

Indian Journal of Pure & Applied Physics
Vol. 55, November 2017, pp. 786-796

Structural, electronic and elastic properties of $RERu_2$ ($RE = Pr, Nd$ and Sm) Laves phase compounds

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Received 5 November 2016; accepted 25 April 2017

Bonding nature, structural, electronic, magnetic and elastic properties of $RERu_2$ ($RE = Pr, Nd$ and Sm) Laves phase compounds have been studied using the full-potential linearized augmented plane wave (FP-LAPW) method based on density functional theory. The LSDA and LSDA+ U approach has been used to get accurate results because of the presence of the highly localized $4f$ electron of RE ($RE = Pr, Nd$ and Sm) atoms. The calculated lattice parameters and magnetic moments are in good agreement with available experimental results. The electronic and bonding properties have been resolved in terms of band structures, DOS, Fermi surfaces and charge density difference plots, which confirm their metallic character. From the charge density difference plots it has been observed that these compounds show mixed covalent-ionic bonding nature simultaneously and metallic bonding is also present. The mechanical properties and Debye temperature have been predicted from the calculated elastic constants. The ductility of these Laves phase compounds have been predicted in accordance with Pugh's criteria.

Keywords: Intermetallic compounds, Elastic properties, Electronic structure, Ab initio calculations

1 Introduction

Laves phase compounds belong to the intermetallics family, crystallize in three different structures: C15 face centered cubic $MgCu_2$ type, C14 hexagonal $MgZn_2$ type and C36 hexagonal $MgNi_2$ type¹⁻³. With the different composition many Laves phase compounds have been studied theoretically as well as experimentally and many are yet to be studied. The Laves phase compounds are of great technological interest due to their physical and mechanical properties, including high melting temperature, low densities and excellent oxidation resistance, which are essential for high-temperature structural applications⁴. In the three different Laves phases, the C15 structure is anticipated to reveal superior deformability as compared to other two phases because the independent slip system are allowed in its fcc-based structure⁵. The fine precipitates of Laves phase improve the fatigue strength of turbine steels⁶. The Laves phase C15 compounds, such as $CeRu_2$ and $(Hf, Zr)V_2$ show superconducting properties^{7,8}, $(Tb, Dy)Fe_2$ compounds manifest a giant magnetostriction⁹, ZrX_2 ($X = V, Cr, Mn, Fe, Co, Ni$), $(Ho, Mn)Co_2$ compounds are used as hydrogen storage materials¹⁰⁻¹², RCO_2 compounds with

($R=Er, Ho$ and Dy) show magnetocaloric effect and are used in magnetic refrigerators^{13,14}.

Saidi *et al.*¹⁵ have calculated the structural and mechanical properties of YCu_2 and YZn_2 by first-principles calculations. FP-LAPW study of electronic properties of the Al_2X ($X = Sc, Y, La, Lu$) Laves phase compounds are reported by Rajagopalan *et al.*¹⁶. Chen *et al.*¹⁷ have reported the ground state properties, electronic structure and mechanical properties of $TiCr_2$, $ZrCr_2$, $HfCr_2$ by *ab-initio* density functional approach. Yakoubi *et al.*¹⁸ have calculated the structural and electronic properties of BaM_2 ($M = Rh, Pd$ and Pt) Laves phase compounds using first principles. Greidanus *et al.*¹⁹ have studied the magnetic properties of PrX_2 ($X = Pt, Ru, Ir, Rh$) by using neutron diffraction measurements. Recently Shrivastava *et al.*²⁰ have studied the effect of pressure on structural, electronic and elastic properties of $REIr_2$ ($RE = Sc, Y$ and La) Laves phase compounds using density functional theory, which is useful for material design and other technological applications.

The rare-earth (RE) with transition metal (TM) based Laves phase compounds have been attractive for the basic understanding of the electronic structure, the high Curie temperature, heavy ferromagnetic behavior, investigating the physical properties and technological applicability²¹. They have, however, not

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investigated the electronic and elastic properties so far in details. Such materials are of great academic interest to understand the role of RE-*f* electron in the electronic properties. The unique nature of *f*-electron of this type of compounds shows extraordinary electronic and magnetic properties which make them important for potential technological applications. In the present paper, we have carried out the structural, electronic, magnetic and elastic properties of RERu₂ (RE = Pr, Nd and Sm) Laves phase compounds using density functional theory (DFT). To obtain a proper understanding of the electronic structures of RERu₂ (RE = Pr, Nd and Sm) Laves phase compound which contain rare-earth element RE (localized 4*f* electron) with partially filled *d* or *f* states or transition metal (3*d* local electrons), we have employed the LSDA+*U* approach and calculated the BS, TDOS, PDOS, Fermi surface topology and charge density difference plots. The LSDA+*U* method distinctly includes the on-site Coulomb interaction term in the conventional Hamiltonian and their effect on the electronic and magnetic properties of highly correlated system.

2 Method of Calculations

The RERu₂ (RE = Pr, Nd and Sm) compounds crystallize in C15 (fcc) MgCu₂ type structure (space group Fd3m, No. 227). In order to study their structural, electronic, magnetic and elastic properties, we have used first-principles full potential linearized augmented plane wave (FP-LAPW) method within the density functional theory^{22,23} (DFT). We have used the GGA, LSDA and LSDA+*U* approach for exchange and correlation effects²⁴⁻²⁶. The atomic positions¹⁸ of RERu₂ is, RE: (0.125, 0.125, 0.125) and Ru: (0.5, 0.5, 0.5). To obtain energy convergence, the basis functions expanded up to $R_{MT} * K_{max} = 7$, where R_{MT} is the smallest atomic radius in the unit cell and K_{max} refers to the magnitude of the largest *k* vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is $l_{max} = 10$, while the charge density is Fourier expanded up to $G_{max} = 12$ (a.u.)⁻¹. The self-consistent calculations are converged when the total energy of the system is stable within 10⁻⁴ Ry. Energy to separate core and valence states is -6.0 Ry. A dense mesh of 2744 *k*-points and the tetrahedral method²⁷ have been employed for the brillouin zone integration.

3 Results and Discussion

3.1 Structural properties

In the present study, the ground state properties of RERu₂ (RE = Pr, Nd and Sm) Laves phase

compounds are obtained by a minimization of total energy as a function of unit cell volume using GGA, LSDA and LSDA+*U* approximations for exchange-correlation (XC) potential²⁴⁻²⁶. The calculated total energies are fitted to the Birch Murnaghan's equation of state²⁸ to determine the ground state properties such as equilibrium lattice constants (a_0), bulk modulus (B), and pressure derivative of bulk modulus (B'). The variation of total energies as a function of volumes using LSDA+*U* is shown in Fig. 1(a-c). The computed ground state properties along with the available experimental and other theoretical data are presented in Table 1 and indicate that the lattice parameters are consistently smaller as compared to

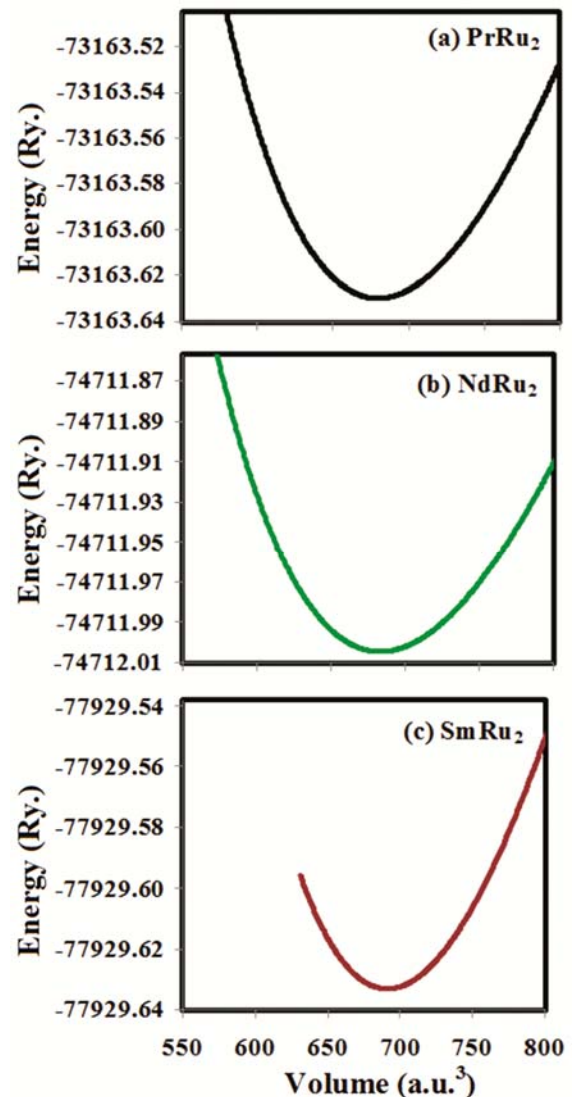


Fig. 1 — Energy versus volume curve for (a) PrRu₂, (b) NdRu₂ and (c) SmRu₂ using LSDA+*U* approximation.

the previously reported results²⁹⁻³² for PrRu₂, NdRu₂ and SmRu₂, respectively. From Table 1, PrRu₂ possesses the largest bulk modulus, which indicates that this compound is the hardest and least compressible as compared to NdRu₂ and SmRu₂. The hardness decreases from PrRu₂ to SmRu₂, due to homologically decrease of bulk modulus from PrRu₂ to SmRu₂. However since the values of lattice parameters do not differ much, the values of bulk modulus also do not differ appreciably in the series.

3.2 Electronic properties and magnetic properties

To understand the electronic properties of RERu₂ (RE = Pr, Nd and Sm) compounds, in which the *f*-electrons are well localized, we have calculated spin polarized band structures, density of states, Fermi surfaces and charge density difference plots by using LSDA+*U* method. The 4*f* orbital of RE (Pr, Nd and Sm) atoms is half filled therefore this method is suitable for strongly correlated RERu₂ (RE = Pr, Nd and Sm) compounds. The electronic properties are calculated with different values of Hubbard parameter ranging³³ from 1 to 9 eV. In the present calculations, we have used the effective parameter $U_{\text{eff}} = U - J$, where *U* is the Hubbard parameter and *J* is the exchange parameter. We set *U* = 5.30 eV (Pr), 5.03 eV (Nd), 4.76 eV (Sm), 4.08 eV (Ru) and *J* = 0.70 eV. The pictorial presentation of the changes of energy of various electronic states along the wave vectors W-L- Λ - Γ - Δ -X-Z-W-K of brillouin zone are shown in Fig. 2(a-c), which are calculated at the

equilibrium lattice constants using LSDA+*U*. From Fig. 2 it is noticed that, the spin up and spin down band profiles in all the RERu₂ (RE = Pr, Nd and Sm) compounds are quite similar except that the spin up RE-*f* bands lie well at the Fermi level (E_F) and the spin down RE-*f* bands are lie well above the Fermi level (E_F). It can be seen from Fig. 2 that in spin up profile, the bands below the Fermi level (-5 eV to -1 eV) appear due to the '*d*' states of Ru atom. It is also noticed that, the hybridized itinerant *f*-states of RE (RE = Pr, Nd and Sm) atoms and '*d*' states of Ru atom make the cluster of bands at the Fermi level which is responsible for the strong metallic behaviour. Pagare *et al.*³⁴ have obtained the itinerant behavior of *f*-electron for NdCd and SmCd, which are almost similar to the present case. The bands above the Fermi level appear due to hybridization of *d*-states of RE and Ru atoms. In spin down profile, the bands around the Fermi level (-5 eV to 1 eV) are mainly due to *d*-states of Ru atom. The unhybridized *f*-state of RE (RE = Pr, Nd and Sm) atoms makes the cluster of bands above the Fermi level, which gradually shifts to the higher energy level in the conduction region when one goes from PrRu₂ to SmRu₂ due to the increase in number of *f*-electron of RE atoms. It can also be noted that there is no band gap for these compounds since the density of states has a non-zero value at the Fermi level which demonstrate the metallic character (Table 1).

The total and partial densities of states demonstrate the elemental contributions of each state of particular

Table 1 — Calculated ground state and magnetic properties of RERu₂ (RE = Pr, Nd and Sm) Laves phase compounds.

Solid	Approach	a_0 (Å)	<i>B</i> (GPa)	<i>B'</i>	$N(E_F)$ (States/eV)		Magnetic moment per RE (Pr, Nd and Sm) atoms (μ_B)	Magnetic moment per Ru atom (μ_B)	Total magnetic moment for RERu ₂ (Re=Pr,Nd and Sm)
					↑	↓			
PrRu ₂ Present study	GGA	7.52	171.11						
	LSDA	7.363	198.34	4.64			1.510	-0.119	2.882
	LSDA+ <i>U</i>	7.385	187.65	4.20	15.4	1.7	1.525	-0.139	2.889
Experimental		7.623 ^a	-	-	-	-	-	-	2.70 ^e , 2.9 ^e
Other		7.624 ^c	-	-	-	-	-	-	
NdRu ₂ Present study	GGA	7.50	174.91						
	LSDA	7.365	192.16	4.81			2.836	-0.244	5.156
	LSDA+ <i>U</i>	7.397	185.13	4.18	20.8	1.2	2.842	-0.246	5.165
Experimental		7.613 ^a	-	-	-	-	-	-	-
Other		7.61 ^b , 7.612 ^c	-	-	-	-	-	-	-
SmRu ₂ Present study	GGA	7.49	169.71						
	LSDA	7.424	186.18	4.90			5.414	-0.412	9.412
	LSDA+ <i>U</i>	7.426	182.48	4.14	36.3	2.4	5.464	-0.430	9.429
Experimental		7.577 ^a	-	-	-	-	-	-	-
Other		7.580 ^c , 7.57 ^d	-	-	-	-	-	-	-

^a:Ref.²⁹; ^b:Ref.³⁰; ^c:Ref.³¹; ^d:Ref.³² and ^e:Ref.¹⁹

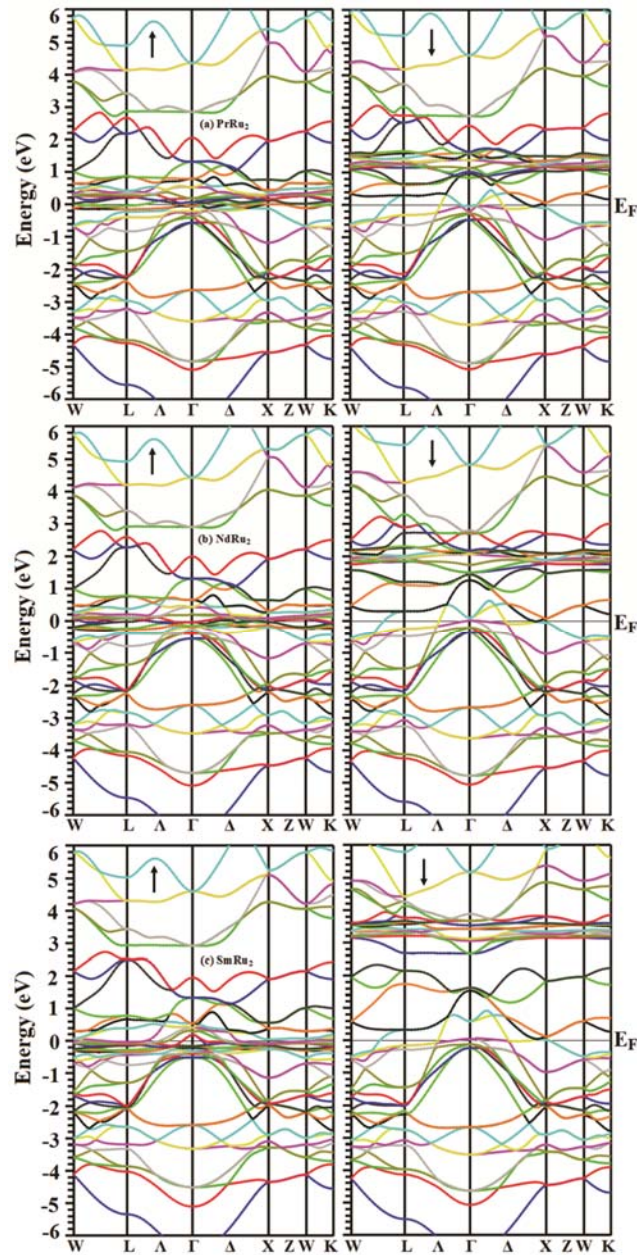


Fig. 2 — Band structures for (a) $PrRu_2$, (b) $NdRu_2$ and (c) $SmRu_2$ using LSDA+ U approximation for majority and minority spin.

atoms to the electronic structures. We have calculated the total and partial density of states for these compounds using LSDA+ U approximation, as shown in Fig. 3(a-c). As is seen in Fig. 3 the sharp peak at Fermi level in the up spin DOS and about 2 eV above the Fermi level in the spin down DOS are due to the f -state of RE (RE = Pr, Nd and Sm) atoms. The d -state of Ru atom are mainly dominated in the energy range (-4 eV to 4 eV) which is hybridized with f -state of RE atoms at the Fermi level in the spin up profile and

d -state of RE atoms in the spin down profile. The density of states at Fermi level $N(E_F)$ from LSDA+ U for $RERu_2$ (RE = Pr, Nd and Sm) compounds are presented in Table 1 for both spins which indicate their metallic nature. From Table 1, we have noticed that, in spin up profile the density of states at Fermi level $N(E_F)$ increase with increasing the number of f -electron in $RERu_2$ compounds on the other hand it decreases in spin down profile except $SmRu_2$.

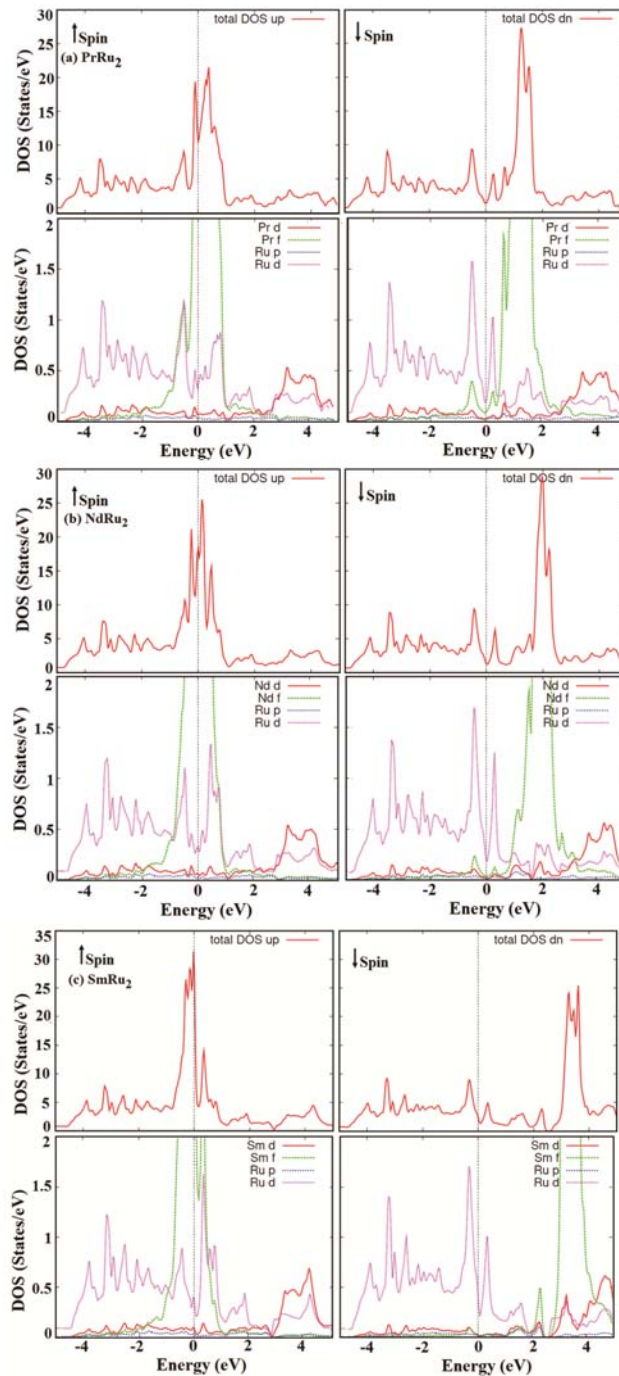


Fig. 3 — Total and partial density of states for (a) PrRu₂, (b) NdRu₂ and (c) SmRu₂ using LSDA+*U* approximation for majority and minority spin.

We have calculated the total and partial magnetic moments with optimized lattice constants using LSDA and LSDA+*U* approach and listed in Table 1. From Table 1, the magnetic moment is mostly located at RE (RE = Pr, Nd and Sm) atoms and the positive

and negative sign of the magnetic moment of RE (RE = Pr, Nd and Sm) and Ru atoms show that, they are aligned opposite to each other. It can also be seen that, the calculated values of total magnetic moment increase from PrRu₂ to SmRu₂ and the same of PrRu₂

is good agreement with experimental data obtained by neutron-diffraction measurement¹⁹. It is clear that, the calculated magnetic moment from LSDA+ U is higher than LSDA which is due to electron-electron correlation and the partial density of states of RE and Ru atoms shows the energy shift. Therefore, the LSDA+ U approximation gives more accurate results.

The Fermi surfaces (FS) of RERu_2 (RE = Pr, Nd and Sm) Laves phase compounds are plotted for the bands which cross the Fermi level for both spin profiles and shown in Figs 4-6. For PrRu_2 , in spin up

profile, there are three bands namely (46, 47, 48) are crossing the Fermi level and make the three FS sheets and fourth is the confluent FS sheet of these three sheets shown in Fig. 4(a-d). The first sheet for band 46 is due to the electron pocket along $W \rightarrow K$ direction. The second sheet for band 47 is due to the hole pocket along $L \rightarrow W$ direction. The third sheet for band 48 is due to the electron pocket along $L \rightarrow W$ direction. The energy ranges for the bands 46, 47 and 48 are 0.85-0.87 Ry., 0.86-0.87 Ry. and 0.86-0.88 Ry. respectively. In spin down profile, 44, 45 bands make

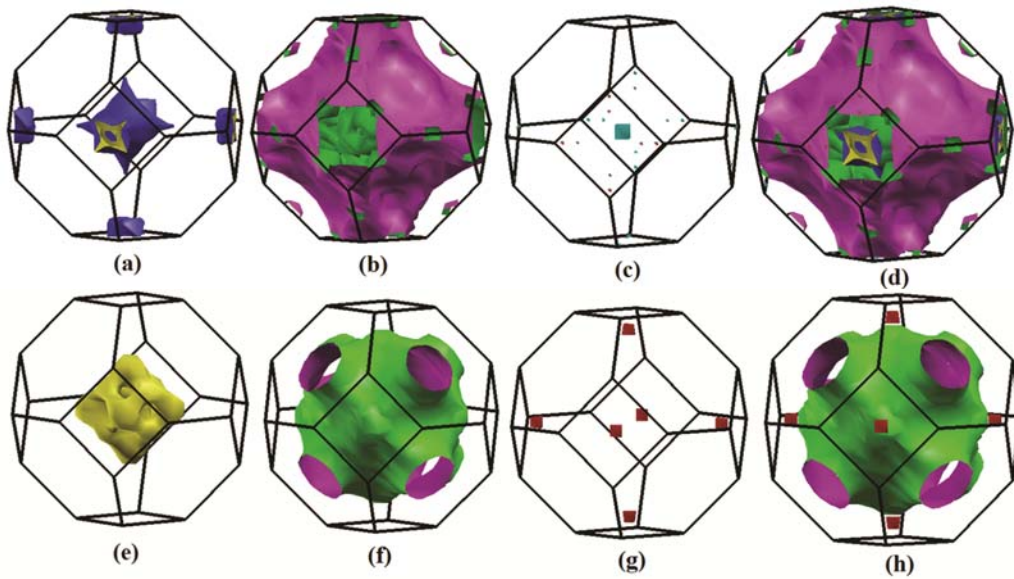


Fig. 4 — Fermi surfaces plots for PrRu_2 using LSDA+ U approximation for both spin.

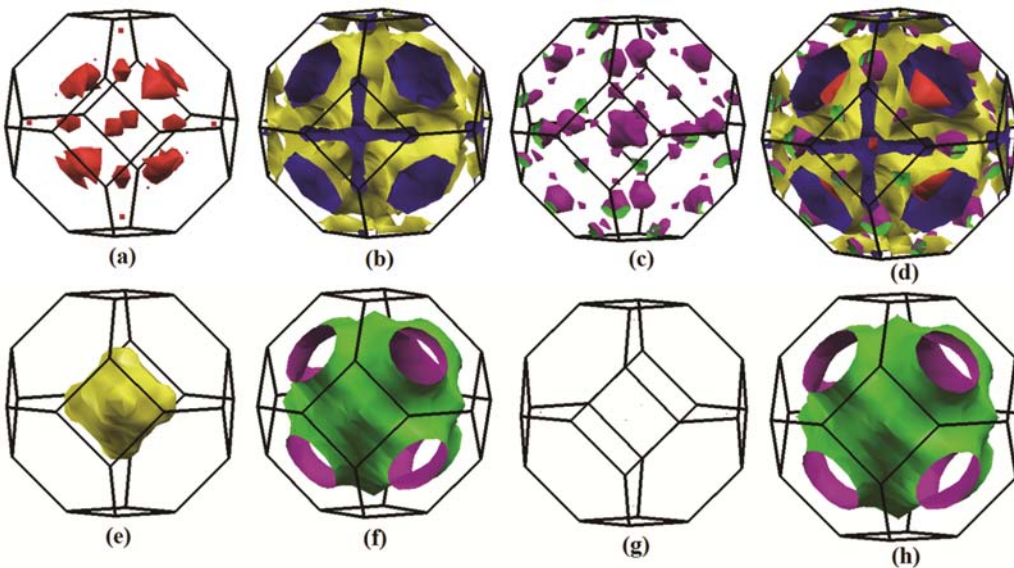


Fig. 5 — Fermi surfaces plots for NdRu_2 using LSDA+ U approximation for both spin

the two FS sheet due to hole pocket at Γ point and 46 band makes the one FS sheet due to electron pocket at X point, shown in Fig. 4(e-h). The fourth sheet is the merged sheet of these three sheets. The energy ranges for the bands 44, 45 and 46 are 0.81-0.89 Ry., 0.82-0.90 Ry. and 0.86-0.93 Ry, respectively. Similarly NdRu₂ gives six FS for both spin in which three sheets are for spin up and remaining for spin down and are shown in Fig. 5(a-h). For spin up, the energy ranges for the bands 48, 49 and 50 are 0.81-0.83 Ry., 0.82-0.83 Ry. and 0.82-0.83 Ry., respectively, and for spin down, the energy ranges for the bands 43, 44 and 45 are 0.78-0.80 Ry., 0.79-0.87 Ry. and 0.82-0.93 Ry., respectively. For SmRu₂, in spin up profile, four FS sheets appear from 51, 52, 53 and 54 bands as shown in Fig. 6(a-e). The first two sheets for 51 and 52 bands are due to the hole pocket at Γ point, The third and fourth sheets for 53 and 54 bands are due to the electron pocket along $L \rightarrow X$ direction. The fifth sheet is the merged sheet of these four sheets. The energy ranges for the bands 51, 52, 53 and 54 are 0.76-0.78 Ry., 0.76-0.78 Ry., 0.76-0.79 Ry. and 0.76-0.80 Ry., respectively. In spin down profile, 43, 44 bands make the two FS sheet due to hole pocket at Γ and electron pocket at X point, as shown in Fig. 6(f-h), the third sheet is the merged sheet of these two sheets. The

energy ranges for the bands 43 and 44 are 0.73-0.81 Ry., 0.73-0.84 Ry., respectively. A common features that one can observe from the band structures and FS is the metallic character for all the studied RERu₂ (RE = Pr, Nd and Sm) compounds.

In order to explore the nature of bonding character and to explain the charge transfer between the constituent elements of RERu₂ (RE = Pr, Nd and Sm) compounds, we have plotted the charge density difference plots for both spin (from $-0.01 \text{ e}/\text{\AA}^3$ to $+0.3 \text{ e}/\text{\AA}^3$) along (110) plane which is obtained by subtracting the superposition of free atoms densities from the total valence charge density. The results are shown in Fig. 7(a-f). From Fig. 7, it can be noted that the difference plots for both spin are quite similar. The overlapping of electron densities between Ru-Ru atoms implies a covalent bonding between them due to hybridization of Ru-*d* states. It can also be noted from Fig. 7 that the charge transfer from RE (Pr, Nd and Sm) atoms towards Ru atom is due to the higher electronegativity of Ru atom as compared to the RE (Pr, Nd and Sm) atoms. This fact suggests the presence of ionic bonding between them. The bonding between Pr-Pr, Nd-Nd and Sm-Sm is metallic. A comparison of our calculated results with those of previously reported results³⁵ of MgCu₂ suggests that

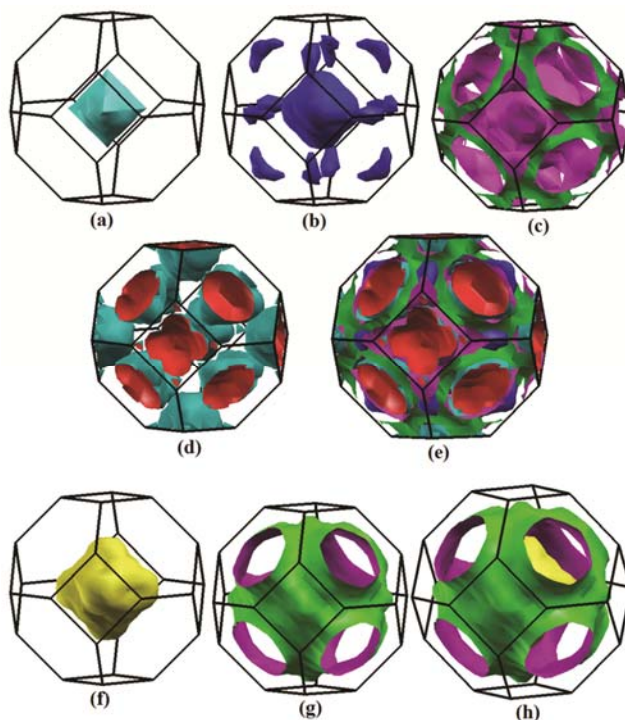


Fig. 6 — Fermi surfaces plots for SmRu₂ using LSDA+*U* approximation for both spin.

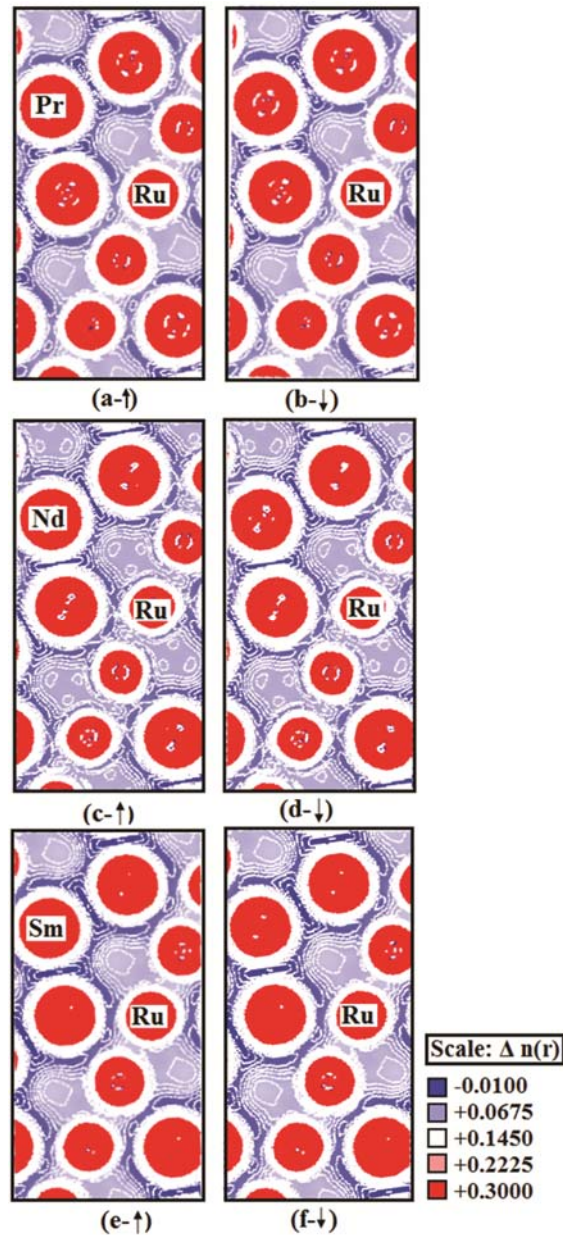


Fig. 7 — Charge density difference plots in (110) plane for (a,b) PrRu₂, (c,d) NdRu₂ and (e,f) SmRu₂ (in units of $e/\text{\AA}^3$) using LSDA+*U* approximation for both spin.

our results are in good agreement. The above discussion shows that the bonding characteristics of RERu₂ (RE = Pr, Nd and Sm) Laves phase compounds are covalent, ionic as well as metallic, leading to structural stability.

3.3 Elastic properties

Elastic constants are required to know how a material undergoes stress deformation and then recovers and returns to its original shape after stress ceases. Elastic

constants are also related to thermal properties such as specific heat, thermal expansion coefficient and Debye temperature. RERu₂ (RE = Pr, Nd and Sm) have cubic symmetry, therefore to understand and describe their mechanical behavior, we have calculated only three independent elastic parameters C_{11} , C_{12} and C_{44} at ambient pressure by using the method developed by Charpin³⁶ and co-ordinate in the WIEN2k package²². For elastic constants calculations, we have used the optimized lattice constants (7.52, 7.50 and 7.49 for

PrRu₂, NdRu₂ and SmRu₂, respectively) using GGA approximations only. Here, a group of three equations are required to resolve all the constants. The first type of equation involves computing the bulk modulus (*B*), given by the formula:

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

The second step represents the volume-conservative tetragonal strain given by the following tensor³⁶:

$$\begin{bmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \frac{1}{(1+\delta)^2} - 1 \end{bmatrix} \quad \dots (2)$$

where $\delta = (1+e)^{1/3}-1$ with *e* as strain tensor. Application of this strain has an effect on the total energy from its unstrained value as follows:

$$E(\delta) = E(0) + 3(C_{11} - C_{12}) + V_0\delta^2 + O(\delta^3) \quad \dots (3)$$

where *V*₀ is the volume of the unit cell.

Finally, for the last type of distortion, we use the volume-conserving rhombohedral strain tensor given by³⁶:

$$\frac{\delta}{3} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \quad \dots (4)$$

which transforms the total energy to:

$$E(\delta) = E(0) + \frac{1}{6}(C_{11} + 2C_{12} + 4C_{44}) + V_0\delta^2 + O(\delta^3) \quad \dots (5)$$

It can be pointed out that our calculated values of elastic constants, presented in Table 2, satisfy the stability criterions^{37,38}: $C_{11}-C_{12} > 0$, $C_{44} > 0$, $C_{11} +$

$2C_{12} > 0$, $C_{11} > B > C_{12}$, which clearly indicate the mechanical stability of these compounds in cubic *C*₁₅ phase. It may be noted that the calculated value of bulk modulus (*B*) from the elastic constants has almost the same value as that obtained by fitting the total energy versus volume to the Birch Murnaghan's equation of state²⁸. This gives us a good estimate of the magnitude and accuracy of the elastic constants of RERu₂ (RE = Pr, Nd and Sm) compounds. The bulk moduli are usually assumed to be a measure of deformation resistant capacity upon applied pressure³⁹. The larger value of bulk modulus gives the stronger capacity to resist deformation. From our calculated result, we can conclude that the ability to resist deformation from strong to weak is NdRu₂, PrRu₂ and SmRu₂, respectively.

By using the calculated elastic constants, we can further study the mechanical properties such as shear modulus⁴⁰ (*G*_H), Young's modulus^{40,41} (*E*), Pugh's ratio³⁹ (*B/G*_H), Poisson's ratio⁴² (σ), Anisotropy ratio⁴² (*A*), Cauchy's pressure⁴¹ (*C*₁₂-*C*₄₄), Kleinman parameter⁴³ (ξ), Lamé's coefficient (λ) and shear constant (*C*_S) which are presented in Table 2. The shear modulus *G*_H describes the material's response to shearing strain using the Voigt- Reuss-Hill (VRH) method^{40,44,45} and is a measure of resist reversible deformation by shear stress³⁸. The larger value of shear modulus gives the stronger capacity to resist shear deformation. The calculated results demonstrate that SmRu₂ has the largest value, followed by NdRu₂ and PrRu₂. Hence, the deformation resistant capacity of SmRu₂ would be much larger than that of NdRu₂ or PrRu₂.

The Cauchy pressure *C*_p (*C*₁₂-*C*₄₄) can also define the ductility (brittleness) of a crystal^{46,47}. The bond character of cubic compounds is also explained with respect to their Cauchy pressure. Ganeshan *et al.*⁴⁸ have established a correlation between the bonding and brittleness/ductility properties. Compounds having more positive Cauchy's pressure tend to form bonds which are primarily metallic in nature. According to Pettifor⁴⁹, this positive value of *C*_p relates to more ionic character of the bonding,

Table 2 — Calculated elastic constants, Young's modulus *E*, shear modulus *G*_H, anisotropic factor *A*, Poisson's ratio σ , *B/G*_H ratio, Cauchy's pressure (*C*₁₂-*C*₄₄), Kleinman parameter (ξ), Lamé's coefficient (λ) and shear constant (*C*_S) of RERu₂ (RE = Pr, Nd and Sm) Laves phase compounds with GGA approximation.

Solids	<i>C</i> ₁₁ (GPa)	<i>C</i> ₁₂ (GPa)	<i>C</i> ₄₄ (GPa)	<i>E</i> (GPa)	<i>G</i> _H (GPa)	<i>A</i>	σ	<i>C</i> ₁₂ - <i>C</i> ₄₄ (GPa)	<i>B/G</i> _H	ξ	λ	<i>C</i> _S
PrRu ₂	182.37	168.28	26.46	45.54	15.63	3.75	0.45	141.82	11.06	6.60	141.33	9.54
NdRu ₂	187.04	174.89	31.86	48.52	16.67	5.24	0.45	143.03	10.72	0.95	150.57	6.07
SmRu ₂	186.81	163.13	44.89	75.44	26.44	3.79	0.42	118.23	6.46	0.91	139.57	11.84

whereas the compounds having more negative Cauchy's pressure form bonds which are more angular or covalent in character. Thus the ductile nature of all RERu₂ (RE = Pr, Nd and Sm) compounds can be correlated to their positive Cauchy's pressure and thereby having mixed ionic and metallic character in their bonds. Using the elastic properties of RERu₂ compounds, we have also analyzed their ductility using the (B/G_H) ratio. As suggested by Pugh³⁹, the ratio of bulk to shear modulus (B/G_H) may be used to determine whether a compound be brittle ($B/G_H < 1.75$) or ductile ($B/G_H > 1.75$). For RERu₂ (RE = Pr, Nd and Sm) compounds, we obtain the value $B/G_H > 1.75$ which shows their ductile nature.

The Young's modulus (E) is important for technological and engineering applications. Larger the value of E , the stiffer is the material. It is reported in the literature that stiffer solids have covalent bonds⁵⁰. It can be seen from the Table 2 that the highest value of E is obtained for SmRu₂, indicating it to be stiffer as compared to NdRu₂ and PrRu₂.

We have calculated another important parameter, the elastic anisotropic factor (A), which gives a measure of the anisotropy of the elastic wave velocity in a crystal. The elastic anisotropy (A) has an important implication in industrial science to detect the micro cracks in materials. For an isotropic crystal A is 1, while a value greater than or less than unity is an anisotropic crystal. According to our results from the Table 2 the RERu₂ (RE = Pr, Nd and Sm) compounds are anisotropic.

Poisson's ratio (σ) provides valuable information about the bonding forces in a material which is related to elastic property⁴¹. In pursuance of Frantsevich rule⁵¹, the critical value of Poisson's ratio of a material is $1/3$. If the value of Poisson's ratio is $\sigma > 1/3$ the material is considered as ductile and if $\sigma < 1/3$ it shows brittle character. In the present case, we find that all the RERu₂ (RE = Pr, Nd and Sm) compounds are ductile in nature.

With the calculated value of the Young's modulus E , bulk modulus B and the shear modulus G_H , one may obtain the Debye temperature, which is an important fundamental parameter plays a key role in the discussions of the temperature dependence of the electrical resistivity of metals and closely related to many physical properties such as specific heat and melting temperature. Debye temperature θ_D can be obtained from the average sound velocity, v_m , by the following relation^{52,53}:

Table 3 — Calculated density ρ , longitudinal v_l , transverse v_t , average elastic wave velocities v_m , Debye Temperature θ_D of RERu₂ (RE = Pr, Nd and Sm) Laves phase compounds with GGA approximation.

Solids	ρ (g/cm ³)	v_l (ms ⁻¹)	v_t (ms ⁻¹)	v_m (ms ⁻¹)	θ_D (K)
PrRu ₂	10.71	4252.7	1207.4	1377.4	172.45
NdRu ₂	10.90	4294.5	1236.1	1409.8	177.17
SmRu ₂	11.14	4302.0	1539.8	1751.3	220.92

$$\theta_D = \frac{h}{k_B} \left[\frac{3n}{4\pi V_a} \right]^{1/3} v_m \quad \dots (6)$$

where h is Plank's constant, k_B is Boltzmann's constant, V_a is the atomic volume, n is the number of atoms per formula unit and v_m is average sound velocity. The average sound velocity⁵²⁻⁵⁴ approximately calculated by using the transverse (v_t) and longitudinal (v_l) sound velocities⁵⁵.

The calculated values of average sound velocities (v_m) and Debye temperatures (θ_D) as well as the densities are reported in Table 3. In the non-appearance of any studied data in the literature, they could not be compared. Hence, our results can be appreciated as predictions for these properties of Laves phase compounds. Further experimental works are required in order to certify our calculated results.

4 Conclusions

We have theoretically investigated the structural, electronic, magnetic and elastic properties of the RERu₂ (RE = Pr, Nd and Sm) Laves phase intermetallic compounds. The calculated lattice constants are in reasonable agreement with the available experimental value but there are no experimental or theoretical data for comparing the other properties except magnetic moment of PrRu₂ which is well agreed with experimental results. The electronic band structures and density of states of RERu₂ confirm their metallic character. ' f ' states of RE and ' d ' states of Ru play an important role in band structures and Fermi surfaces. We have also observed from the charge density difference plots that RERu₂ show ionic-covalent bonding nature simultaneously and metallic bonding is also present. The computed elastic constants obey the necessary mechanical stability conditions suggesting that all the RERu₂ Laves phases are mechanically stable.

Acknowledgement

The authors are thankful to UGC, New Delhi for the award of a UGC-BSR Fellowship to DS.

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