



Structural, elastic and dynamical properties of $YP_{1-x}As_x$ alloys from first principles calculations

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Abstract. The structural, elastic and lattice vibration properties of the ternary alloys $YP_{1-x}As_x$ at various As concentrations (x) from 0 to 1, $x = 0, 0.25, 0.5, 0.75$ and 1, are presented. The calculations were performed using the density functional perturbation theory (DFPT) within the generalised gradient approximation (GGA) and employing virtual crystal approximation (VCA). We studied the effect of arsenic (As) composition on structural parameters, the phase transition pressure, the elastic constants, the optical and acoustic phonon frequencies at high symmetry points Γ , X and L , the static and electronic dielectric constants, and the Born effective charge. It is established that all these properties follow a quadratic law in the concentration (x). There is a good agreement between our results and the available data for binary compounds YP and YAs. Our results are for $YP_{1-x}As_x$ predictions.

Keywords. Virtual crystal approximation; $YP_{1-x}As_x$ alloys; elastic properties; dynamical properties; pseudopotentials.

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1. Introduction

The calculation of quantum properties of materials has attracted a lot of attention in predicting and studying important properties, where the experimental data are not available. Among these qualities, elastic and dynamic properties represent excellent methods of investigation for estimating the quality of a theoretical approach [1].

In fact, many physical properties such as band gap, lattice parameters, elastic properties, optical and magnetic properties of the compounds can be changed scientifically by adding another substance with known properties. The principal reason for this study is to further the understanding of the lattice parameters, elastic as well as dynamical properties of the $YP_{1-x}As_x$ alloys, with x varied from 0 to 1 in the stable rock-salt phase.

There are several research papers on both theoretical and experimental methods, in particular on the change of phase as structural properties, which is called phase transition, and elastic coefficients for yttrium pnictide

compounds YN, YP, YAs and YSb because these compounds are systems with hard correlations [2–11]. They show a number of attractive properties such as hardness and very high melting points. Because of these properties, these compounds have very wide applications in coating and magnetic storage [12,13] and also in optoelectronic devices such as light detectors and emitters [14].

These materials have two phases: (1) NaCl (B1) phase, which is a stable phase under ambient conditions and (2) the unstable CsCl (B2) phase under pressure conditions [15,16].

There are lot of studies on yttrium pnictide compounds (YN, YP, YAs and YSb) concerning their structural stability, electronic properties, dynamical properties, thermodynamic properties and optical properties using theoretical methods such as full potential linearised augmented plane wave (FP-LAPW) method and pseudopotentials [17–21]. Recently, first principles calculations with pseudopotential method were used to obtain stable and unstable phases from phonon

spectrum and thermodynamic properties of yttrium pnictide compounds [15]. However, there is no study, to the best of our knowledge, on the ternary $YP_{1-x}As_x$ alloys using the first principles calculations.

In this work we focus on the effect of the addition of As on the lattice parameter (a_0), bulk modulus (B), elastic constants (C_{11}, C_{12}, C_{44}), phonon frequencies at high symmetry points Γ, X and L , the Born effective charge (Z^*), and the static $\varepsilon(0)$ and electronic $\varepsilon(\infty)$ dielectric constants. The calculations are performed using the plane-wave pseudopotentials method within the density functional theory and linear response technique using the virtual crystal approximation (VCA).

This paper is organised as follows: the description of the detailed calculations is given in the next section, the discussion of the results obtained by pseudopotentials method are given in the penultimate section and in the end, the conclusions are given.

2. Details of the calculations

In this study, our calculations are carried out using the pseudopotentials and plane-wave method (PP-PW) and VCA to obtain structural, elastic and lattice dynamics properties of $YP_{1-x}As_x$ alloys as a function of the composition (x) in the rock-salt phase. The calculations were performed using the ABINIT package [22–25] in the density functional perturbation theory (DFPT) using the generalised gradient approximation of Perdew–Burke–Ernzerhof (GGA-PBE) parametrisation for the exchange-correlation potential [26]. In the literature, the pseudopotentials of Troullier and Martins type, generated by FHI (Fritz-Haber-Institut) code (GGA-FHI), agree very well with the results of the transition compounds, as used here for yttrium compounds. These pseudopotentials are used for describing the interaction between the valence electrons and the nuclei and core electrons [27–29]. To agree a very well convergence, we have performed convergence tests that proved the choice of the inputs: $4 \times 4 \times 4$ face centred cubic (FCC) grid, equivalent to $8 \times 8 \times 8$ Monkhorst Pack [23,30] mesh of k points for the Brillouin zone and the plane wave energy cut-off to expand the wave function is set to be 80 Hartree to obtain a total energy accuracy that is better than 10^{-5} Hartree.

The method of Hamann *et al* [31] in the framework of perturbation theory based on ABINIT code is used to compute the elastic constants. Using this method, one can also compute the elastic response of the system with respect to the strain perturbation and obtain the second derivatives of the total energy with respect to all perturbations. On the other hand, by using DFPT [32–36], we determined the phonon frequencies

at high symmetry points, the Born effective charges and dielectric constants. To treat the disordered ternary alloys, we applied the VCA [37]. The retention of a crystal with primitive periodicity is allowed. Within the first principles VCA format, we produced the pseudopotentials of the alloy which is composed of virtual atomic potentials, averaging those of the atoms in the parent compounds. As shown in relation (1), to build the virtual pseudopotentials of the ($P_{1-x}As_x$) atom we combined both pseudopotentials of P and As:

$$V_{VCA}^{PS}[x] = xV_{As}^{PS} + (1-x)V_P^{PS}. \quad (1)$$

3. Results

3.1 Structural parameters and phase transition pressure

The yttrium pnictide alloys $YP_{1-x}As_x$ have been investigated in NaCl phase to show the effect of As concentration on the structural properties, lattice parameters and bulk modulus, and to compare with Vegard law and linear composition dependence (LCD) [38,39]. Initially, the stability lattice coefficients have been determined via minimising the total energy, which were in accordance with the different values of the lattice constants. Secondly, by using the Murnaghans [40] equation of states (EOS), we could fit the calculated total energy to determine the lattice constant and bulk modulus by changing the concentration x of As in the ternary alloy at concentrations from 0 to 1 ($x = 0, 0.25, 0.50, 0.75$ and 1). Under normal conditions, the binary compounds crystallise in the B1 phase, which have experimental lattice constants of: $a = 5.652$ (Å) [41] and $a = 5.786$ (Å) [42], respectively, for YP and YAs. In this work, at $x = 0$, $a = 5.659$ (Å) for YP and at $x = 1$, $a = 5.818$ (Å) for YAs. Hence, it shows a good agreement between our obtained results of equilibrium lattice and theoretical data by other computations and available experimental values, as shown in table 1 for $x = 0$ to 1. However, for $YP_{1-x}As_x$ alloys as a function of composition (x), we have fitted the lattice constants with a quadratic relation, in general, of $YP_{1-x}As_x$:

$$a_{YP_{1-x}As_x} = xa_{YAs} + (1-x)a_{YP} - bx(1-x), \quad (2)$$

where a_{YAs} and a_{YP} are the stability lattice parameters of the binary yttrium compounds YAs and YP, respectively. $a_{YP_{1-x}As_x}$ is the lattice constant of the alloy and the quadratic expression b stands for the bowing parameter (represents the disordered parameter). Our values, obtained by using the GGA approximation, are listed in table 1 for $YP_{1-x}As_x$ alloys with various compositions of x (0.25, 0.50, 0.75 and 1). An increase in lattice

Table 1. The computed lattice parameter a_0 in Å, bulk modulus B in GPa and its pressure derivative B' of $YP_{1-x}As_x$ alloys.

Alloys	Parameters	This work	Others	Expt.
($x = 0$)	a_0	5.659	5.659 [15], 5.673 [16], 5.683 [4], 5.6439 [3]	5.652 [41]
YP	B	81.250	79.99 [15], 86.285 [4], 87 [3]	–
	B'	3.500	3.64 [15], 3.805 [4], 3.68 [3]	–
($x = 0.25$)	a_0	5.702		–
$YP_{0.75}As_{0.25}$	B	78.461		–
	B'	3.851		–
($x = 0.50$)	a_0	5.742		–
$YP_{0.50}As_{0.50}$	B	75.760		–
	B'	3.828		–
($x = 0.75$)	a_0	5.780		–
$YP_{0.25}As_{0.75}$	B	73.125		–
	B'	3.742		–
($x = 1$)	a_0	5.818	5.818 [15], 5.835 [4], 5.7665 [3]	5.786 [42]
YAs	B	70.679	70.012 [15], 76.198 [4], 77 [3]	–
	B'	3.725	3.563 [15], 3.821 [4], 3.89 [3]	–

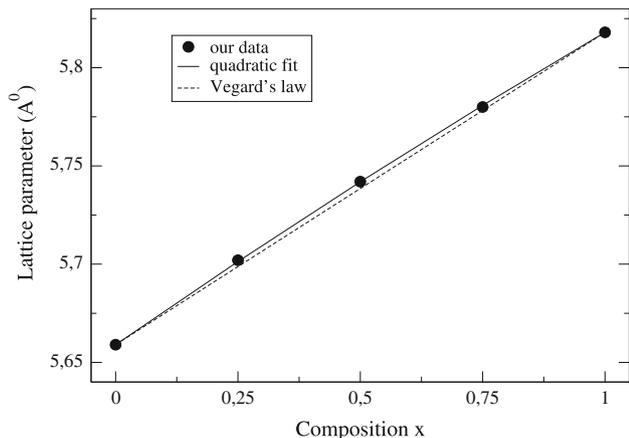


Figure 1. The lattice constant (solid circles) as a function of As concentration (x). Solid line is the quadratic fit to our data and the dashed line represents Vegard’s law.

constant as a function of the As concentration is shown in figure 1.

The deviation of the computed lattice parameter with the addition of an As atom is approximately linear, and it can show a minor difference from Vegard’s law through a tiny growing bowing factor of -0.0136 \AA . This may be explained by the relatively weak mismatches that enter the lattice constants of its binary parents ($a_0(\text{YP}) - a_0(\text{YAs}) = 0.159 \text{ \AA}$). The lattice constant of YAs ($x = 1$) is higher than that of YP ($x = 0$), whereas the bulk modulus value for YP is larger than that of YAs, showing an opposite relation between unit cell volume and bulk modulus.

Figure 2 plots the effect of As concentration on the bulk modulus for $YP_{1-x}As_x$ alloys, compared to the values predicted via the LCD.

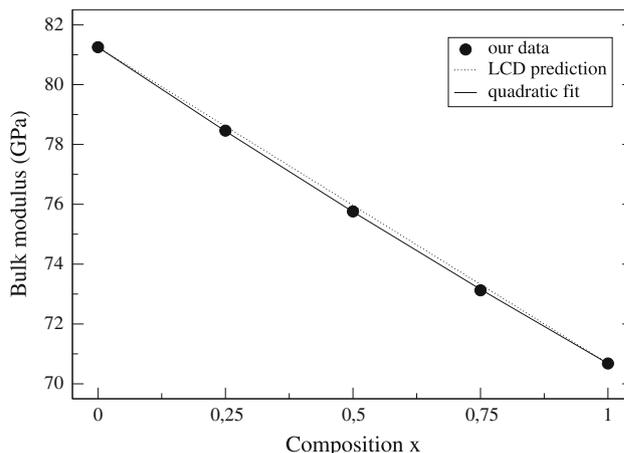


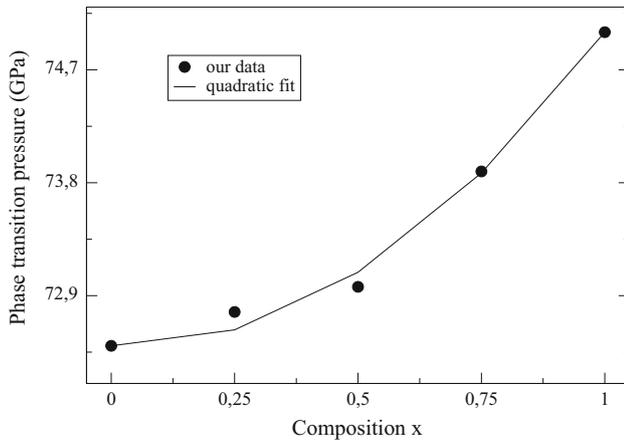
Figure 2. The bulk modulus (solid circles) as a function of As concentration (x). Solid line is the quadratic fit to our data and the dashed line is the LCD prediction.

A significant variation from LCD with downward bowing is equal to 0.8691 GPa for $YP_{1-x}As_x$ alloys. Another physical factor influences the relationship between As concentration and bulk modulus: with the increase in the increment of As concentration (x), the bulk modulus decreases, thus the alloys usually become more compressible.

In general, the bulk modulus B is related to the variation in the volume of a material with a change in pressure (assuming constant temperature): $B = -V dP/dV$. If all dimensions of a cell are simultaneously decreased (increased) (as for the $E(V)$ calculation), then this corresponds to putting positive (negative) external pressure on the cell. The pressure (at constant temperature) follows from the energy change according to $P = -dE/dV$. Therefore, for the bulk modulus, we find $B = V d^2 E/dV^2$.

Table 2. The computed phase transition pressure P_t of $YP_{1-x}As_x$ alloys in GPa.

Alloys	This work	Others	Expt.
($x = 0$) YP	72.5	72.5 [15], 63.8 [3], 55.94 [4]	–
($x = 0.25$) $YP_{0.75}As_{0.25}$	72.77		–
($x = 0.50$) $YP_{0.50}As_{0.50}$	72.97		–
($x = 0.75$) $YP_{0.25}As_{0.75}$	73.89		–
($x = 1$) YAs	75	75 [15], 58.25 [3], 50.45 [4]	–

**Figure 3.** The plot of phase transition pressure (solid circles) as a function of As concentration (x). Solid line is the quadratic fit to our data.

In normal conditions, the binary compounds of the yttrium (Y), YP and YAs, have two phases: one is the stable phase NaCl (B1) with the space group Fm3m (#225). These compounds change their phase to an unstable phase CsCl (B2) with the space group Pm3m (#221) under pressure. They modify from the six-fold coordinated NaCl phase to the eight-fold coordinated phase (B2). This structure transition is a first-order phase transition.

In order to determine the transition pressure at $T = 0$ K, the enthalpy, $H = E_0 + PV$, should be calculated. The stable structure at a given pressure is the structure for which the enthalpy has its lowest value. The transition pressures are obtained, at which the enthalpy of phase B1 is equal to that of phase B2. Table 2 presents the results of transition pressure of $YP_{1-x}As_x$ alloys at different concentrations of As, from $x = 0$ to 1 with other available theoretical data. The results of the transition phase are plotted in figure 3 and they show that the values of P_t increase with the increasing concentration of As from 0 to 1. From figure 3, we observe that the transition pressure has a quadratic variation with composition x :

$$P_{tYP_{1-x}As_x} = xP_{tYAs} + (1-x)P_{tYP} - b_{Pt}x(1-x). \quad (3)$$

We define the phase transition (P_t) and the bowing factor (b_{Pt}). The value of b_{Pt} is 2.6541 GPa. For all concentrations of x in $YP_{1-x}As_x$, the B1 structure becomes unstable at a volume reduction $V_{Pt}/V_0 = 0.66 \pm 0.012$, where V_0 is the equilibrium volume and V_{Pt} is the volume at the phase transition pressure.

3.2 Elastic properties

The elastic constants C_{ij} determine the response of the crystal to external forces. They are among the fundamental properties (that can be predicted from the first principles ground-state total energy) and are closely related to various fundamental solid-state phenomena [43]. The cubic crystal is usually defined via three independent elastic constants. The C_{11} tensor provides information concerning resistance in the direction of $\langle 100 \rangle$. The C_{44} tensor expresses resistance against shear deformation along the plane (100) in the $[110]$ direction. The other elastic constant, namely C_{12} has no physical significance, except that if we do the arrangement of C_{12} with C_{11} and C_{44} it gives other information apropos the elastic behaviour of the compounds. However, we can also provide the mechanical stability conditions for cubic crystal by computing the elastic coefficients which satisfy the relations [44,45]:

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

In this study, the obtained values of C_{11} for yttrium alloys $YP_{1-x}As_x$ are greater than their C_{12} and C_{44} values for each concentration of As. This high value of C_{11} is an indication that the compression resistance is more resistant than shear. By comparing the values of elastic constants of yttrium alloys $YP_{1-x}As_x$ with respect to the As concentration (x), $x = 0, 0.25, 0.50, 0.75$ and 1, a decrease in the values of C_{11} and C_{44} is observed, indicating that $YP_{1-x}As_x$ is less resistant to shear deformation with the increase of concentration (x). The results obtained by the pseudopotentials method with VCA approximation show that they satisfy the mechanical stability criteria. The calculated elastic coefficients C_{11} , C_{12} and C_{44} of $YP_{1-x}As_x$ are given in

Table 3. The computed elastic constants in GPa with GGA approximation of $YP_{1-x}As_x$ alloys.

Alloys	Parameters	This work	Others	Expt.
$(x = 0)$ YP	C_{11}	182.4341	204.66 [13], 116.0 [45], 205 [46], 199.4 [47]	–
	C_{12}	32.853	20.07 [13], 31.0 [45], 39 [46], 28.7 [47]	–
	C_{44}	52.011	40.46 [13], 86.28 [45], 21 [46], 46.3 [47]	–
$(x = 0.25)$ $YP_{0.75}As_{0.25}$	C_{11}	181.9102	–	–
	C_{12}	31.6258	–	–
	C_{44}	50.3965	–	–
$(x = 0.50)$ $YP_{0.50}As_{0.50}$	C_{11}	168.2177	–	–
	C_{12}	30.5120	–	–
	C_{44}	47.9940	–	–
$(x = 0.75)$ $YP_{0.25}As_{0.75}$	C_{11}	162.8106	–	–
	C_{12}	29.3761	–	–
	C_{44}	45.9081	–	–
$(x = 1)$ YAs	C_{11}	157.731	184.22 [13], 192 [46], 177.8 [47]	–
	C_{12}	28.355	30.75 [13], 23 [3], 41 [46], 24.4 [47]	–
	C_{44}	43.869	42.71 [13], 39 [3], 19 [46], 38 [47]	–

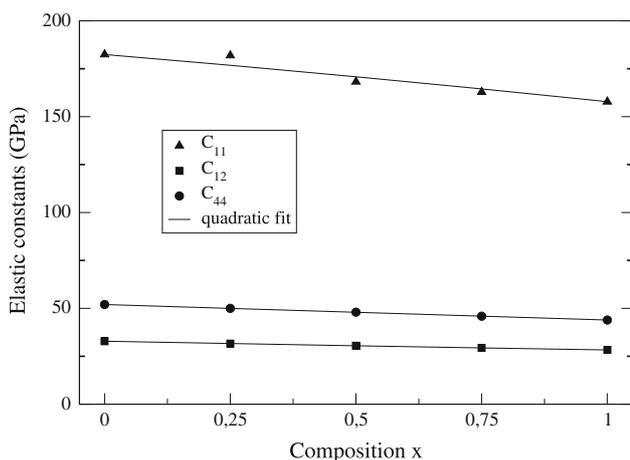
**Figure 4.** The plot of the elastic constants with respect to As composition (x). Solid line is the quadratic fit to our data.

table 3 and are plotted in figure 4 with different concentrations of As. To confirm our results of elastic constants, we have done the convergence tests for energy cut-off, total energy and k -points as shown in table 4. The plane-wave energy cut-off to expand the wave functions is set to 80 Hartree. The Brillouin-zone integration is done using special k -points sampled within the Monkhorst Pack scheme. It is found that a mesh of k -points $4 \times 4 \times 4$ FCC grid is required to describe well the stability and mechanical properties.

It can be observed that the elastic constants decrease with As composition (x). Their dependence on As concentration (x) is quadratically fitted by means of the following relation (4):

$$C_{ij}^{YP_{1-x}As_x} = xC_{ij}^{YAs} + (1-x)C_{ij}^{YP} - b_{ij}x(1-x). \quad (4)$$

We define C_{ij}^{YAs} and C_{ij}^{YP} as, respectively, the elastic coefficients of binary materials YAs and YP. $C_{ij}^{YP_{1-x}As_x}$ is the elastic coefficient of the alloys and b_{ij} is the bowing factor. These parameters are determined to be $b_{11} = -2.7146$, $b_{12} = 0.3594$ and $b_{44} = -0.03449$ GPa.

3.3 Dynamical properties

3.3.1 Phonon frequencies. We start by listing in table 5 the calculated values of the phonon frequencies at the high symmetry points Γ , X and L together with the other theoretical data. As can be seen from this table, our results agree very well with the data from ref. [15] for $x = 0$ and 1. Furthermore, our results for $x = 0.25$, 0.5 and 0.75 have been predicted for the first time and may serve as a reference for future investigation. Our results are plotted in figure 5 at Γ , X and L points. Figure 5 shows the longitudinal and transversal modes of acoustic and optic branches. As can be seen from this figure, the computed phonon frequencies illustrate a nonlinear decrease with increasing As composition x , and their dependence is quadratically fitted by means of the following equation:

$$W^{YP_{1-x}As_x} = xW^{YAs} + (1-x)W^{YP} - bx(1-x), \quad (5)$$

where W^{YP} and W^{YAs} are the phonon frequencies at Γ , X and L points of the binary compounds, $W^{YP_{1-x}As_x}$ is the phonon frequency of the alloys and b is the bowing parameter. In this study of $YP_{1-x}As_x$ alloys, we can use this relation to predict the frequency of every mode of As concentration (x). The obtained values for the bowing

Table 4. The convergence test results of the k -point mesh of $YP_{1-x}As_x$ alloys.

Alloys	k -Points	C_{11}	C_{12}	C_{44}	Total energy
$(x = 0)$ YP	$2 \times 2 \times 2$	166.15384	38.70255	56.28671	-8.29377
	$4 \times 4 \times 4$	182.43410	32.85312	52.01111	-8.29452
	$6 \times 6 \times 6$	182.43420	32.85322	52.01119	-8.29451
	$8 \times 8 \times 8$	182.43425	32.85305	52.01121	-8.29453
$(x = 0.25)$ $YP_{0.75}As_{0.25}$	$2 \times 2 \times 2$	165.12221	37.64521	56.12331	-8.21056
	$4 \times 4 \times 4$	168.21779	30.51203	47.99405	-8.21106
	$6 \times 6 \times 6$	168.21765	30.51206	47.99404	-8.21106
	$8 \times 8 \times 8$	168.21762	30.51204	47.99403	-8.21106
$(x = 0.50)$ $YP_{0.50}As_{0.50}$	$2 \times 2 \times 2$	164.43312	36.88765	55.66544	-8.13879
	$4 \times 4 \times 4$	168.21779	30.51203	47.99405	-8.13910
	$6 \times 6 \times 6$	168.21782	30.51204	47.99406	-8.13910
	$8 \times 8 \times 8$	168.21781	30.51202	47.99404	-8.13910
$(x = 0.75)$ $YP_{0.25}As_{0.75}$	$2 \times 2 \times 2$	154.33245	34.23441	53.22398	-8.07217
	$4 \times 4 \times 4$	162.81069	29.37616	45.90818	-8.07235
	$6 \times 6 \times 6$	162.81072	29.37619	45.90821	-8.07235
	$8 \times 8 \times 8$	162.81071	29.37618	45.90820	-8.07235
$(x = 1)$ YAs	$2 \times 2 \times 2$	142.22431	30.99871	49.88776	-8.00955
	$4 \times 4 \times 4$	157.81883	28.31055	43.92109	-8.00966
	$6 \times 6 \times 6$	157.81883	28.31055	43.92109	-8.00966
	$8 \times 8 \times 8$	157.81883	28.31055	43.92109	-8.00966

Table 5. The obtained values of phonon frequencies (in units of cm^{-1}) of $YP_{1-x}As_x$ alloys with As concentration.

	YP	$YP_{0.75}As_{0.25}$	$YP_{0.50}As_{0.50}$	$YP_{0.25}As_{0.75}$	YAs
TO(Γ)	244.144	221.636	199.118	186.606	177.201
Other	244.615 [15] 235.69 [16]				177.79 [15] 175.33 [16]
LO(Γ)	261.521	257.346	251.166	233.609	218.944
Other	260.626 [15] 250.69 [16]				218.362 [15]
TA(X)	113.063	108.311	103.521	98.435	89.768
Other	113.063 [15] 116.54 [16]				89.768 [15]
LA(X)	145.322	140.550	135.142	128.406	116.024
Other	145.322 [15] 149.72 [16]				116.024 [15]
TO(X)	251.557	220.991	209.297	202.506	177.685
Other	251.557 [15] 246.41 [16]				177.685 [15]
LO(X)	278.860	241.191	224.741	215.213	188.908
Other	278.860 [15] 277.90 [16]				188.908 [15]
TA(L)	130.650	127.994	131.102	133.943	122.254
Other	130.650 [15]				122.254 [15]
LA(L)	213.862	204.029	185.924	172.597	148.467
Other	213.862 [15]				148.467 [15]
TO(L)	240.155	211.538	212.321	212.871	183.880
Other	240.155 [15]				183.880 [15]
LO(L)	302.559	259.800	233.049	213.324	199.363
Other	302.559 [15]				199.363 [15]

parameter b at Γ , X and L points are listed in table 6. We can observe that it has the highest bowing values for almost all modes.

3.3.2 Dielectric and Born effective charge. By using the DFPT method with GGA approximation and employing VCA, we computed the Born effective

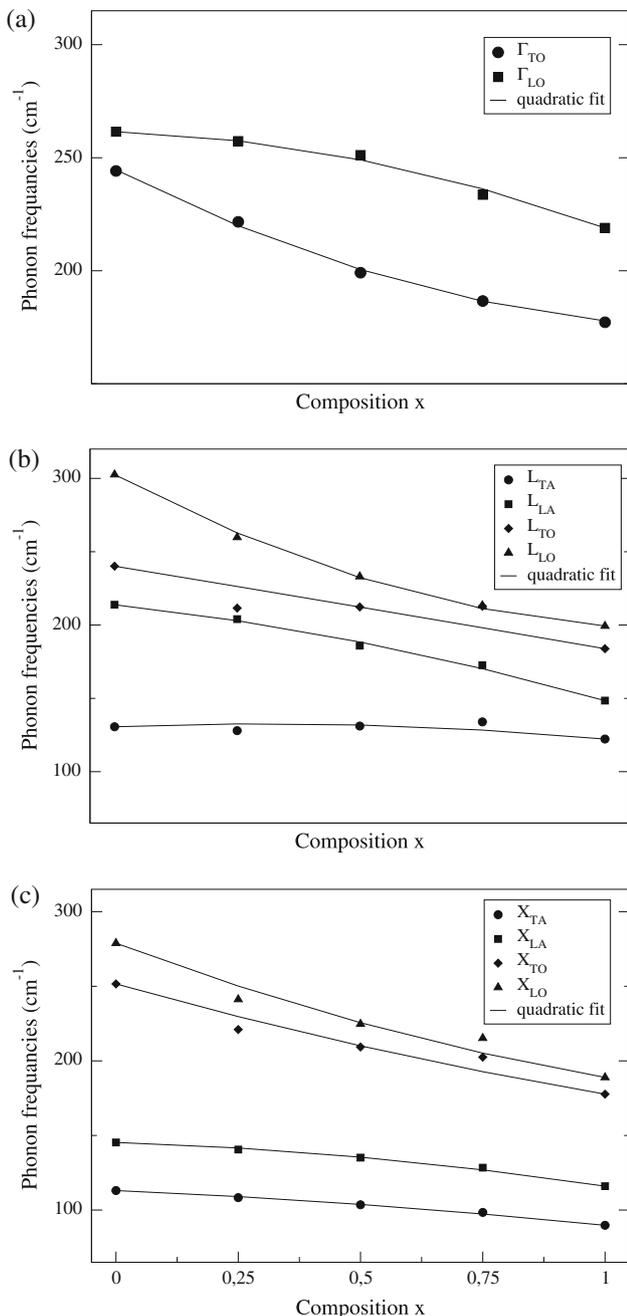


Figure 5. Phonon frequencies at high symmetry points as a function of composition (x) of As atom at (a) Γ point, (b) L point and (c) X point. Solid line is a quadratic fit to our data.

charge (Z^*), the electronic $\epsilon(\infty)$ and static dielectric $\epsilon(0)$ constants for different x compositions. The Born effective charges give dynamic response of the system to a displacement and electric field perturbation of the system. We obtain the Born effective charge by VCA which has two atoms: the first atom is yttrium (Y) and the second atom is the whole virtual atom ($P_{1-x}As_x$). We have two equal and opposite Born effective charges on the anion and cation which satisfy the acoustic sum

Table 6. The bowing constants (in units of cm^{-1}) at the high symmetry points Γ , X and L of $YP_{1-x}As_x$ alloys.

	Parameters	This work
Γ point	b_{TO}	42.7392
	b_{LO}	-35.3904
X point	b_{TA}	-9.4903
	b_{LA}	-19.1557
	b_{TO}	18.1312
	b_{LO}	33.2588
L point	b_{TA}	-21.5054
	b_{LA}	-29.1431
	b_{TO}	-1.09929
	b_{LO}	74.3727

Table 7. The values of the Born effective charge, static and electronic dielectric constants.

Alloys	Parameters	This work	Others	Expt.
$(x = 0)$ YP	Z^*	3.2111	-	-
	$\epsilon(0)$	21.4498	-	-
	$\epsilon(\infty)$	13.2148	-	-
$(x = 0.25)$ YP _{0.75} As _{0.25}	Z^*	3.1873	-	-
	$\epsilon(0)$	21.2821	-	-
	$\epsilon(\infty)$	13.4949	-	-
$(x = 0.50)$ YP _{0.50} As _{0.50}	Z^*	3.18280	-	-
	$\epsilon(0)$	21.5711	-	-
	$\epsilon(\infty)$	13.5571	-	-
$(x = 0.75)$ YP _{0.25} As _{0.75}	Z^*	3.1703	-	-
	$\epsilon(0)$	21.8277	-	-
	$\epsilon(\infty)$	13.9282	-	-
$(x = 1)$ YAs	Z^*	3.1523	-	-
	$\epsilon(0)$	22.1456	-	-
	$\epsilon(\infty)$	14.3737	-	-

rule [48,49]. The results of these properties are obtained and presented in table 7 and are shown in figures 6 and 7. The obtained values of the Born effective charge and dielectric constants are given by the quadratic relations as follows:

$$Z_{YP_{1-x}As_x}^* = xZ_{YAs}^* + (1-x)Z_{YP}^* - b_Z x(1-x), \quad (6)$$

$$\epsilon_{YP_{1-x}As_x} = x\epsilon_{YAs} + (1-x)\epsilon_{YP} - b_\epsilon x(1-x). \quad (7)$$

We define $b_Z = 0.0061$ as the bowing parameter for Z^* . It can be seen that the computed Born effective charge decreases with the increasing composition (x) of As atoms. This signifies that the Y-As bond is less ionic than the Y-P bond in $YP_{1-x}As_x$ alloys. Unfortunately, no experimental and theoretical data are given for Z^* for

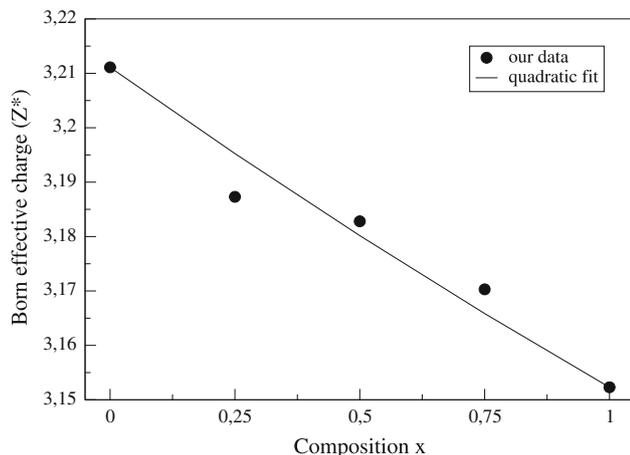


Figure 6. The plot of the Born effective charge as a function of As concentration (x). Solid line is the quadratic fit to our data.

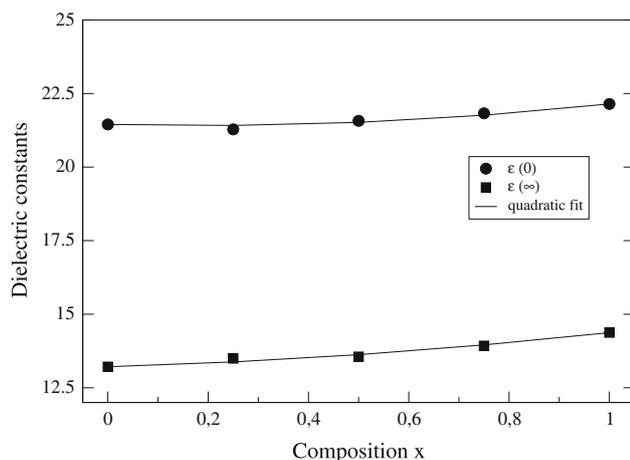


Figure 7. The plot of the dielectric constants as a function of As concentration (x). Solid line is the quadratic fit to our data.

a comparison. The bowing parameters of $\epsilon(0)$ and $\epsilon(\infty)$ are 1.1117 and 0.6795, respectively. It can be seen that the computed static dielectric constant increases with increasing As concentration (x). This is mostly due to the softening of the optical phonon at Γ points. The computed electronic dielectric constant increases with x , and we were able to estimate that when the number of core electrons increase, the atoms of the alloys become more polarisable [50]. We note here that our results are predictions as no experimental or theoretical data are available for comparison.

4. Conclusion

Using DFPT we have studied the structural, phase transition, elastic and vibrational properties of ternary alloys of yttrium compounds $YP_{1-x}As_x$ in the stable phase

NaCl (B1). The calculations were done using the GGA approximation and employing VCA with respect to As concentration (x) at different points: $x = 0, 0.25, 0.50, 0.75$ and 1. For the binary compounds YP and YAs, respectively, for $x = 0$ and 1, our results are in reasonable agreement and are close to the available theoretical and experimental data. The obtained values of the elastic constants, the phonon frequencies at the high symmetry points Γ , X and L points, the Born effective charge, the electronic and static dielectric constants follow the quadratic form as a function of the concentration (x) of As atom. The disordered parameter b , called bowing parameter, is predicted. Finally, although there is no existing experimental data, it may be reasonably safe to consider that the current calculations predict the elastic and dynamical properties of the $YP_{1-x}As_x$ ternary alloys.

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