considered materials have the same behavior as the high frequency dielectric constants.

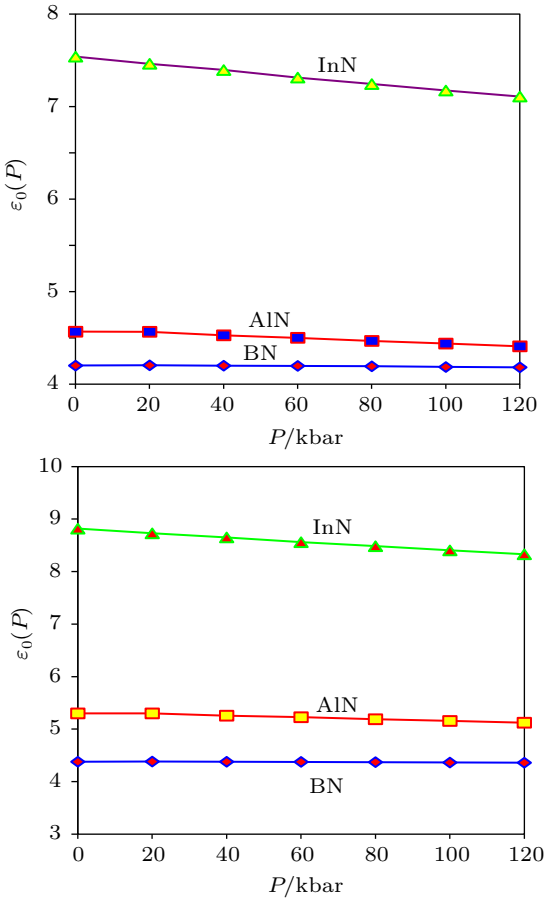


Fig. 4. (color online) Variations of optical and static dielectric constants of BN, AlN, and InN with pressures.

From the final adjusted symmetric $W^{S}(P)$ and antisymmetric $W^{A}(P)$ form factors at $G(1, 1, 1)$, the polarities of the considered materials at various pressures are calculated and shown in Table 3. The polarities of the considered materials slightly increase with pressure increasing. The calculated values of polarities for the considered materials are in excellent accordance with the published values. Knowing the polarities of BN, AlN, and InN, their elastic constants (C_{11}, C_{12}, and C_{44}) at various pressures can be calculated. The calculated values of elastic constants (C_{11}, C_{12}, and C_{44}) and the linear compressibility C_0 of BN, AlN, and InN at various pressures are listed in Table 3 and shown in Fig. 5. The elastic constants increase with pressure rising and the increasing rates of BN and AlN is higher than that of InN which has lower sensitivity of pressure. The linear compressibility decreases with pressure rising. The knowing of the elastic constants may assist us in obtaining information about the stability of the crystal over the whole region of pressure. The requirements for mechanical stability of a cubical crystal are $C_{11}(P) + 2C_{12}(P) > 0$, $C_{44}(P) > 0$, $C_{11}(P) - |C_{12}(P)| > 0$,[32,33] which are fulfilled in our calculations over the whole region of pressure, reflecting that BN, AlN, and InN compounds are more stable in their zinc-blende structures. Our results for C_{11}, C_{12}, C_{44} of the studied material are in good accordance with the published data.

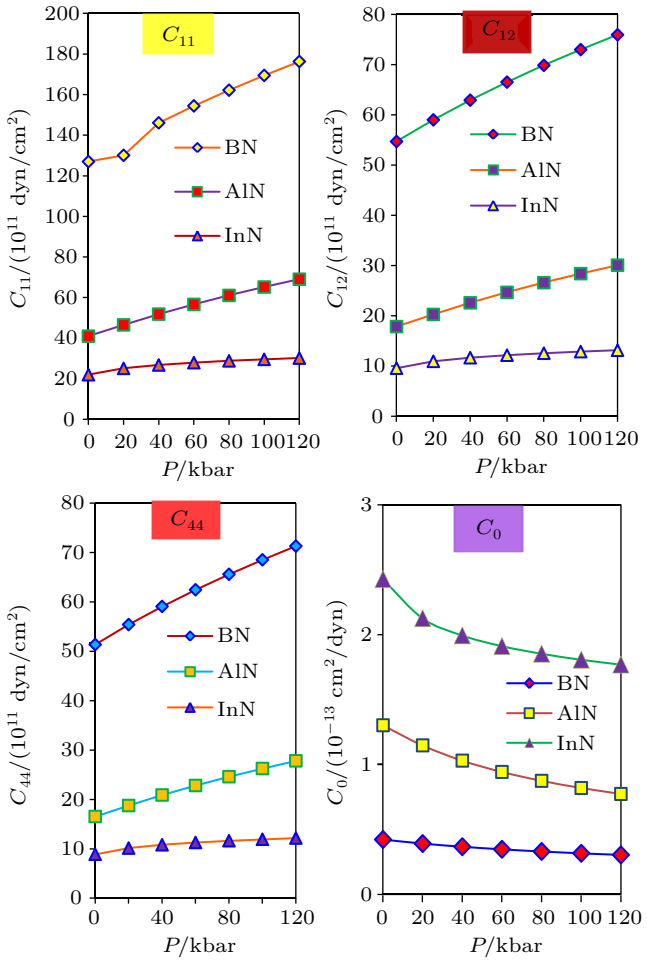


Fig. 5. (color online) Variations of elastic constants (C_{11}, C_{12}, and C_{44}) and C_0 of BN, AlN, and InN with pressures.

Table 3. Values of polarity α_p, elastic constants C_{ij}, and the linear compressibility C_0 of BN, AlN, and InN at different pressures.

BN							
P/kbar	0	20	40	60	80	10	12
α_p	0.22698, 0.226[a]	0.2270	0.2271	0.2272	0.2273	0.2274	0.2275
$C_{11}/(10^{11}$ dyn/cm$^2)$	127.0, 83.7[c], 120.44[a]	130.1	146.1	154.45	162.19	169.46	176.32
$C_{12}/(10^{11}$ dyn/cm$^2)$	54.707, 50.28[a], 42.0[d]	59.02	62.935	66.531	69.868	72.999	75.954
$C_{44}/(10^{11}$ dyn/cm$^2)$	51.355, 59.19[a], 49.3[a]	55.403	59.079	62.454	65.586	68.525	71.298
$C_0/(10^{-13}$ cm^2/dyn)	0.42299, 0.3846[a]	0.39208	0.36768	0.34781	0.3312	0.317	0.30467
AlN							
α_p	0.39764, 0.397[a]	0.3979	0.3983	0.3991	0.3995	0.3999	0.4005
$C_{11}/(10^{11}$ dyn/cm$^2)$	41.033, 42.99[a]	46.571	51.875	56.659	61.088	65.211	69.066
$C_{12}/(10^{11}$ dyn/cm$^2)$	17.871, 18.71[a]	20.283	22.595	24.68	26.61	28.407	30.088
$C_{44}/(10^{11}$ dyn/cm$^2)$	16.518, 16.0[d]	18.747	20.882	22.807	24.589	26.248	27.799
$C_0/(10^{-13}$ cm^2/dyn)	1.3025	1.1476	1.0302	0.94322	0.87483	0.8195	0.77375
InN							
α_p	0.39, 0.39[b]	0.3904	0.3907	0.3915	0.3925	0.39	0.3935
$C_{11}/(10^{11}$ dyn/cm$^2)$	22.022, 21.632[b]	25.143, 25.775[e]	26.81	27.962	28.843	29.581	30.207
$C_{12}/(10^{11}$ dyn/cm$^2)$	9.5846, 9.4[b]	10.943	11.669	12.171	12.556	12.878	13.151
$C_{44}/(10^{11}$ dyn/cm$^2)$	8.8676, 8.6[d]	10.124	10.795	11.259	11.613	11.91	12.162
$C_0/(10^{-13}$ cm^2/dyn)	2.4277	2.1263	1.9941	1.9119	1.8534	1.8071	1.7696

[a]Ref. [49], [b]Ref. [50], [c]Ref. [51], [d]Ref. [52], [e]Ref. [53].

The determining of the elastic constants C_{11}, C_{12}, C_{44} may help us to proceed with calculating the bulk (B_u), shear (S_h), and Young's (Y_0) moduli. Table 4 and figure 6 show the calculated values of bulks, shears, and Young's modul of BN, AlN, and InN and their functions of pressure, respectively. These moduli have the same behaviors under pressure as elastic constants C_{11}, C_{12}, and C_{44}. The Young modulus is desired to supply information about the measure of the stiffness of the material. The stiffness increases with the increase of Young modulus of the material. The present values of Young moduli decrease from BN to InN which indicates that BN is stiffer than AlN and InN. One can estimate the brittle and ductile behaviors of the studied compounds by calculating the values of ductility index (μ_d) of the considered materials, according to the empirical formula of Pugh:[35] this formula states that the value of μ_d that separates the ductile behavior and brittle behavior of material is around 1.75. If $\mu_d > 1.75$ the material behaves as a ductile material, otherwise the material behaves as a brittle manner.[32] Table 4 also contains the calculated values of μ_d for the considered materials which are approximately constants over the whole region of pressure and greater than 1.75, indicating that the considered materials are ductile materials.

Table 4. Values of bulk, shear, Young's moduli, and the ductility indices of BN, AlN, and InN at various pressures.

BN							
P/kbar / Elastic parameters	0	20	40	60	80	100	120
$B_u/(10^{11}$ dyn/cm$^2)$	78.805, 73.67[a], 55.7[b]	85.017	90.657	95.837	100.64	105.15	109.41
$Y_0/(10^{11}$ dyn/cm$^2)$	94.059, 90.61[c]	101.47	108.21	114.39	120.12	125.51	130.59
$S_h/(10^{11}$ dyn/cm$^2)$	36.147, 31.4[c]	38.996	41.583	43.959	46.163	48.232	50.184
μ_d	2.1801	2.1801	2.1801	2.1801	2.1801	2.1801	2.1802
AlN							
$B_u/(10^{11}$ dyn/cm$^2)$	25.592, 26.81[a]	29.046	32.355	35.34	8.103	40.675	43.08
$Y_0/(10^{11}$ dyn/cm$^2)$	30.189, 29.231[d]	34.263	38.165	41.683	44.94	47.972	50.805
$S_h/(10^{11}$ dyn/cm$^2)$	11.581, 11.7[d]	13.144	14.64	15.99	17.239	18.402	19.489
μ_d	2.2098	2.2098	2.21	2.2101	2.2103	2.2104	2.2105
InN							
$B_u/(10^{11}$ dyn/cm$^2)$	13.73, 13.8[b]	15.677	16.716	17.435	17.985	18.445	18.836
$Y_0/(10^{11}$ dyn/cm$^2)$	16.209, 23.10[c], 11.6[e]	18.506	19.732	20.58	21.227	21.769	22.229
$S_h/(10^{11}$ dyn/cm$^2)$	6.2188, 6.51[c]	7.1	7.5704	7.8953	8.1436	8.3515	8.528
μ_d	2.2078	2.208	2.2081	2.2083	2.2085	2.2086	2.2087

[a]Ref [49], [b]Ref. [52], [c]Ref. [54], [d]Ref. [55], [e]Ref. [56].

Table 5 lists the values of bond-stretching (α), bond-bending (β) force constants, internal strain parameter (ζ), transverse effective charge (e_T^*), Cauchy ratio (C_a), anisotropy factor (I_s), and Poisson ratio (P_o) of BN, AlN, and InN at different pressures. From this table, it can be seen that the bond-stretching (α), bond-bending (β) force constants increase with the increase of pressure. Our results of (α, β), at normal pressure agree well with those obtained experimentally.[49,50,54–56] The Poison ratio is also a very significant property for manufacturing investment; it supplies more information about the distinction of the bonding force than any of the other elastic parameters. For the fulfillment of hardness of present materials, the elastic properties, e.g., anisotropy factor, Poisson's ratio of these materials are measured. From Table 5, one can say that all calculated results except the bond-stretching (α), bond-bending (β) force constants, are slightly influenced by pressure.

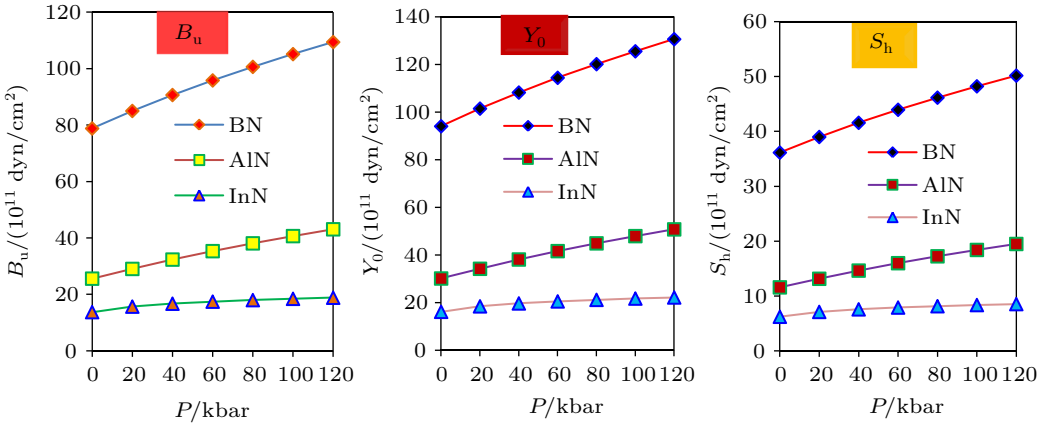


Fig. 6. (color online) Variations mechanical parameters (B_u, Y_0, and S_h) of BN, AlN, and InN with pressures.

Table 5. Values of bond-stretching α, bond-bending (β) force constants, anisotropy factor (I_s), Poisson ratio (P_o), internal strain parameter (ζ), Cauchy ratio (C_a), and transverse effective charge (e_T^*) of BN, AlN, and InN at different pressures.

				BN			
P/kbar	0	20	40	60	80	100	120
α/(N/m)	263.14, 261.54[e]	279.6	294.34	307.71	320	331.42	342.1
β/(N/m)	65.345, 62.2[e]	69.433	73.093	76.413	79.463	82.298	84.951
I_s	0.70386, 1.473[a]	0.70386	0.70386	0.70386	0.70386	0.70386	0.70386
P_o	0.30107, 0.18[b]	0.30107	0.30107	0.30107	0.30107	0.30107	0.30108
ζ	0.56555, 0.55[e]	0.56555	0.56555	0.56555	0.56556	0.56556	0.56556
C_a	1.0653	1.0653	1.0653	1.0653	1.0653	1.0653	1.0653
e_T^*	1.8634	1.8637	1.8641	1.8644	1.8647	1.865	1.8652
				AlN			
α/(N/m)	103.4, 121.1[e]	114.41	124.71	133.81	142.1	149.7	156.72
β/(N/m)	25.305, 24.9[e]	27.999	30.517	32.740	34.767	36.625	38.339
I_s	0.70113	0.70112	0.70111	0.70109	0.70108	0.70107	0.70106
P_o	0.30339, 0.346[b]	0.3034	0.30341	0.30342	0.30343	0.30344	0.30345
ζ	0.56971, 0.663[c], 0.57[e]	0.56972	0.56973	0.56976	0.56977	0.56979	0.56981
C_a	1.0819	1.082	1.082	1.0821	1.0822	1.0823	1.0823
e_T^*	2.3734	2.3741	2.3753	2.3772	2.3781	2.3793	2.3807
				InN			
α/(N/m)	62.962, 83.3[e]	69.999	73.680	76.189	78.086	79.670	81.007
β/(N/m)	15.423, 15.5[e]	17.145	18.046	18.659	19.122	19.508	19.834
I_s	0.7013	0.70129	0.70128	0.70126	0.70124	0.70123	0.70122
P_o	0.30324, 0.369[b]	0.30325	0.30326	0.30327	0.30329	0.3033	0.30331
ζ	0.56944, 0.58[e]	0.56946	0.56947	0.5695	0.56953	0.56955	0.56956
C_a	1.0809	1.0809	1.081	1.0811	1.0812	1.0813	1.0813
e_T^*	2.354, 2.35[d]	2.3551	2.356	2.358	2.3604	2.3617	2.363

[a]Ref. [54], [b]Ref. [56], [c]Ref. [55], [d]Ref. [50], [e]Ref. [49].

4. Conclusions

In this study, we use the EPM for performing our calculations. The values of energy band gap, n, ε_∞, ε_0 of the nitride semiconductors, BN, AlN, and InN are calculated at different pressures. The polarities of considered materials are determined from the adjusted form factors at $G(1, 1, 1)$ and are

used to obtain the elastic constants C_{11}, C_{12}, and C_{44} and their relevant elastic parameters namely, bulk (B_u), shear (S_h), and Young's (Y_0) modulus. Other important parameters such as α, β, ζ, e_T^*, P_0, C_0, C_a, μ_D, and A are also calculated. The variations of the studied parameters with pressure are also studied. Our results at normal pressure are compared with the available published data and show they are in satisfactory accordance. The effects of pressure on most of our results have not yet been measured nor calculated, so, our results can serve as a prediction for future investigations.

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