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Study of electronic and lattice dynamical properties of antiperovskite-type nitrides $XNNi_3$ (X= Pd, Sn and Sb)

Abstract

First principles study of electronic and lattice dynamical properties of the $XNNi_3$ (X=Pd, Sn and Sb) ternary nitrides with $E2_1$ structure (space group Pm3$\bar{m}$ (221)) has been reported using the plane-wave pseudo-potential technique based on density functional theory. The calculated equilibrium parameters are in good agreement with other works. The relationship between anisotropy and mechanical properties are also analyzed. Mechanical stability and stiffness of these materials are determined and $XNNi_3$ (X=Pd, Sn and Sb) ternary nitride compounds are found mechanically stable at zero pressure. Shear Modulus (*G*), Young's Modulus (*E*), maximum and minimum Poisson ratios (υ), Zener anisotropy factor (*A*) and compressibility (β) values are calculated and evaluated in calculations of elastic properties. The electronic properties are studied and presented by plots with total and partial density of states with charge density distributions. The $XNNi_3$ (X=Pd, Sn and Sb) ternary nitrides are metallic behavior and have covalent bonding due to the hybridization. The vibrational properties are investigated to explain lattice dynamics of these types of ternary nitrides.

Keywords: first-principles, lattice dynamical properties, electronic properties, ternary nitrides, antiperovskite

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Introduction

The antiperovskite type Ni-rich ternary nitrides $XNNi_3$ researches have been increased since the discovery of superconductivity (8 Kelvin) for cubic antiperovskite $MgCNi_3$ compound.[1] This discovery has strongly motivated to study antiperovskite series. The studies of the family of Ni-rich carbides have been investigated theoretically and experimentally.[2–15] In recent years, the investigations on some new antiperovskite type nitrides have gained wide interest also some biosensor applications in bioelectronics industry.[16–30] Despite of the fact that there are number of studies related with their properties for some cubic antiperovskite type Ni-rich ternary nitrides, in particular, the mechanical properties of $XNNi_3$-type compounds with X= Al, Ga, In, Zn, Cd, Mg, Sn, Sb, Pd, Cu, Ag and Pt have been studied in theory,[15] it is not mentioned on especially lattice dynamical and electronic properties of $XNNi_3$ (X= Pd, Sn and Sb). One of interesting study is about a new Ni-based antiperovskite nitride, $CuNNi_3$ that shows the superconductivity at 3.2 K and it is reported with X-ray diffraction, magnetization, resistivity and heat capacity measurements.[16] The structural and mechanical properties of the antiperovskite $XNNi_3$ (X=Zn, Mg, Al) with pressure effect are studied by Hong-Cun et al.,[26] by using CASTEP code. Optical functions of $SnNNi_3$, $ZnNNi_3$ and $CuNNi_3$ compounds are studied until 40 eV.[29] In this study, by means of the ab-initio calculations, we have analyzed in details the comparative study of electronic and elastic properties of the $XNNi_3$ (X=Pd, Sn and Sb). Optimized lattice parameters and electronic band structures are reported by using ultra soft pseudo potential.[31,32] In addition, anisotropic independent second order elastic constants (C_{ij}). These constants give permissions us to get the mechanical parameters of $XNNi_3$ (X=Pd, Sn and Sb). Additionally, vibrational properties of $XNNi_3$ (X=Pd, Sn and Sb) compounds are investigated and summarized.

Method of calculation

The density functional theory (DFT) [33,34] has successfully been applied to the ab-initio calculations of the ground-state properties. In view of these circumstances, we have applied to the Generalized Gradient Approximation (GGA)[35] for the exchange-correlation functional. All properties of calculations are investigated by using the Vienna Ab-initio Simulation Package (VASP).[36–39] The calculations are performed for Pd($4d^{10}$), Sn($5s^2 5p^2$), Sb($5s^2 5p^3$), N($2s^2 2p^3$), Ni($4s^1 3d^9$). In our calculations, plane-wave basis sets with cut-off energy 500 eV and the 12x12x12 Monkhorst and Pack[40] k-points are used in the Brillouin zone for $XNNi_3$ (X=Pd, Sn and Sb). To obtain mechanical anisotropic properties, EIAM code is used for calculations.[41] The elastic properties are exploited to estimate with stress-strain method.[42,43]

Results and discussion

Structural and elastic properties

The unit cell of $SnNNi_3$ compound is shown in Figure 1. The crystal structures of $SbNNi_3$ and $PdNNi_3$ compounds are the same with $SnNNi_3$ compound as shown in Figure 1. In our case $E2_1$-type structure which is illustrated in Figure 1. The Wyckoff positions of atoms are located as follow: Sn (0, 0, 0); N (0.5, 0.5, 0.5); and Ni (0, 0.5, 0.5) (Figure 2). Firstly, the equilibrium lattice constants, bulk modulus and its pressure derivative have been obtained by minimizing the total crystal energy calculated for different values of lattice constants using the Birch-Murnaghan equation of states (eos)[44] and the calculation results are given in Table 1 for cubic perovskite ($E2_1$) structure (space group Pm3$\bar{m}$ (221)) of $XNNi_3$ (X=Pd, Sn and Sb). (Table 1) the present structural results are listed in the Table 1, along with the other theoretical and experimental works. The present lattice constants are obtained as 3.905 Å, 3.944 Å and 3.808 Å, respectively, for $XNNi_3$ (X=Pd, Sn and Sb) compounds. Our lattice constants are very good convenient parameters with the other theoretical studies. Our lattice constants in $E2_1$-type crystal structure for $SnNNi_3$ is nearly 0.127% lower, for $SbNNi_3$ is nearly 0.051% higher and for $PdNNi_3$ is nearly 0.132% higher than the reference value.[28] These deviations may stem from the using of GGA approximations with different ab-initio codes. Additionally, the volume values and bulk modulus values of $SnNNi_3$ compound are in convenient with other theoretical values and also the same values are in very good agreement of $SbNNi_3$ and $PdNNi_3$ compounds. The effect of hydrostatic pressure indicated by the derivative of bulk modulus under pressure (B′) is given in Table 1 for each of ternary nitride compounds. According to Table 1, the pressure derivatives of bulk modulus are calculated 4.440, 4.399 and 4.590, respectively, for $XNNi_3$ (X=Pd, Sn and Sb) compounds and sequenced like as $B'(SbNNi_3) > B'(PdNNi_3) > B'(SnNNi_3)$. The derivative of bulk modulus is evaluated with anisotropy. From Table 3, the anisotropy values of $XNNi_3$ (X=Pd, Sn and Sb) compounds are, respectively, 1.19, 1.28 and 1.21. The magnitudes of anisotropy factors are arranged with $A(SbNNi_3) > A(PdNNi_3) > A(SnNNi_3)$. Due to both of these equalities, derivative of bulk modulus are confirmed by anisotropy as an expected. The thermodynamic stability of $XNNi_3$ (X=Pd, Sn and Sb) compounds can be reflected by the formation enthalpy (ΔH). Negative formation enthalpy has been explained as an exothermic process, and formation energy in the lower ones shows the stability related with the decomposition to the constituents of an element. The formation enthalpy could be expressed by the relation:[45]

$$\Delta H=(E_{top}-\ (\Sigma\, n_i\, E_i)\ /\ n \tag{1}$$

where E_{tot} is the total energy of the compound with n_i atoms of all i (X(Pd, Sn, Sb), N and Ni). n: total number of atoms in the primitive cell, E_i: total energy of a pure i the atom with equilibrium lattice constants. The calculated theoretical formation enthalpies of $XNNi_3$ (X=Pd, Sn and Sb) compounds are included in Table 1. As far as we known, there are no data for evaluation the formation energy in the literature to compare with ours. $SbNNi_3$ shows the lowest value of formation enthalpy, which indicates that $SbNNi_3$ compound has the highest stability of these nitride structures. It is important to investigate the second order elastic properties because of the fact that the calculations provide an accuracy and comparison of the calculations of mechanical properties. Herein, C_{ij} elastic constants are the second-order elastic constants of the structure and has been optimized under a given set of exchange–correlation (XC) potential functions and attained an equilibrium structure with a minimum total energy. The elastic parameters are obtained from the second-order derivatives of the total energy:

$$C_{ij}=\frac{1}{V_0}\frac{\partial^2 E_{total}}{\partial\xi_i\partial\xi_j} \tag{2}$$

The cubic crystal has only three independent parameters, C_{11}, C_{12} and C_{44}. The traditional rules on the elastic constants: $C_{11}>0$, C_{11}-$C_{12}>0$, $C_{44}>0$, $C_{11}+2C_{12}>0$ and $C_{11}>B>C_{12}$. These traditional mechanical stability conditions (called that Born's stability criteria) *(P=0 GPa)*[46] are investigated by using the obtained second-order elastic constants all our three nitride compounds. The calculated values of C_{ij} are summarized and given in the table for $XNNi_3$ (X=Pd, Sn and Sb), respectively (Table 2). Second-order elastic constants of $XNNi_3$ (X=Pd, Sn and Sb) meant to Born's stability conditions Table 2. According to Table 2, it is obvious that $XNNi_3$ (X=Pd, Sn and Sb) compounds satisfy stability conditions. For $SbNNi_3$ compound in reference,[28] C_{44} is found as -8.6 GPa although our present calculated value is 34.79 GPa for C_{44}. All other theoretical references are compatible with present values. As it can be seen from Table 2, our ternary nitride compounds have different elastic constants due to their classifications of elements. Elastic properties of our nitride compounds are effected owing to the fact that Tin (Sn) is post-transition metal, antimony (Sb) is metalloid and palladium (Pd) is transition metal. The Zener anisotropy factor (*A*), Poisson ratio ($\tilde{\sigma}$), and Young's modulus (*E*) that are important parameters to see all image of elastic properties are also calculated using by these formulas:[47]

$$A=\frac{2C_{44}}{C_{11}-C_{12}} \tag{3}$$

$$\tilde{\sigma}=\frac{1}{2}\left[\frac{(B-\frac{2}{3}G)}{(B+\frac{1}{3}G)}\right], \tag{4}$$

$$E=\frac{9GB}{G+3B} \tag{5}$$

where G is the an isotropic shear modulus as a function of crystal orientation and is given like that $G=(G_V+G_R)/2$, herein G_V is Voigt's shear modulus (it is related with the upper bound of G values) and G_R is Reuss's shear modulus (it is related with the lower bound of G values) and can be written as $G_V=(C_{11}-C_{12}+3C_{44})/5$ and $5/G_R= 4/(C_{11}-C_{12})+3/C_{44}$, resopectively. The calculated an isotropic shear modulus, Young's modulus, Poisson ratios, Zener anisotropy factor, and compressibility (β) of the $XNNi_3$ (X=Pd, Sn and Sb) are presented in Table 3. The Shear and Young's modulus are calculated with their Voigt and Reuss values and Poisson ratios with maximum and minimum values at zero pressure by ElAM code[41] for anisotropic behaviors of three ternary nitrides (Table 3). Obtained by Voigt and Reuss values of isotropic shear modulus (*G*) are 152.21 GPa, 129.39 GPa and 129.11 GPa, respectively, for $PdNNi_3$, $SnNNi_3$ and $SbNNi_3$ compounds. Using ratio of isotropic shear modulus and bulk modulus, elastic manners of materials are estimated. Ratios of G/B that is called Pugh ratio of $XNNi_3$ (X=Pd, Sn and Sb) compounds are given in Table 3. Providing that G/B<0.5, the material exhibits in a ductile behavior, and while G/B>0.5, the material exhibits in a brittle behavior.[47,48] As can be seen in Table 3, all of $XNNi_3$ (X=Sn, Sb and Pd) ternary nitrides compounds indicate brittle manners due to the fact that their G/B ratios are greater than 0.5. In fact, they behave nearly at brittle/ductile border like in reference.[13] It has also observed that for all of our three antiperovskite type nitrides B>G. As mentioned that parameters limit the mechanical stability of these materials. As a comparison, the Young's modulus of $PdNNi_3$ compound has the biggest one in our ternary nitrides systems. From the literature it is well-known that, if the rate of Poisson is less than 0.25, the material shows covalent bond character, otherwise it is bigger than or equal to 0.25 it shows ionic bond character.[49] The minimum value Poisson's ratio of $SbNNi_3$ is calculated as zero and maximum value Poisson's ratio of $SbNNi_3$ is calculated as 0.14. It might have originated from directions or maximum stability. The other values of Poisson's ratios of $XNNi_3$ (X=Pd, Sn and Sb) are obtained similar values for each of three nitride compounds. Three ternary $E2_1$ structure nitrides show metallic-like systems as indicated in reference.[13] In bulk materials, to see the elastic anisotropy behavior, the Zener anisotropy factor is using to determine the degree of anisotropy. Providing that it gives the value of 1, our compound shows entirely isotropic. Otherwise, this value exhibits anisotropic behavior. The values of our three nitrides are greater than 1. Our materials partially exhibit anisotropic behaviors. The compressibility is a measure of elasticity and is defined as following relations:[50]

$$\beta = \frac{C_{11} - C_{12}}{\Omega} \tag{6}$$

$$\Omega = (C_{11} + C_{12})C_{11} - 2C_{12}^2 \tag{7}$$

The calculated compressibility values are found as 0.0023 GPa^{-1}, 0.0029 GPa^{-1} and 0.0031 GPa^{-1}, respectively, for $PdNNi_3$, $SnNNi_3$ and $SbNNi_3$ compounds. The calculated present values of compressibility are compatible with other theoretical data for $SbNNi_3$ and $PdNNi_3$ compounds.

Table 1 Calculated lattice parameter (a_{cal}), volume (*V*), bulk modulus (*B*), pressure derivative of bulk modulus (*dB/dP*), formation energy (Δ*H*)

Material	a_{cal} (Å)	*V* (Å³)	*B* (GPa)	*dB/dP*	Δ*H* (eV)
$PdNNi_3$	3.808 3.803[b] 3.783[c] 3.809[d]	55.219 55.002[b]	190.4 212.10[b] 217.40[d]	4.44	-2.977
$SnNNi_3$	3.905 3.768[a] 3.910[b] 3.927[c]	59.547 53.497[a] 59.776[b] 60.559[c]	159.203 182.30[b] 176.80[c]	4.399	-3.095
$SbNNi_3$	3.944 3.942[b] 3.766[c]	61.349 61.256[b]	156.405	4.59	-3.109

Abbreviations: [a], numerical study according to empirical model,[8]; [b], theoretical study with APW+lo (FLAPW) implemented in WIEN2k code, GGA-PBE,[28]; [c], theoretical study with CASTEP code, GGA,[29]; [d], theoretical study with CASTEP code, GGA-PBE[30]

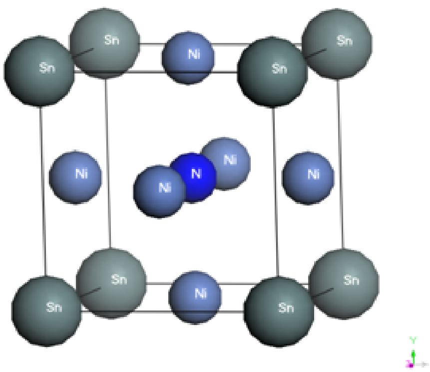

Figure 1 The unitcell of $SnNNi_3$.

Table 2 Second-order elastic constants (C_{ij}), bulk modulus (B), stability

Material	C_{11} *[GPa]*	C_{12} *[GPa]*	C_{44} *[GPa]*	*B [GPa]*	*Stability*
$PdNNi_3$	324.67 313.3[a] 315.6[b]	164.5 161.5[a] 168.3[b]	53.71 81.1[a] 42.8[b]	190.4 212.1[a]	Stable
$SnNNi_3$	272.33 239.9[a]	138.75 153.5[a]	39.28 2.2[a]	159.203 182.3a 176.8b	Stable
$SbNNi_3$	257.48 226.7[a]	142.52 154.3[a]	34.79 -8.6[a]	156.405	Stable

Abbreviations: [a], GGA-PBE[28]; [b], GGA[29]; [c], GGA-PBE[30]

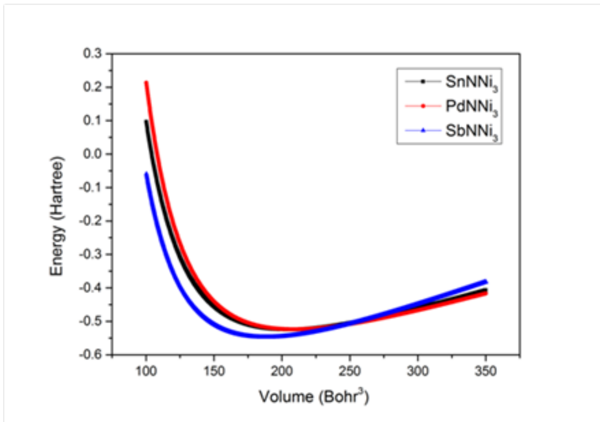

Figure 2 Total energy versus volume curves of $XNNi_3$ (X=Pd, Sn and Sb).

Table 3 Voigt's shear modulus (GV), Reuss's shear modulus (GR), voigt's young's modulus (EV), reuss's Young's modulus (ER), Maximum and minimum poisson ratios (υ), zener anisotropy factor (A), compressibility (β)

	$PdNNi_3$	$SnNNi_3$	$SbNNi_3$
GV [GPa]	152.89	129.86	130.05
GR [GPa]	151.52	128.91	128.17
G/B	0.8	0.81	0.83
EV [GPa]	338.8	284.35	279.15
ER [GPa]	336.54	282.83	276.25
υ_{max}	0.16	0.14	0.14
υ_{min}	0.05	0.04	0
A	1.21 1.06[a] 0.58[b]	1.19	1.28
β[GPa^{-1}]	0.0023 0.0047[a] 0.0046[b]	0.0029 0.0055[a]	0.0031

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Electronic properties

In this section, the main features of electronic properties of $XNNi_3$ (X=Pd, Sn and Sb) compounds are described by analyzing the density of states as total and partial with their related charge densities in Figure 3 & Figure 4. The energy zero is chosen to be at the Fermi energy E_F. All of the three total densities of states have nearly similar features. For all compounds conduction band minimum values are upper than from Fermi energy level. As a comparison of DOS of $SbNNi_3$ with other compounds, its DOS is lower at Fermi energy level. The DOS of $PdNNi_3$ are above at Fermi energy level according to $SbNNi_3$ compound. These all compounds exhibit metallic character in consideration of rate for impletion at Fermi energy levels. The metallic behavior of $XNNi_3$ (X=Pd, Sn and Sb) compounds are mostly owing to the addition of Ni-d states at the Fermi level and a little addition of Pd-d states for $PdNNi_3$ compound. It is clearly seen that Sn-s state and N-p state contribute at Fermi level, and this emerges to a sp-hybridization between metal-s state and N-p states. As it is seen from partial density of states explanations, owing to the covalent bonding, there is hybridization and clarifies the charge densities in Figure 4. The lower valance band is because of the 2s-states electrons for $XNNi_3$ (X=Pd, Sn and Sb) compounds. The charge densities of $XNNi_3$ (X=Pd, Sn and Sb) compounds are depicted in Figure 4. The computed charge density distributions are evident that the covalent bonding that nature of our three ternary nitrides is obtained as covalent due to the sp-hybridization that is also confirmed by partial density of states plots. It is easy to observe that from Figures 3 and 4, the $SbNNi_3$ compound is much more covalent according to $PdNNi_3$ and $SnNNi_3$ compounds. The charges are more accumulated between atoms. Moreover, a high ratio of G/B is related with brittleness. Considering that $SbNNi_3$ compound has the greatest value of G/B, consolidates that $SbNNi_3$ compound has more covalent character than $PdNNi_3$ and $SnNNi_3$.

Additionally, stability of $XNNi_3$ compounds is also confirmed by Band Filling Theory.[51,52] Considering the Band Filling Theory, the numbers of bonding states increase, the stability of material increases and anti-bonding states decrease the stability of compounds. If we called the ratio the width of the occupied states (W_{occ}) and the width of bonding states (W_b), we can explain the work about the material stability. If the ratio of W_{occ}/W_b is closer to 1.0, the stability increases. In this work, these quantities predict the structural stability, namely, the pseudo-gaps (W_p), gaps of occupation (W_{occ}), gaps of bonding (W_b) and the W_{occ}/W_b values are calculated for each compound and presented in Table 4 for $XNNi_3$ compounds. Also shown in Table 4, using this band theory formulation, the ratio of W_{occ}/W_b equals 0.987 and is closer to 1 for $SbNNi_3$ compound. It is obvious that $SbNNi_3$ compound is the most stable material. This result confirms that the previous presented partial density of states for our nitrides and charge density distributions for our nitrides.

Vibrational properties

The phonon dispersion curves of $XNNi_3$ (X=Pd, Sn and Sb) were obtained using by the PHONOPY code.[53] The partial atomic phonon density of states (DOS) for $XNNi_3$ ternary nitrides were calculated along the high symmetry directions using a 2x2x2 super cell and given in Figure 5A-5C. The 0.03 Å for displacement is adopted for each atom of the 2x2x2 supercell in to determine the forces of the atoms. The primitive cells of $XNNi_3$ contains 5 atoms with 15 phonon branches have 3 acoustic and 12 optical modes. For $PdNNi_3$ compound, a gap between acoustic and optic modes is found in the phonon dispersion curves owing to the bigger ratio of mass cation and anions. But, accordin to the $SnNNi_3$ and $PdNNi_3$ compounds there is not a gap between acoustic and optic modes. The lack of soft phonon imaginariy modes in the phonon spectra that supports the stable character as dynamically for the $XNNi_3$ (X=Pd, Sn and Sb) nitrides. In the literature, there is no study of the lattice dynamics of these compounds to compare with our data. It can be seen from Figure 5 that the low-lying optical phonon modes have interactions with phonon modes for $SnNNi_3$ and $SbNNi_3$ as the acoustic. For the phonon DOS of $XNNi_3$ ternary nitrides the acoustic modes are emerged by the vibrations of Sn, Sb and Pd atoms, while the optical modes are emerged by the vibrations of Ni atoms at low modes, with less addition from N and Ni atoms. At higher optical mode, the main contributions emerge from N atoms, with less contributions comes from Ni atoms. $PdNNi_3$ has upper phonon energies than $SnNNi_3$ and $SbNNi_3$ at Gamma point. The main distinction of the three nitrides is due to difference in the chemical bonding and masses for $XNNi_3$ (X=Pd, Sn and Sb) nitrides (Figure 5).

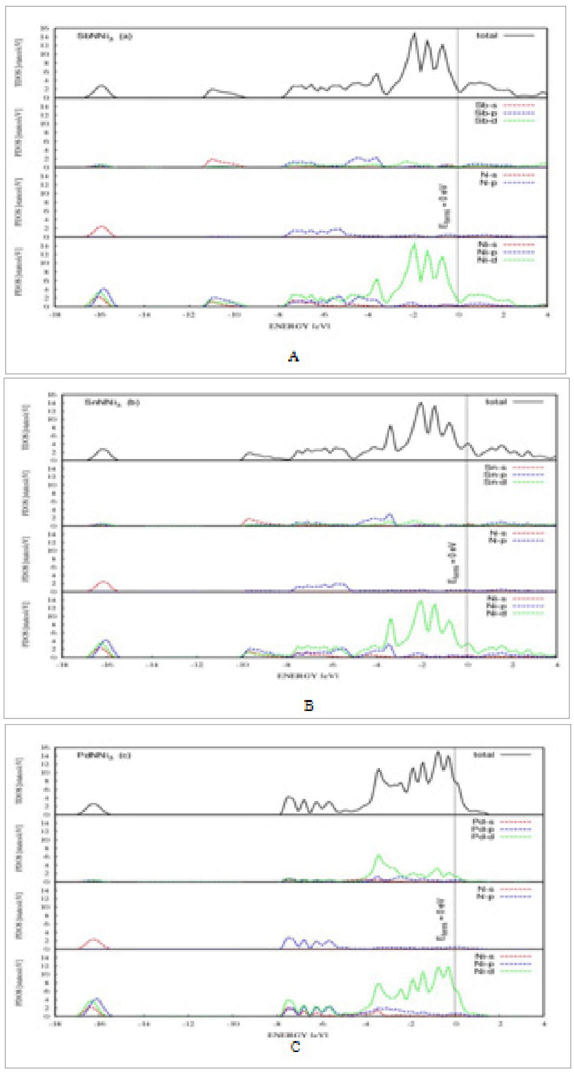

Figure 3 Partial and total DOS of A) $PdNNi_3$, B) $SnNNi_3$ C) $SbNNi_3$.

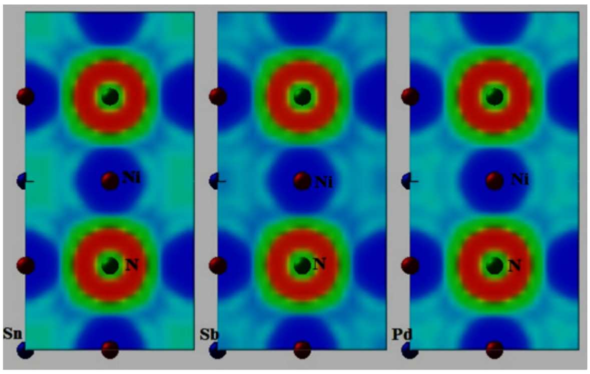

Figure 4 Charge density distribution of (110) plane of $XNNi_3$ (X=Pd, Sn and Sb) compounds.

Table 4 The calculated pseudogap W_p (eV), the width of occupied states W_{occ} (eV), bonding states W_b (eV), electron numbers at fermi levels n (Fermi) for $XNNi_3$ compounds

Materials	W_p	W_{occ}	W_b	W_{occ}/W_b	*n*
$PdNNi_3$	0.773	9.453	10.185	0.928	7.829
$SnNNi_3$	0.481	11.677	12.158	0.96	4.162
$SbNNi_3$	0.166	13.082	13.248	0.987	1.526

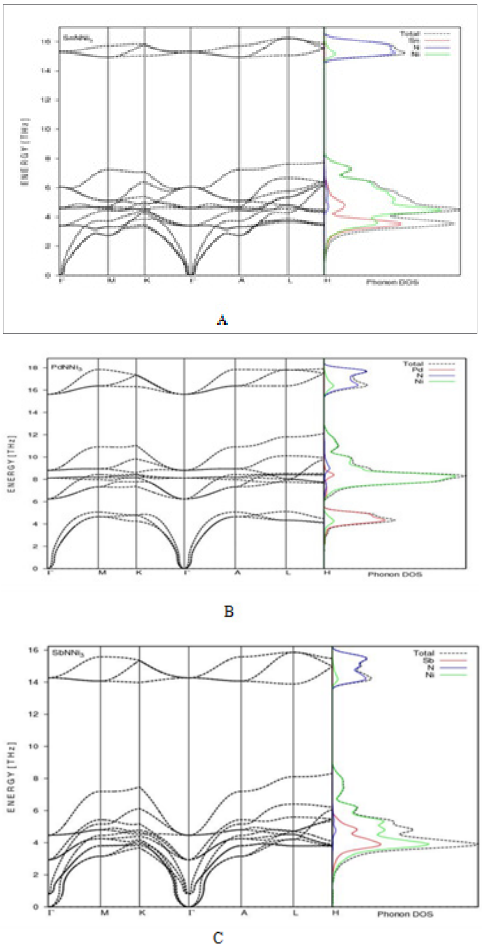

Figure 5 Calculated phonon dispersion curves and partial density of states throughout the high-symmetry directions in the BZ of XNNi3 (X=(A)Pd, (B) Sn and (C)Sb).

Conclusion

In this work, we have studies structural, elastic, electronic and vibrational properties of antiperovskite type nitrides $XNNi_3$ (X=Pd, Sn and Sb) compounds with E21 crystal structure using the GGA. The found lattice constants, volume, bulk modulus as structural parameters at zero pressure are in convenient with the previous work. Mechanical stability of $XNNi_3$ (X=Pd, Sn and Sb) compounds are predicted by Born's stability criteria and found that three nitrides show stability at zero pressure. In elastic calculations, isotropic shear modulus, Poisson's ratios and Young's modulus were estimated using with Voigt and Reuss approximations. In addition to good understand of mechanical behaviors of these compounds, anisotropy factor and compressibility are determined. From our first-principles calculations, the stoichiometric $XNNi_3$ (X=Pd, Sn and Sb) compounds are very similar in both structural and elastic properties. The three ternary nitrides have metallic behavior and exhibit covalent characters. The mechanical behavior of $XNNi_3$ (X=Pd, Sn and Sb) compounds are corroborated with electronic properties as given in the results section. The calculated phonon spectra and phonon DOS indicate that $XNNi_3$ (X=Pd, Sn and Sb) compounds are dynamically stable. To best of our knowledge is there is no experimental or theoretical study in vibrational properties of $XNNi_3$ (X=Pd, Sn and Sb) ternary nitrides has been reported yet for comparison. We predict that, our results are good and qualified estimations for future investigations.

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Conflicts of interest

There are no conflicts to declare.

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