Structural phase stability, elastic parameters and thermal properties of YN from first-principles calculation

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Abstract : The structural phase stability, elastic parameters and thermodynamic properties of YN at normal and under high pressure are reported. The calculations are mainly performed using the full-potential linearized augmented plane wave method within the density functional theory. Both local density approximation (LDA) and generalized gradient approximation (GGA) are used to model the correlation-exchange potential. The calculated equilibrium lattice parameter and the bulk modulus show good accordance with the experimental and previous theoretical reports. The phase transition from the NaCl (B1) structure to the CsCl (B2) structure is found to occur at 131 GPa within GGA and 115 GPa within LDA. The linear pressure coefficients of the different elastic moduli being addressed here are also determined along with the mechanical and dynamical stability criteria which are shown to be satisfied for YN with B1 phase under normal conditions. Besides, the heat capacity and other thermodynamic parameters are examined and discussed versus temperature.

1. Introduction

Yttrium is a chemical element of symbol Y that resembles lanthanides. It belongs to a group of elements with very interesting properties known as transition metals. It is very common in rare earth ores, relatively stable in air and resembles scandium in appearance. It may appear to gain a faint pink glow when exposed to light [1]. By combining yttrium with nitrogen, a compound (yttrium nitride YN) can be obtained with excellent physical properties such as hardness, chemical inertness, electrical and thermal conductivities [2], [3]. From an industrial point of view, YN plays a major role as an electrical contact, diffusion barrier, buffer layer, etc. [4].

The elastic properties of materials play a very important role not only in the study of the mechanical and vibrational properties of the material, but also when dealing with the study and conception of numerous devices [5], [6], [7]. Indeed, these properties are essential starting points in the study and design of all optoelectronic components based on heterojunctions such as laser diodes (LDs), light emitting diodes (LEDs) and photovoltaic solar cells to name but a few [8]. In addition, the elastic constants provide very valuable information on the bonds between the adjacent atomic planes, the anisotropic nature of the bond and the structural stability [9], [10], [11].

The study of the phase stability of semiconductor materials from both mechanical and dynamical point of view can provide a basic model for understanding their physical properties [12], [13], [14]. NaCl phase (B1) is one of the simplest and most thoroughly studied ionic crystals. Thus, its phase transformation might be useful for studying the fundamental properties of more complex ionic crystals. Upon compression, it is well established that NaCl with a rocksalt structure (the B1 phase) transforms into a CsCl structure (the B2 phase) [15]. In this respect, the structural phase transition in YN has been studied by Mancera et al. [16] using ab initio calculations. Their results reported a B1-B2 structural phase transition that occurred at pressure of 138 GPa. Moreover, Haglund et al. [17] have calculated the electronic band structure and cohesive properties of YN in the B1 phase. Other physical properties of YN have also been carried out by Stampfl et al. [18] and Takeuchi [19]. The results of Takeuchi using first-principle calculations within the local density approximation (LDA) showed that YN is a semimetal. The electronic band structure and structural parameters of YN have also been reported recently by Zerroug et al. [1] who predicted that at zero pressure YN is a semiconductor with an indirect band gap of 0.8 eV and showed a phase transition of the material of interest from NaCl to CsCl (B1→B2) at pressure of about 134 GPa. Besides, Singh et al. [20] have examined the phase transition of YN from the NaCl (B1) to the CsCl (B2) by using a three-body potential model showing a phase transition pressure of 140 GPa.

The present contribution deals with the structural stability, phase transition, elastic parameters and thermal properties of a novel and less explored material YN. The motivation behind this work is the lack or at least the scarcity of bibliographic data on these fundamental properties of YN. All properties of interest are investigated at zero pressure and under compression. The calculations are performed using ab initio full-potential linearized augmented plane wave (FP-LAPW) method in the framework of the density functional theory (DFT) using both the LDA and the generalized gradient approximation (GGA). The present results are compared where possible with the experimental and previous theoretical data. Other case, they are predictions which may serve as a reference for future studies of YN material.

2. Computational methodology

In the present work, calculations are performed using the WIEN2K [21] code within the full potential linearized augmented plane wave (FP-LAPW) method [22] in the frame work of DFT [23], [24]. To model the correlation-exchange potential. we have used both the LDA [25] and the GGA as parameterized by Perdew et al. [26]. In the adopted approach, the wave function and the potential are decomposed into spherical harmonics inside non-overlapping spheres surrounding the atomic sites (Muffin-Tin, MT, spheres), and a plane wave basis set in the interstitial region. The cut-off plane wave is defined in such a manner that $k_{max} = 7 / R_{MT}$ (where R_{MT} is the smallest radius of the muffin-tin sphere in the unit cell). The muffin-tin radius was chosen as equal to 1.9 and 1.8 a.u. for Y and N atoms, respectively. The self-consistent calculation is considered to converge when the error on the total energy of the system becomes equal or less than 10^{-5} Ry. For the wave vector k-integrations over the Brillouin zone (BZ), this BZ is sampled into $10 \times 10 \times 10$ points according to Monkhorst-Pack scheme [27] for the two phases rocksalt (B1) and CsCl (B2) being considered here. The cutoff energy and the number of k-points have been varied so as to ensure the convergence of the total energy. The theoretical equilibrium lattice parameter, the zero pressure bulk modulus, and the first order derivative of the bulk modulus with respect to the pressure, are determined by fitting the total energy of our system (YN) as a function of volume to the Murnaghan's equation of state [28] for both B1 and B2 phases.

For the calculation of elastic constants, we used the same scheme as that described by Charpin and reported in Ref. [5]. It is well known that in the cubic structure, the number of the independent elastic constants reduces to only three elastic constants, namely C_{11} , C_{12} , and C_{44} . Therefore the

determination of these constants requires a set of three equations [5]. The first equation is that relating the bulk modulus (B) to the elastic constants [5], [29],

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \quad (1)$$

The second equation involves performing volume-conservative tetragonal strain tensor δ .

$$\bar{\delta} = \begin{pmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \frac{1}{1+\delta^2} - 1 \end{pmatrix} \quad (2)$$

The application of this strain has an effect on the total energy from its unstrained values as follows,

$$E(\delta) = (C_{11} - C_{12})6V_0\delta^2 + O(\delta^3) \quad (3)$$

where V_0 is the volume of the unit cell. Finally, the last type of deformation, we used the volume-conserving rhombohedral strain tensor given by,

$$\bar{\delta} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \quad (4)$$

from which the total energy can be derived as,

$$E(\delta) = \frac{1}{3}V_0(C_{11} + 2C_{12} + 4C_{44})\delta^2 + O(\delta^3) \quad (5)$$

3. Results and discussion

3.1. Structural properties

The calculated total energy E of our system YN as a function of the volume V/V_0 of the unit cell for the two phases B1 and B2 is plotted in Fig. 1(a) and (b) using respectively the LDA and GGA approaches. In agreement with previous published works [1], [30], it can be stated from these curves that the NaCl (B1) structure is more stable than the CsCl (B2) one.

The total energy is calculated for a set of selected lattice parameters and then fitted to the Murnaghan's equation of state so as to determine the ground-state properties namely the equilibrium lattice parameter a_0 , the zero pressure bulk modulus B_0 and the first-order derivative of the bulk modulus with respect to the pressure B_0' . The obtained results are assembled in Table 1 along with experimental and other theoretical data reported in the literature. It should be noted that compared to the experimental value, the lattice parameter a_0 is slightly overestimated when using the GGA approach, whereas the use of the LDA approach leads to the underestimation of a_0 . Such a fact is consistent with the general trend of these approximations [1], [5], [8], [34], [35]. The deviation of our calculated values from experiment is estimated to be within 4% and 5.8% when using the LDA and GGA approaches, respectively. Our result regarding B_0 has also been compared to that of ZrN

which has been reported by Asvini Meenaatci et al. [36] to be 250 GPa. The comparison to ZrN is due to the fact that this material is close to YN. The B_0 calculated for YN seems to be less than that of ZrN. This indicates that YN is less harder than ZrN.

Fig. 1. Total energy versus normalized volume for YN in B1 and B2 phases using (a) LDA, and (b) GGA approaches.

Table 1

Equilibrium lattice parameter (a_0), bulk modulus (B_0), and the pressure derivative of the bulk modulus (B'_0) for YN in B1 and B2 phases using LDA and GGA approaches.

YN Phase	Structural parameter	Present work		Experiment	Previous calculations
		LDA	GGA		
B1	a_0	4.84	4.94	4.877 ^a	4.93 ^b , 4.93 ^c , 4.827 ^d , 4.913 ^e , 4.90 ^f , 4.93 ^g , 4.85 ^h , 4.77 ⁱ
	B_0	168.62	147.91		151 ^b , 157 ^c , 181 ^d , 158 ^e , 160 ^f , 163 ^g , 163 ^h , 204 ⁱ
	B'_0	3.73	3.59		3.86 ^b , 3.50 ^c , 4.77 ⁱ
B2	a_0	2.94	3.01		3.00 ^b , 3.01 ^c
	B_0	160.87	138.60		153 ^b , 136 ^c
	B'_0	3.91	3.70		3.46 ^b , 4.11 ^c

^a Ref. [31].

^b Ref. [1] using FP-LAPW within GGA approximation.

^c Ref. [32] using FP-LAPW within GGA approximation.

^d Ref. [33] using PP-PW within LDA approximation.

^e Ref. [33] using PP-PW within GGA approximation.

^f Ref. [18] using PP-PW within GGA approximation.

^g Ref. [18] using GW calculations within PAW-GGA as implemented in VASP code.

^h Ref. [25] using FP-LAPW within GGA approximation.

ⁱ Ref. [25] using FP-LAPW within LDA approximation.

The estimation of the transition pressure (P_t) from the phase B1 to the phase B2 of the YN at zero temperature is determined by using the usual condition of equal enthalpies. P_t is given as the abscissa of the intersection point between the curves representing the enthalpy $H = E + PV$ for both considered phases. Fig. 2 shows the enthalpy of YN as a function of pressure for both B1 and B2 phases using both the LDA and GGA approaches. It can be seen that the transition pressure from B1 phase to the B2 phase is around 131 GPa when using GGA and 115 GPa when using LDA. Our results are in very good agreement with those reported in Refs. [1], [30].

3.2. Electronic band structure

The computed electronic band structure of YN with rocksalt structure along representative directions of high symmetry points in the Brillouin zone at zero pressure using the GGA approach is illustrated in Fig. 3. The maximum of the valence band is taken to be the zero energy reference. The valence band is due to 2p of N electrons with a small contribution from 4d of Y electrons. The first conduction band at Γ is predominantly of cationic s character. The band structure of rocksalt YN is topologically similar to that of rocksalt ZrN [36]. The main difference with that of rocksalt ZrN is, of course, the value of the fundamental energy gap. Note that at zero pressure the top of the valence band occurs at the Γ point, whereas the minimum of the conduction band is at the X point. One may thus conclude that rocksalt YN is an indirect (Γ -X) band gap semiconductor. The value of the fundamental band gap of rocksalt YN is found to be 0.78 eV. This value is in good accord with that of about 0.85 eV reported by Stampfl et al. [18], [37] for rocksalt YN using screened-exchange LDA approach. Nevertheless, Soto et al. [4] have reported a value of about 0.3 eV for the material of interest using the FP-LAPW method which seems to be much smaller than our obtained value. The lowest valence state is a singlet that originates from the bonding Y-N like orbitals.

3.3. Elastic parameters and mechanical stability

Because of their great importance in the study of optoelectronic materials and components, the elastic constants of the material under investigation in B1 phase are determined at zero pressure and under hydrostatic pressure. The elastic constants C_{11} , C_{12} and C_{44} vary linearly as the pressure varies on going from 0 up to 120 GPa as shown in Fig. 4. Our results for different pressures

between 0 and 120 GPa are summarized in Table 2. Note that the calculated values of the elastic constant C_{11} using

Fig. 2. Enthalpy versus pressure for YN in B1 and B2 phases using (a) LDA, and (b) GGA approaches.

GGA approach are less than the corresponding ones obtained from the LDA. The same conclusion can be drawn for the elastic constant C_{44} . Nevertheless, as far as C_{12} is concerned the results of the

GGA approach appear to be larger than those of the LDA. In the absence of both theoretical and experimental results regarding the elastic constants of rocksalt YN, to the best of our knowledge, our results are predictions. However, when compared to the elastic constants of the transition metal nitride ZrN in the phase B1 at zero pressure which were reported to be: $C_{11}=550$, $C_{12}=100$ and $C_{44}=108$ GPa [36], our obtained C_{11} and C_{12} elastic constants are smaller than those reported in Ref. [36], whereas the opposite can be noticed for C_{44} .

The calculation of the elastic constants allowed us to determine the bulk modulus B , the shear modulus G and the Young modulus Y using Eq. (1) and the following relations [38], [39],

$$G = \frac{(C_{11} - C_{12})}{2} \quad (6)$$

$$Y = \frac{(C_{11} + 2C_{12})(C_{11} - C_{12})}{C_{11} + C_{12}} \quad (7)$$

The calculated elastic moduli B , G and Y vary monotonically and quasi-linearly with increasing pressure from 0 up to 120 GPa as shown in Fig. 5. It is obvious that the behavior of these studied parameters when using LDA differs quantitatively from that obtained from GGA, although the qualitative behavior seems to be almost similar. Due to the lack of bibliographic data, our results are predictions. In Table 3, we present the first derivatives of elastic constants, bulk modulus, shear modulus, and Young's modulus with respect to pressure for YN in B1 phase using the LDA and GGA approaches. To the best of our knowledge, these values are reported for the first time and may serve as a reference for future works. At zero pressure, Asvini Meenaatci et al. [36] reported values of $G = 154$ GPa and $Y = 376$ GPa for rocksalt ZrN. These values are larger than those obtained in our case for rocksalt YN. This suggests that the rigidity of rocksalt ZrN is larger than that of rocksalt YN, i.e. rocksalt ZrN material is more resistant to transverse deformations than rocksalt YN material.

As well known, crystals can undergo crystallographic phase transitions depending on the constraints (for example pressure) exerted on them. For a crystal to remain stable in a crystalline phase, its elastic constants must fulfill a set of conditions constituting the so-called mechanical stability criteria. These stability criteria at zero pressure are given as [40], [41],

$$C_{11} - C_{12} > 0, \quad C_{44} > 0, \quad \text{and} \quad C_{11} + 2C_{12} > 0 \quad (8)$$

We observe that the stability criteria are all fulfilled for YN with B1 phase at zero pressure. One may thus conclude that YN is mechanically stable in the B1 structure at normal conditions.

Fig. 3. Band structure for rock salt YN.

Fig. 4. Elastic constants (C_{11} , C_{12} , C_{44}) versus pressure for YN in B1 phase using GGA (solid line) and LDA (dotted line) approaches.

Table 2

Calculated elastic constants C_{11} , C_{12} , C_{44} , bulk modulus, shear modulus, and Young's modulus (GPa) for YN in B1 phase at various pressure values using LDA and GGA approaches.

YN	Present work						
Pressure (GPa)	0	20	40	60	80	100	120
C_{11}	289 ^a 445 ^b	396 ^a 530 ^b	504 ^a 615 ^b	611 ^a 700 ^b	719 ^a 784 ^b	826 ^a 869 ^b	933 ^a 960 ^b
C_{12}	91 ^a 52 ^b	147 ^a 123 ^b	204 ^a 94 ^b	260 ^a 264 ^b	317 ^a 335 ^b	374 ^a 406 ^b	430 ^a 465 ^b
C_{44}	128 ^a 137 ^b	125 ^a 132 ^b	122 ^a 126 ^b	118 ^a 120 ^b	115 ^a 115 ^b	111 ^a 109 ^b	108 ^a 108 ^b
B_0	157 ^a 183 ^b	230 ^a 259 ^b	304 ^a 334 ^b	377 ^a 409 ^b	451 ^a 485 ^b	524 ^a 560 ^b	598 ^a 630 ^b
G	99 ^a 196 ^b	125 ^a 204 ^b	150 ^a 211 ^b	175 ^a 218 ^b	201 ^a 225 ^b	226 ^a 232 ^b	252 ^a 247 ^b
Y_0	246 ^a 434 ^b	317 ^a 484 ^b	386 ^a 522 ^b	456 ^a 555 ^b	525 ^a 584 ^b	593 ^a 611 ^b	662 ^a 657 ^b

^a This work using GGA.

^b This work using LDA.

Fig. 5. Elastic moduli (B , G , Y) versus pressure for YN in B1 phase using GGA (solid line) and LDA (dotted line) approaches.

Table 3

Linear pressure coefficients of the elastic constants C_{11} , C_{12} , C_{44} (GPa), the bulk modulus B , the shear modulus G , and the Young's modulus Y (GPa) for YN in B1 phase using LDA and GGA approaches.

	$\frac{dC_{11}}{dp}$	$\frac{dC_{12}}{dp}$	$\frac{dC_{44}}{dp}$	$\frac{dB_0}{dp}$	$\frac{dG}{dp}$	$\frac{dY}{dp}$
LDA	4.24	3.54	-0.28	3.77	0.35	1.74
GGA	5.37	2.83	-0.17	3.68	1.27	3.47

3.4. Phonon spectrum and dynamical stability

The characterization of the phonon dispersions for the investigation of materials is desirable and may give information in the material dynamical stability [42], [43], [44], [45], [46], [47], [48]. Using the density functional perturbation theory (DFPT) the phonon-dispersion curves along several symmetry directions in the Brillouin zone for YN in the rocksalt structure have been obtained. Our results are illustrated in Fig. 6. A gap between the LO and TO phonon branches can be observed. This gap disappears in the case of the wurtzite structure as reported for AlN [46]. This is essentially due to the difference in the ionicity degree and elastic forces strengths of the structures. The picture is qualitatively similar to that reported by Saib et al. [46] for rocksalt AlN. At the X symmetry point the LO phonon frequency seems to be larger than the TO one. The mass ratio between the cation (Y) and anion (N) has been reported to influence significantly the relative frequencies of the LO and TO modes [49]. In this contribution, the cation mass is about seven times larger than that of the anion. According to Srivastava et al. [49] hypothesis, the condition LO phonon frequency is greater than TO phonon frequency at the symmetry point X is satisfied for all zinc-blende and rocksalt materials with mass ration either cation/anion or anion/cation greater than approximately two. Note that there is no imaginary phonon frequency in the whole Brillouin zone as shown by the phonon dispersion curves (see, Fig. 6).

Fig. 6. Phonon dispersion spectrum for rock salt YN at zero pressure.

This clearly indicates the dynamical stability of the material of interest.

3.5. Thermodynamic properties

Let us now turn our attention to the thermodynamic properties of the material of interest. In this respect the heat capacity at constant volume C_V has been calculated using the relation,

$$C_V = \left(\frac{dU}{dT} \right)_V \quad (9)$$

In Eq. (9), V is the volume, T is the temperature, and U is the total internal energy.

Fig. 7 displays the computed C_V versus T for rocksalt YN. Note that C_V increases exponentially with raising temperature up to around $T = 300$ K. However, beyond this temperature, the C_V behavior follows the Debye model and approaches the Dulong-Petit limit.

Fig. 7. Heat capacity at constant volume versus temperature for YN.

This suggests that at high temperatures, the thermal energy excites all phonon modes and the anharmonic effects on C_V are highly reduced. Qualitatively, a similar behavior was reported for C_V as a function of T for InN [50], CdSe and CdTe [51] and CuX ($X = \text{Cl}, \text{Br}$) [52] binary semiconductor compounds.

Fig. 8 displays the variation of the entropy (multiplied by temperature), free energy and enthalpy as a function of temperature for YN material. We observe that at low temperature the entropy increases rapidly and monotonically with increasing the temperature T ; then the entropy behaves more like a sublinear versus T . The thermodynamic free energy is the energy in a physical system that can be converted to do work. We note from Fig. 8 that this energy increases monotonically with raising the temperature. On the other hand, the enthalpy of the material system of interest can be seen as decreases with increasing the temperature. As a matter of fact, the change in enthalpy is the heat absorbed or released by the material system of interest through a chemical reaction or by external heat transfer.

Fig. 8. T^* entropy, free energy and enthalpy versus temperature for YN.

4. Conclusion

In summary, the structural phase stability, electronic band structure, elastic moduli, lattice vibration spectrum, and thermal properties of YN in B1 phase were investigated. The calculations were carried out by using the FP-LAPW method in the framework of the DFT within both LDA and GGA approaches and DFPT. Our results were found generally to be in reasonably good accord with experiment and previous reported calculations in the literature. The mechanical and dynamical stability of the material of interest was verified at zero pressure and found to be fulfilled. Upon compression, rocksalt YN is found to undergo a phase transition to the B2 phase at transition pressure of 131 GPa (calculated using GGA) and 115 GPa (obtained from LDA). The electronic band structure of rocksalt YN showed that the material in question is an indirect (Γ -X) band gap semiconductor with a fundamental band gap energy of about 0.78 eV. The thermal properties such as the heat capacity, entropy, free energy and enthalpy were also examined and discussed. The pressure dependence of all features being studied here were analysed.

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