



Electronic structure, phase stability and elastic properties of ruthenium based four intermetallic compounds: Ab-initio study



Ekta Jain ^{a,*}, Gitanjali Pagare ^{a,*}, Sunil Singh Chouhan ^{b,1}, Sankar P. Sanyal ^{b,1}

^a Department of Physics, Government M.L.B. Girls P.G. College, Bhopal 462-002, India

^b Department of Physics, Barkatullah University, Bhopal 462-026, India

ARTICLE INFO

Article history:

Received 4 February 2014

Received in revised form

7 May 2014

Accepted 8 May 2014

Available online 11 June 2014

Keywords:

B. Brittleness and ductility
B. Density functional theory
B. Mechanical properties
B. Elastic properties
E. Ab-initio calculations

ABSTRACT

The structural, electronic and elastic properties of four RuX (X = Sc, Ti, V and Zr) intermetallic compounds have been investigated by using density functional theory within full potential linearized augmented plane wave method and using generalized gradient approximations in the scheme of Perdew, Burke and Ernzerhof (PBE), Wu and Cohen (WC) and Perdew et al. (PBEsol) for the exchange correlation potential. The relative phase stability in terms of volume-energy and enthalpy-pressure for these compounds is presented for the first time in three different (B₁, B₂ and B₃) structures. The total energy is computed as a function of volume and fitted to Birch equation of states to find the ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B'). It is found that the lattice parameters in B₂-phase agree well with the existing experimental and previous theoretical results. The second order elastic constants (SOECs) are also predicted for the above compounds. All the four compounds show ductile behavior. The ductility of these compounds has been analyzed using Pugh's rule. From the plots of electronic density of states (DOS), it can be concluded that these intermetallic compounds are metallic in nature.

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1. Introduction

Intermetallic compounds have drawn considerable attention over the past decades in the field of research in material science. They are composed of a solid phase containing two or more metallic elements, whose crystal structure differs from that of its constituents [1]. Ruthenium can be considered the most reactive element in platinum group-metals (PGM). The most important characteristic for practical applications is an excellent catalytic activity [2]. Ruthenium is extensively used as an alloying agent in applications for the chemical and electronics industries [3]. The mixing of ruthenium improves the corrosion resistance and mechanical properties of titanium and other metals based super alloys with applications including the turbine blades in jet engine [4]. At high temperatures, ruthenium alloys show excellent chemical and

electrical stabilities. Particularly RuX (X = Sc, Ti, V and Zr) compounds are 'd' block transition metal intermetallics; they have high corrosion resistance, good ductility, high tensile strength and thermal stability [5–9].

Mehl et al. [10] have reported first principles calculations within the framework of local-density approximation (LDA) for elastic properties of many binary compounds including RuAl and RuZr using density functional theory. They concluded that these compounds exhibit high melting temperatures and large elastic constants and are found to be ductile in nature. Nguyen et al. [11] computed the electronic structure, phase stability and elastic moduli of AB-type transition metal aluminides including RuAl in twelve different structures using FP-LMTO method with local-density approximation (LDA). Ab-initio FP-LAPW calculation has been performed by Novakovic et al. [12] to investigate structural stability of some CsCl structured HfTM (TM = Co, Rh, Ru, Fe) compounds.

The various potential applications of ruthenium have encouraged many theoretical investigations based on density functional theory as an alloy and an element. A comprehensive study of ruthenium binary alloys was performed using first principles calculations by Jahnatek et al. [13]. They performed the phase stability

* Corresponding author. Tel.: +91 755 2560462; fax: +91 755 2661783.

E-mail addresses: gita_pagare@yahoo.co.in (G. Pagare), sankarsanyal@gmail.com (S.P. Sanyal).

¹ Co authors: Department of Physics, Barkatullah University, Bhopal 462026, MP, India. Tel.: +91 755 4224989, +91 755 2488530; fax: +91 755 2491823.

of Ru based transition metal alloys by calculating the formation enthalpy in different structures. The study of properties of carbides of ruthenium and other transition metal were performed by density functional theory using plane wave pseudo potential within generalized gradient approximation [14].

In spite of so many distinctive properties there is no systematic calculations reported in the literature on structural, electronic and elastic properties of RuX (X = Sc, Ti, V and Zr) compounds. In the present paper we study specially the phase stability for these intermetallics in terms of volume-energy and enthalpy-pressure in three different crystal structures, e. g. B₁, B₂ and B₃. The lack of data on above investigations motivated us to explore these properties for RuX intermetallics which will provide new reference data for the future research prospect. In this study we also have used PBE-GGA, WC-GGA and PBEsol-GGA approximations within the density functional theory to study above mentioned properties and analyzed the ductile nature of these RuX compounds. The remainder of this paper is organized as follows. The method of calculations has been given in Section 2. In the Section 3 the results and discussion are presented.

2. Method of calculation

The FP-LAPW method as implemented in WIEN2k code [15] is employed for the calculations based on density function theory (DFT) within generalized gradient approximations. The schemes of Perdew, Burke and Ernzerhof (PBE), Wu and Cohen (WC) and Perdew et al. (PBEsol-GGA) is applied for the exchange and correlation effects [16]. The basis function was expanded up to $R_{MT}^*K_{max} = 7.0$ for both B₁ and B₂ phases in order to achieve convergence, where R_{MT} is the minimum sphere radius and K_{max} is the maximal value of the reciprocal lattice vector used in the plane wave expansion. For calculations of RuTi by WC-GGA in B₂-phase this function is expanded up to 6.0. For B₃-phase, in the case of RuTi and RuZr, the $R_{MT}^*K_{max}$ has taken 6.0 and 7.5 respectively. The spherical harmonics inside the muffin-tin are taken with an angular momentum $l_{max} = 10$ while the charge density is Fourier expanded up to $G_{max} = 12$. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1000 k points and the tetrahedral method [17] have been employed for the Brillouin zone integration. The total energies are fitted to Birch equation of state [18] to obtain the ground state properties.

All binary RuX (X = Sc, Ti, V and Zr) intermetallic compounds have a cubic B₂-type (CsCl) ordered structure. For the cubic crystals, there are three independent elastic constants, referred to as C_{11} , C_{12} and C_{44} . The equation involves calculation of bulk modulus (B), which is related to the elastic constants as:

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

The thermal loss mechanisms (temperature dependence) of a material is most suitably described in terms of the Debye temperature (θ_D) which is a fundamental parameter closely related to many physical properties such as elastic constants, specific heat and melting temperature. One of the standard methods to calculate the Debye temperature is from elastic constants data, since θ_D may be estimated from the average sound velocity v_m by the following equation [19,20]:

$$\theta_D = \frac{h}{k_B} \left[\frac{3n}{4\pi V_a} \right]^{\frac{1}{3}} v_m \quad (2)$$

where h is a Planck'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, which is approximately calculated from [19,21]:

$$v_m = \left[\frac{1}{3} \left(\frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{-\frac{1}{3}} \quad (3)$$

where v_t and v_l are the transverse and longitudinal sound velocities respectively obtained by using the elastic constants as follows:

$$v_l = \sqrt{\frac{C_{11} + \frac{2}{3}(2C_{44} + C_{12} - C_{11})}{\rho}} \quad (4)$$

$$v_t = \sqrt{\frac{C_{44} - \frac{1}{3}(2C_{44} + C_{12} - C_{11})}{\rho}} \quad (5)$$

where C_{11} , C_{12} and C_{44} are second order elastic constants and ρ is mass density per unit volume.

3. Result and discussion

3.1. Structural properties

The phase stability of ruthenium based four intermetallic compounds RuX (X = Sc, Ti, V and Zr) has been presented in Fig. 1(a)–(d) in terms of total energy and volume. To investigate the stability of crystal structure many authors [22–25] have reported the enthalpy theoretically. It is essential to estimate the Gibbs free energy (G) [26] which is given by $G = E_0 + PV - TS$, where E_0 is the total energy, P is the pressure, V is the volume, T is the temperature and S is the entropy. Since the theoretical calculations are performed at $T = 0$ K, Gibbs free energy becomes the enthalpy $H = E_0 + PV$. The stability of a particular structure is decided by the minima of the Gibbs free energy (enthalpy at absolute T and at given pressure). The stability of these compounds has been shown from its enthalpy vs. pressure curves in Fig. 2(a)–(d). The stability of above compounds has been determined in B₁ (NaCl), B₂ (CsCl) and B₃ (Zinc Blende) structures using FP-LAPW method. From these (Figs. 1 and 2) curves it is revealed that all the compounds are most stable in B₂-type crystal structure having minimum energy and enthalpy. Therefore, all the further calculations have been performed in their B₂-phase only. The calculated total energy was fitted to Birch equation of states [18]. The pressure as a function of volume is plotted in Fig. 3(a)–(d). From Fig. 2, it can be noticed that the volume decreases with increasing pressure. The calculated results for ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') in all the three crystal structure are presented in Table 1 and compared with the experimental [27,28] and other theoretical results [10,29]. It is noticed from Table 1 that our calculated lattice parameters for all the compounds are close to the experimental and other theoretical results. It is also seen that the calculated value of bulk modulus for period 4 elements (Sc, Ti and V) increases with respect to atomic number as we go across the period whereas the lattice parameter decreases. Thus RuSc is more compressible amongst the three compounds. Moreover RuTi and RuZr belonging to the same group show the opposite behavior showing RuZr to be more compressible. The same trend follows for bulk modulus in B₁-phase but there is some deviation in B₃-phase due to its less stability at ambient pressure.

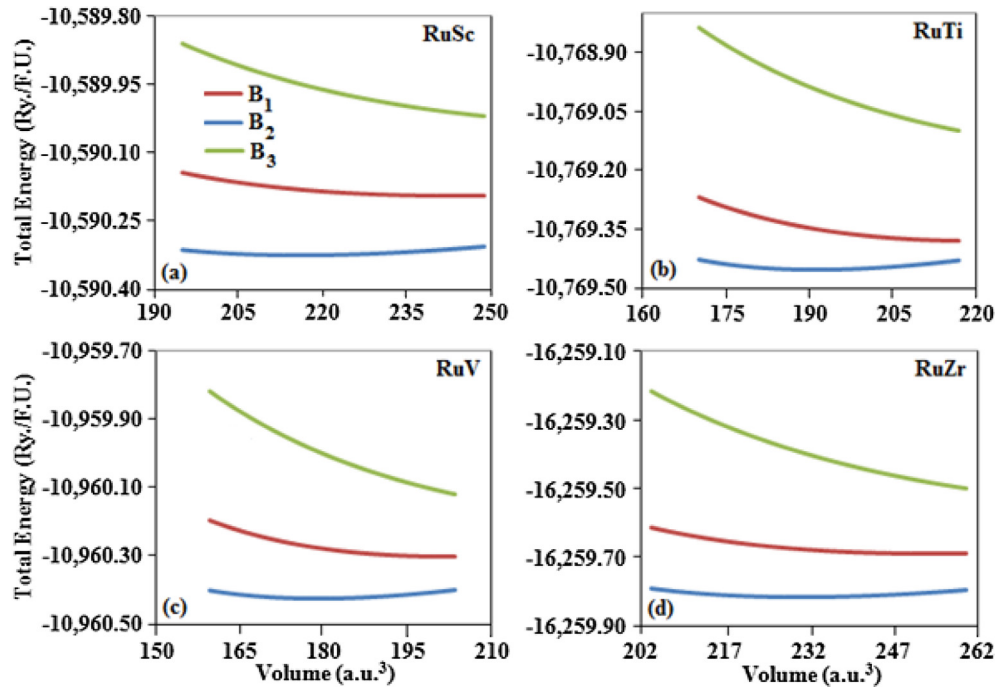


Fig. 1. (a)–(d) Phase stability curves (Energy vs. volume) of RuX compounds in B₁, B₂ and B₃-phase using WC-GGA.

3.2. Electronic properties

In order to get insight into the bonding mechanism for four RuX intermetallic compounds, the self-consistent relativistic total and partial density of states (DOS) along the principal symmetry direction in B₂-phase are plotted in Fig. 4(a)–(d) by using WC-GGA. The Fermi level is set at the zero. For all the compounds, below the Fermi level the major contribution is observed only due to 'd' like state of

Ru in the energy range between −4 and 0 eV, −5 to −1 eV, −6 to −2 eV and −4 to −1 eV respectively. The metallic behavior in RuSc is noticed mainly due to 'd' like states of Ru while for RuTi and RuZr the metallicity is observed due to hybridized 'd' like states of Ru with 'd' like states of Ti and Zr at the Fermi level. For RuV the metallic nature is mainly due to 'd' like states of V with a little contribution of 'd' like states of Ru at the Fermi level. The DOS values are found to be 1.98, 0.39, 3.25 and 0.49 states/eV/F.U. respectively for RuSc, RuTi,

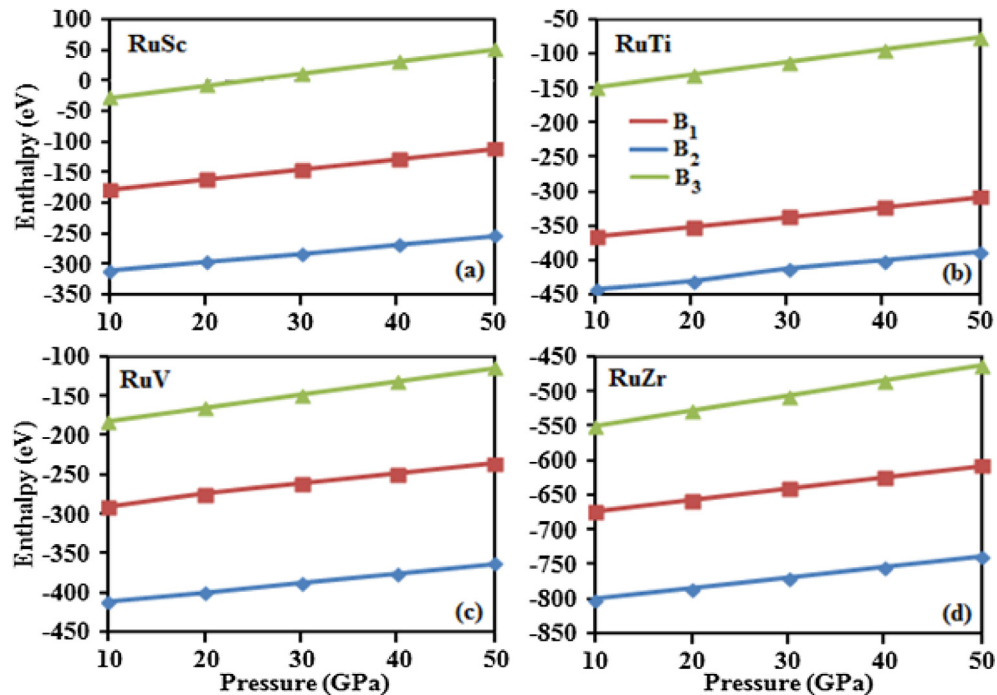


Fig. 2. (a)–(d) Phase stability curves (Enthalpy vs. pressure) of RuX compounds in B₁, B₂ and B₃-phase using WC-GGA.

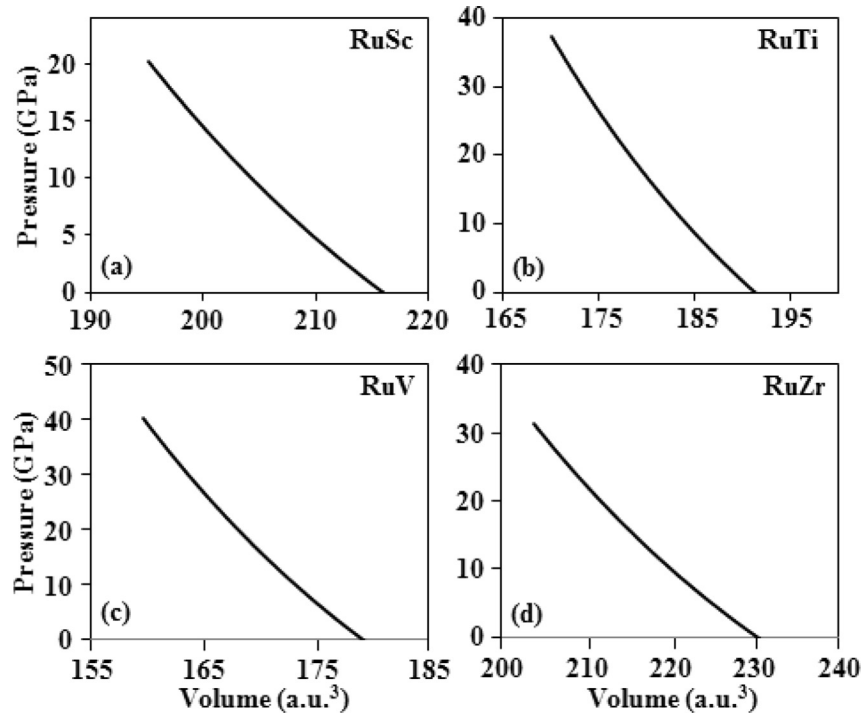


Fig. 3. (a)–(d) Variation of volume with pressure of RuX compounds in B₂-type (CsCl) structure using WC-GGA.

RuV and RuZr which verifies the metallic nature of RuX compounds. The DOS value for RuV is found to be the largest amongst the group of Ru compounds. It might be due to presence of the highest number of 3 'd' electrons in the outermost orbit of vanadium.

Fig. 5(a)–(d) presents the electronic charge density plots for all RuX (X = Sc, Ti, V and Zr) compounds in (1,1,0) plane at ambient conditions. Here Ru is the corner atom while X is the central one. The electron density is the measure of the probability of an electron

Table 1

The calculated ground state properties, density of states at the Fermi level $N(E_F)$ and elastic properties for RuX (X = Sc, Ti, V and Zr) at ambient pressure.

Solids	Work	Approx.	a_0 (Å)	B (GPa)	B'	$N(E_F)$ (states/eV)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
RuSc	Present B ₂	PBE-GGA	3.2138	143.65	4.22	—	256.14	86.83	75.22
		WC-GGA	3.1748	159.29	4.48	1.9867	201.15	139.10	37.11
		PBEsol-GGA	3.1713	158.31	4.23	—	205.33	133.76	25.76
	Exp.	—	3.203 ^a	—	—	—	—	—	—
	Oth. the.	—	3.288 ^b	67.00 ^b	—	—	—	—	—
	B ₁	WC-GGA	5.2395	107.93	4.31	—	—	—	—
RuTi	Present B ₂	PBE-GGA	5.5915	73.86	4.47	—	—	—	—
		WC-GGA	3.0865	220.97	4.07	—	386.97	135.37	109.27
		WC-GGA	3.0501	242.25	3.91	0.3919	484.63	118.07	108.03
	Exp.	PBEsol-GGA	3.0525	237.91	3.89	—	477.26	125.48	105.60
		—	3.06 ^a	—	—	—	—	—	—
		—	3.102 ^b	165.90 ^b	—	—	—	—	—
RuV	Present B ₂	WC-GGA	5.0436	185.63	4.42	—	—	—	—
		WC-GGA	5.6181	53.43	5.50	—	—	—	—
		PBE-GGA	3.0101	250.70	4.56	—	324.07	216.89	164.29
	Exp.	WC-GGA	2.9826	276.74	4.18	3.2448	361.04	240.96	107.63
		PBEsol-GGA	2.977	277.59	4.12	—	374.27	236.16	202.72
		—	2.996 ^a	—	—	—	—	—	—
RuZr	Present B ₂	—	2.995 ^b	228.77 ^b	—	—	—	—	—
		—	4.9238	224.30	4.61	—	—	—	—
		WC-GGA	5.4848	76.56	4.91	—	—	—	—
	Exp.	PBE-GGA	3.2752	185.53	4.24	—	338.49	108.76	63.95
		WC-GGA	3.2440	201.64	3.95	0.4977	348.63	130.00	75.78
		PBEsol-GGA	3.2383	204.11	4.57	—	402.21	103.50	42.99
RuZr	Present B ₂	—	3.25 ^a	—	—	—	—	—	—
		—	3.241 ^b	110.26 ^b	—	—	—	—	—
		—	3.22 ^c	228.00 ^c	3.60 ^c	—	375.00 ^c	154.00 ^c	78.00 ^c
	Exp.	LDA	5.3071	157.68	4.41	—	—	—	—
		WC-GGA	5.8714	65.83	5.08	—	—	—	—
		—	—	—	—	—	—	—	—

Exp. — Experimental, Oth. the. — Other theory, Approx. — Approximations.

^a Ref [27,28].

^b Ref [29].

^c Ref [10].

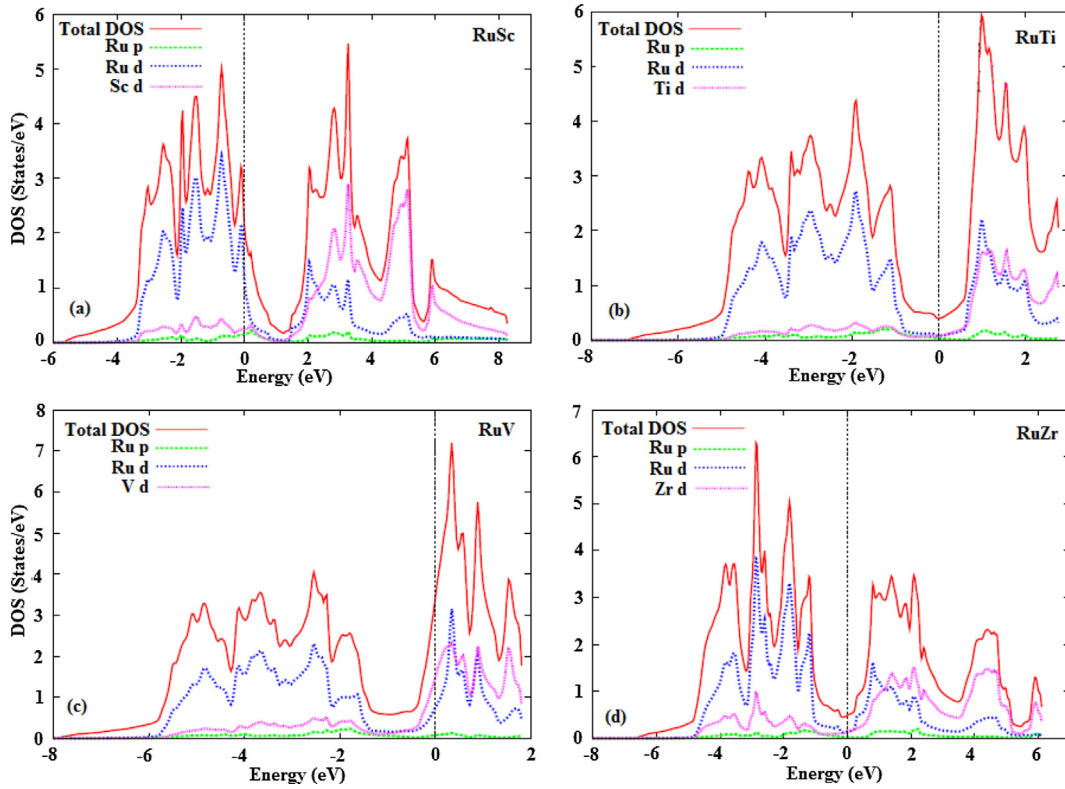


Fig. 4. (a)–(d) Density of states for RuX compounds using WC-GGA.

being present at a specific location. These figures show that the charge distribution on each ion in an ionic crystal will have approximately spherically symmetric concentration with some distortion near the region of contact with neighboring atoms [30] centered on Ru, Sc, Ti, V and Zr atoms (see Fig. 5(a)–(d)). From these Figs., it can be seen that the electronic charge density in the domain of Ru is larger than its complementary atoms Sc, Ti, V and Zr, which might be due to higher electronegativity of Ru atom. The higher the electronegativity of an element, the more electrons are attracted towards it. For covalent and ionic materials, the typical relation between bulk and shear moduli are $G_H = 1.1B$ and $G_H = 0.6B$ [31], respectively. In the present study, the G_H/B ratio for RuSc, RuTi, RuV and RuZr are 0.21, 0.55, 0.30 and 0.43 respectively, indicating them to have weak ionic bonding.

3.3. Elastic properties

The second order elastic constants (SOECs) for all the RuX compounds have been calculated using three different approximations of GGA in their B_2 -phase at ambient pressure. For this calculation, the method introduced by Charpin as integrated in Wien2k code [15] was used. The results of predicted elastic constants are shown in Table 1 together with the other available theoretical data [10]. Our calculated elastic constant in cubic crystal obey the mechanical stability criteria, i. e. $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$. This clearly indicates the stability of ruthenium compounds in B_2 -phase. The elastic constants for RuX intermetallics are calculated for the first time and will provide useful data for comparison in future theoretical and experimental studies.

3.4. Mechanical properties

The calculated values of mechanical properties such as Young's modulus (E), Shear modulus (G_H), Poisson's ratio (ν),

Anisotropic ratio (A) etc. of RuX intermetallic compounds are presented them in Table 2. The bulk and shear moduli can be deduced by using the present values of calculated elastic constants. The shear modulus is calculated using Voigt-Reuss-Hill (VRH) method [32–34]. The effective modulus for the polycrystals could be approximated by the arithmetic mean of the two well known bounds for mono crystals. The Hill shear modulus G_H is given as:

$$G_H = \frac{G_V + G_R}{2} \quad (6)$$

where

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5} \quad (7)$$

is the Voigt shear modulus, and

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})} \quad (8)$$

is the Reuss shear modulus.

Generally Young's modulus (E) is defined as the ratio of stress and strain. It is given by

$$E = \frac{9BG_H}{3B + G_H} \quad (9)$$

When a material is compressed in one direction it is usually tends to expand in other two direction perpendicular to the direction of compression. The ratio of fractional change in cross

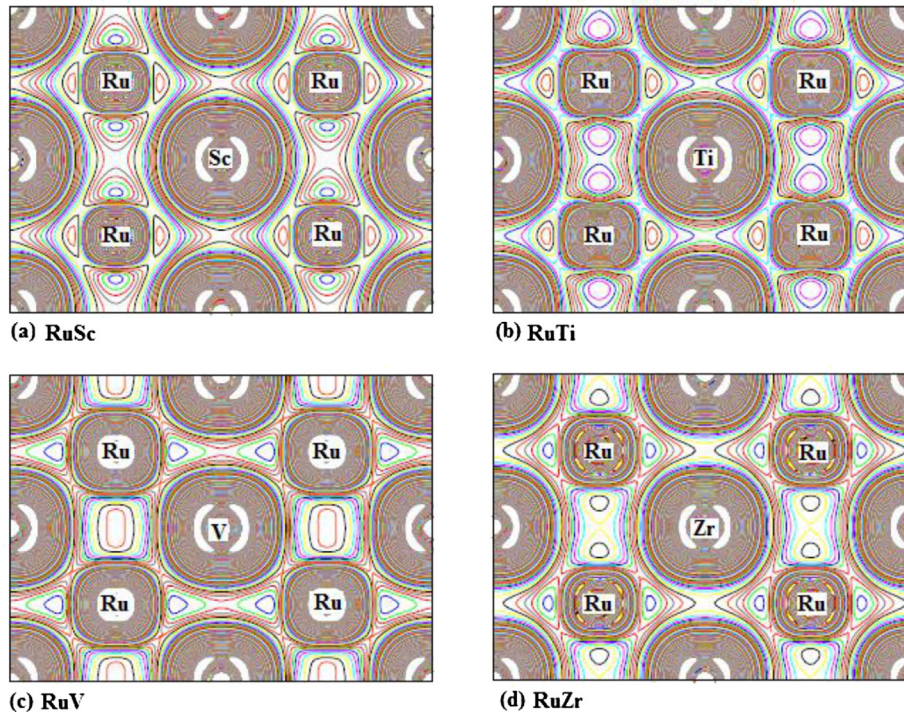


Fig. 5. (a)–(d) Electron density plots in the (110) for RuX compounds using WC-GGA.

sectional direction to the change in length of material is known as Poisson's ratio (ν). This is given by

$$\nu = \frac{3B - 2G_H}{2(3B + G_H)} \quad (10)$$

The Young's modulus E characterizes the stiffness of a material. When it is higher for a given material, the material seems to be stiffer and the stiffer solids have covalent bonds [35].

The calculated values of ν obtained for RuX compounds range between 0 and 0.5. It is observed from Table 2, that value of Poisson's ratio for RuSc is 0.39, which is the largest value among all the compounds, suggesting that when it is compressed, it shows larger lateral expansion.

The bulk modulus represents the resistance to the volume change against the external forces. The shear modulus represents the resistance to shear deformation against the external force. The quotient of shear to bulk modulus (G_H/B) can be used to estimate the brittleness/ductility of intermetallic compounds [36]. If this ratio is larger than 0.57 then materials are considered to be brittle otherwise ductile [36]. This ratio for RuX compounds is found to be

0.21, 0.55, 0.30 and 0.43 respectively, indicating that all the ruthenium compounds studied here are ductile in nature. Due to its lowest G_H/B ratio, RuSc is found to be the most ductile as compared to other compounds. Therefore G_H/B ratio represents the relative directionality of the bonding. Based on this ratio we may conclude that the bonding in these compounds is metallic in nature.

The Cauchy's pressure, defined as the difference between the two particular elastic constants $C_{12}-C_{44}$ is considered to serve as an indication of ductility. Ganesham et al. [37], have established a correlation between the binding properties and ductility. The bonding character of cubic compounds is explained with respect to their Cauchy's pressure ($C_{12}-C_{44}$). Compounds having more positive Cauchy's pressure tend to form bonds which are primarily metallic in nature, whereas compounds having more negative Cauchy's pressure form bonds which are more angular or covalent in character [38]. Thus, the ductile nature of all the RuX compounds, can be correlated to their positive Cauchy's pressure and thereby the metallic character in their bonds. For a good evidence of such conclusion we may also refer Frantsevich [39] who distinguished the ductility and brittleness of materials in terms of Poisson's ratio (ν). The critical value of Poisson ratio of a material is $1/3$. The value of Poisson's ratio $\nu > 1/3$ ($< 1/3$) reveals ductile (brittle) character. According to the above criteria all the compounds possess ductile nature. The Young's modulus (E) can also be considered as an important parameter regarding the bonding character of the material. The lowest value of Young's modulus indicating the presence of metallic bonding while the highest value of it is the evidence of the presence of covalent bonds along with the metallic bonding [35]. For a material ductility (ability to deform) is essential property for the fabrication and its reliable performance. The high degree of ductility occurs due to metallic bonds. In metallic bonds valence shell electrons are delocalized and shared between many atoms. These electrons allow metal atoms to slide past one another in a bulk solid via dislocations and other mechanism. The materials which are ductile in nature change their crystalline symmetry from one type to another before structure

Table 2

The calculated Anisotropy factor (A), Shear modulus (G_H), Young's modulus (E), Poisson's ratio (ν), (G_H/B) ratio, Cauchy's pressure ($C_{12} - C_{44}$) and Plasticity measurement (B/C_{44}) for RuX ($X = \text{Sc, Ti, V and Zr}$) at ambient pressure using WC-GGA in B_2 -phase.

Solids	Work	A	G_H (GPa)	E (GPa)	ν	G_H/B	$C_{12}-C_{44}$ (GPa)	B/C_{44}
RuSc	Present	1.19	34.54	96.66	0.39	0.21	101.99	4.29
RuTi	Present	0.58	133.69	138.32	0.26	0.55	10.04	2.24
RuV	Present	1.79	85.15	232.03	0.36	0.30	133.33	2.57
RuZr	Present	0.69	87.78	230.16	0.31	0.43	54.22	2.66
	Oth. the. LDA	0.70 ^a	90 ^a	237 ^a	0.33 ^a	—	—	—

Oth. the. — Other theory.

^a Ref [10].

Table 3

The calculated density (ρ), longitudinal (v_l), transverse (v_t), average elastic wave velocities (v_m) and Debye temperature (θ_D) for RuX (X = Sc, Ti, V and Zr) at ambient pressure using WC-GGA B₂-phase.

Solids	$\rho \times 10^3$ (kg/m ³)	v_l (m/s)	v_t (m/s)	v_m (m/s)	θ_D (°K)
RuSc	30.34	2605.58	1068.97	1209.07	140.72
RuTi	34.71	3496.73	1994.81	2215.27	267.88
RuV	38.13	3235.13	1524.21	1714.17	212.43
RuZr	37.40	2933.22	1544.25	1725.48	230.16

failure while brittle materials tend to keep their crystalline symmetry until the moment that they fail.

The crystal elastic anisotropy has an important implication in engineering science. To quantify this, we have computed the anisotropy factor A , which gives a measure of the anisotropy of the elastic wave velocity in a crystal and it is given as:

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (11)$$

For isotropic material, A is equal to 1, while any value smaller or larger than 1 indicates anisotropy. The magnitude of the deviation from 1 is a measure of the degree of elastic anisotropy possessed by the crystal. From the computed anisotropy values listed in Table 2, it is clear that the anisotropy factor value for all compounds deviates from unity, meaning that they are characterized by a profound anisotropy. The ratio of bulk modulus (B) to C_{44} may be interpreted as a measure of plasticity [40]. This ratio is also calculated and given in Table 2. From the table one can see that this ratio is the highest for RuSc and lowest for RuTi. This shows that RuSc contains more delocalized bonds than RuTi. Due to the largest B/C_{44} ratio, RuSc may possess lubricating properties.

The Debye temperature (θ_D) can be used in characterizing the excitation of phonons and to describe various lattice thermal phenomena. It is calculated from equation (2). At low temperature the vibrational excitations arise solely from acoustic vibrations. Hence, at low temperature the Debye temperature calculated from elastic constants. The mass density (ρ), longitudinal (v_l), transverse (v_t) and average elastic wave velocities (v_m) including Debye temperatures in B₂-phase have been also calculated and tabulated in Table 3 using the values of calculated elastic constants for all RuX compounds. As far as the author's knowledge is concerned, there is still no experimental and theoretical data regarding thermal behavior of the presented compounds, therefore the obtained theoretical results could consider as a future experimental and theoretical suggestion.

4. Conclusions

We have performed ab-initio calculations on the phase stability of four ruthenium based intermetallic compounds in B₁, B₂ and B₃-phases. The calculated total energy is fitted to the Birch equation of state. The ground state properties such as lattice constants, bulk modulus and its pressure derivative are calculated in all the three phases. The B₂-type (CsCl) crystal structure is found to be the most stable. The electronic, elastic and mechanical properties have also been estimated. The obtained lattice constants in B₂-phase for all the compounds are in good agreement with the experimental and available theoretical data. The computed band structures and density of states show that the studied RuX compounds are metallic in nature. From charge density plots it can be concluded that Ru and X possesses weak ionic bond. Calculated elastic constants satisfy

the mechanical stability criterion for the group of Ru compounds. The ductility for these compounds is analyzed by $G_H/B < 0.57$ ratio and Cauchy's pressure $C_{12}-C_{44} > 0$. RuSc is found to be the most ductile amongst all Ru compounds, which is due to the delocalized single 'd' electron present in the outermost orbit of Sc. The mechanical and thermal properties for these compounds are reported for the first time.

Acknowledgement

The authors are thankful to University Grants Commission Delhi India (New Delhi) No. F. 38-83/2009 (SR), 19.12.2009 for the financial support for Major Research Project. SPS is thankful to UGC (SAP).

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