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Structural, Electronic and Elastic Properties of TMAl (TM=Co, Ni and Ru) Intermetallics: An ab-initio Study

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Abstract

The structural, electronic, elastic, mechanical and thermal properties of transition metal aluminides (CoAl, NiAl and RuAl) have been investigated systematically using first principle density functional theory (DFT). Ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') are calculated which show well agreement with the experimental and other theoretical results. The electronic properties have been analyzed quantitatively. The values of elastic constants are also reported. The ductility of these compounds has been analyzed using the Pugh's rule, Cauchy's pressure (C_{12}-C_{44}) and electronic structure. Our calculated results indicate that NiAl is ductile while CoAl and RuAl are brittle. The elastic properties such as Young's modulus (E), Poisson's ratio (σ) and anisotropic ratio (A) are also reported. We have also correlated the ductility and bonding behaviour of these compounds.

Keywords: Density functional theory; intermetallic compounds; electronic properties; ductility; thermal properties.

1. Introduction

Intermetallic compounds comprise the class of metallic materials which today enjoy intense study by materials scientists and engineers. These materials are already indispensable in many applications and offer the possibility of providing additional breakthroughs in performance in, for example, high temperature structural materials, magnetic materials, and hydrogen storage devices [1, 2]. These materials have ordered arrangement of mixed atom species of metal-metal or metal-semimetal types, generally in a near-stoichiometric composition. For example, TiAl, FeAl, Ni_3AI, $MoSi_2$, etc are of great use. Here titanium (Ti), iron (Fe), nickel (Ni) and molybdenum (Mo) play the role of metal and aluminium (Al) or silicon (Si) the role of metal/semimetal. In such cases the metal-metal or metal-semimetal bonding takes on a partially metallic and partially covalent (or ionic) nature. There are also important intermetallic compounds of metal-metal combinations where atomic size differences are responsible for the ordered arrangement, notably for the Laves phases. The existence of strong interatomic bonding leads to higher elastic moduli -stiffer materials. The presence of a reactive species, aluminium or silicon, leads to the formation of a protective surface layer which endows good oxidation and corrosion resistance.

The transition metal aluminides are generally the most interesting group of intermetallic compounds. These compounds containing aluminium such as NiAl, offer new opportunities for developing low density, high strength structural alloys which might be used at temperatures higher than possible with conventional titanium and nickel-based alloys [3]. Strong bonding between aluminium and nickel, which persists at high temperatures, can provide high strength at elevated temperatures such that the specific strength could be competitive with superalloys and ceramics. However, the high strength is usually associated with poor ductility [4, 5]. With respect to ductility, intermetallics fall between metals and ceramics. Intermetallics are not as brittle as ceramics because the bonding is predominantly metallic, compared to ionic or covalent bonding of ceramics. However it is noticed that in intermetallic compounds, the absence of '*d*' like electrons near the Fermi level accounts for the observed ductility in 90% of the compounds [6].

Of the many intermetallic compounds identified to date, only a relatively small number are candidates suitable for further development as high-temperature applications. In particular, the CsCl type structure (B_2 phase) intermetallics constituted by one transition and another simple metal atom, display diverse physical phenomena and hence are ideally suited for a systematic study of electronic structure, cohesive properties, charge transfer and chemical bonding. The self consistent band structure calculations were done on CsCl-type intermetallics by Pether *et al.* using the APW method. Using angle-resolved photoemission with synchrotron radiation Lui *et al.* [7] have measured the valence band structure of NiAl and compared it with their full potential linear augmented slater-type orbitals (FP-LASTO) calculations. The electronic structure of other homologous material such as CoAl and NiAl were also studied using KKR method by Moruzzi *et al.* [8].

In the present paper, we primarily aim to understand the electronic, elastic and mechanical properties of two groups of transition metal aluminides namely RuAl, NiAl and CoAl which crystallize in CsCl-type structure, using ab-initio theoretical method. We have studied the ground state properties (equilibrium lattice constant, bulk modulus and pressure derivative of bulk modulus) and electronic structure (density of states, band structure) of these compounds. We have also critically examined their ductility by calculating the elastic constants and various mechanical properties. The ductility of these compounds has also been analysed by using electronic structure.

2. Method of calculation

We have performed first-principles total energy calculations within the local density approximation (LDA) and generalized gradient approximation (GGA) using DFT codes WIEN2k [9] and Quantum ESPRESSO [10]. While WIEN2k is based on the full-potential linearized augmented plane-wave (FP-LAPW) method, the quantum ESPRESSO software package uses a plane-wave basis set in the pseudopotential approximation. In both these codes, the electronic states and density are obtained by solving the self-consistent Kohn-Sham equations of DFT [11].

For Quantum ESPREESO irreducible **k**-points are generated according to the Monkhorst-Pack scheme [12]. The Kohn-Sham single-particle functions were expanded on a basis of plane-wave set with a kinetic energy cut-off of 34 Ry. Brillioiun-zone was sampled with 6x6x6 **k**-point mesh, in order to get well converged ground state energy. The exchange and correlation effects have been treated within the LDA. The lattice parameter, bulk modulus and pressure derivative of the bulk modulus were determined by the standard procedure of computing the total energy for different volumes and fitted to Murnaghan's equation of state [13]. While for WIEN2k the generalized gradient approximation (GGA) and local spin density approximation (LSDA) are used for the exchange and correlation effects [14]. In order to achieve convergence, we expand the basis function up to $R_{MT}*K_{max} = 7$ where R_{MT} is the smallest atomic radius in the unit cell and K_{max} gives 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 $G_{max} = 12$. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mash of 1000 **k**- points and the tetrahedral method [12] have been employed for the Brillioiun zone integration. The total energies are fitted to Birch [15] equation of state to obtain the ground state properties.

The elastic moduli require knowledge of the derivative of the energy as a function of the lattice strain. It is well known that a cubic system has only three independent elastic constants namely, C_{11}, C_{12} and C_{44}. Hence, a set of three equations is needed to determine all the constants. The first equation involves calculation of bulk modulus (B), which is related to the elastic constants as:

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

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 etc. One of the standard methods to calculate the Debye temperature is from elastic constants, since θ_D may be estimated from the average sound velocity v_m by the following equation [16, 17]:

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

where h is a 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 velocity is approximately calculated from [16, 18]:

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

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

$$v_l = \sqrt{\frac{\left[C_{11} + \frac{2}{5}(2C_{44} + C_{12} - C_{11})\right]}{\rho}} \tag{4}$$

$$v_t = \sqrt{\frac{\left[C_{44} - \frac{1}{5}(2C_{44} + C_{12} - C_{11})\right]}{\rho}} \tag{5}$$

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

3. Results and discussion

3.1 Structural Properties

For ground state properties of transition metal aluminides (TMAl, TM = Co, Ni and Ru), the total energies are calculated as a function of lattice constant in CsCl-type structure using the first principles pseudopotential (PWSCF) method. For Quantum Espresso these energy values have been fitted to the Murnaghan's equation of state [13] to obtain the equilibrium lattice constant (a_0), bulk modulus (B) and its pressure derivative ($B^{'}$*)* at minimum equilibrium volume V_0.

$$P(V) = \frac{B}{B^{'}}\left[\left(\frac{V_0}{V}\right)^{B^{'}} - 1\right] \tag{6}$$

Where the fit parameter are the equilibrium volume V_0, the bulk modulus B:

$$B = -V\frac{\partial P}{\partial V} = V\frac{\partial^2 E}{\partial V^2} \tag{7}$$

And its derivative with respect to the pressure, B' = dB/dP

For WIEN2k we performed the structural optimization by minimizing the total energy with respect to the volume using FP-LAPW method. The calculated total energies are fitted to the Birch equation of states [15] to determine the ground state properties, such as equilibrium lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') which are listed in Table 1

$$E(V) = E_0 + \frac{BV}{B'}\left[\frac{(V_0/V)^{B'}}{(B'-1)} + 1\right] - \frac{BV}{B'-1} \tag{8}$$

Pressure is obtained by taking volume derivative of the total energy

$$P(V) = \frac{B}{B'}\left[\left(\frac{V}{V_0}\right)^{B'} - 1\right] \tag{9}$$

Figure 1, shows the variation of total energy as a function of lattice constant for the three TMAl. We have also calculated the total energy as a function of volume using the first principle FP-LAPW method using non-spin generalised gradient approximation (GGA) and local spin density approximation (LSDA). The calculated values of lattice constant (a_0), bulk modulus (B), its pressure derivative ($B^{'}$) are listed in Table 1 and compared with the experimental [19-22] and other theoretical results [7, 23-25]. We observed from Table 1, that the result obtained from LDA and LSDA using respectively the Pseudopotential and FP-LAPW method are approximately same while GGA result are slightly overestimated. To the best of our knowledge no data are available for pressure derivative of bulk modulus and density of state at Fermi level $N(E_F)$ for comparison.

3.2 Electronic Properties

The calculated electronic band structure along the principal symmetry directions of TMAl (TM= Co, Ni and Ru) compounds using PWSCF method within LDA (local density approximation) are presented in Figure 2(a-c). It is clear that all TMAl compounds exhibit metallic behaviour. To further elucidate the nature of the electronic band structure, we have also calculated the total and partial density of states of these compounds at ambient pressure and presented them in Figure 3(a-c). In Figure 2(a) for CoAl, the lowest lying bands are due to Co and Al '*s*' like states. The peak just below the Fermi level near -1.0 eV are mainly due to Co '*d*' states. The delocalized band cross the Fermi level at point A and B from valence band to conduction region and at point C and D from conduction band to valence band which are mainly due to hybridization of '*d*' states of Co and '*p*' states of Al. It is also seen from the partial DOS in Figure 3(a), the number of density of states at the Fermi level $N(E_F)$ is 0.97 states/eV (see Table 1). In case of NiAl from Fig 2(b), we observed that Al and Ni '*s*' states dominate the bottom of the valence band. The peak just below the Fermi level near -2.0 eV are mainly due to Ni '*d*' states. The delocalized band cross the Fermi level at points A and B from valence region to conduction region which is due to hybridization of Ni '*d*' states and Al '*p*' states and the delocalized bands cross the Fermi level at points C and D from conduction region to valence region are mainly due to hybridization of '*d*' and '*p*' states of Ni with '*p*' states of Al. It also seen from the Figure 3 (b) that the hybridization of Ni '*d*' and Al '*p*' states are delocalized from valence to conduction region. The finite DOS at Fermi level is found to be 1.29 states/eV. In NiAl we observed that the bands near Fermi level are slightly shifted below the Fermi level as compared to CoAl.

In Figure 2 (c) and 3 (c) for RuAl, Al '*s*' like states dominate the bottom of the valence band. A small peak is observed near -6.0 eV which is due to Ru '*d*' and Al '*s*' states. The hybridization of Ru '*d*' and Al '*p*' states are delocalized from valence to conduction region. Ru '*d*' bands are much wider than the Ni/Co '*d'* bands which may be due to 4*d* electrons of Ru atom. The bands are crossing the Fermi level at 9 points. The bands at the first 5 points (A to E) mostly around the Γ point consist of '*d*' states of Ru with admixed small amount of Al '*p*' like states. For the other four points around e.g. the R point (F, G, H and I) the bands are identified more or less as hybridized Ru-Al hybridized. Overall, the states around the Fermi level consist predominantly of Ru '*d*' orbital's compared to the Ni/Co '*d*' like states for NiAl/CoAl. The number of density of states at the Fermi level N(E_F) is 1.48 states/eV (see Table 1).

From the analysis of band structure of these TMAl we have observed that all the three compounds have similar band structure that mainly differ from each other by the energy level of each band relative to the Fermi level. The strong hybridization between the TM-*d* and Al-*p* states are spread from valence to conduction region. Therefore, the *p-d* hybridization provides the cohesion and leads to a high formation energy of these compounds. From Figure 3 (a) for CoAl, a peak is observed at the Fermi level reveals that this compound is brittle [26] whereas for NiAl (Figure 3 (b)) the peak shifted below the Fermi level reveals the ductility in it. From closely examine of the electronic structure of these compounds we observed that TM '*d*' bands are found near and at Fermi level for CoAl and RuAl respectively, while for NiAl it is little far from Fermi level due to which CoAl and RuAl are found to be brittle and NiAl ductile [6] which will be discuss in detail later.

3.3 Elastic Properties

The elastic constants provide a link between the mechanical and dynamical behaviour of crystals and provide important information concerning the nature of the interatomic forces. In particular, they provide information on the stability and stiffness of materials. We have calculated the elastic constants of the TMAl (TM= Co, Ni and Ru) at ambient pressure by using the method developed by Charpin and integrated it in the WIEN2k package [9]. The calculated values of elastic constants are given in Table 2. It can be noted that our calculated elastic constants satisfy the stability criterions, C_{11}-C_{12}>0, C_{44}>0, $C_{11}+2C_{12}>0$ and $C_{12}<B<C_{11}$ which clearly indicate the stability of these compounds in their respective phase. It can be seen from Table 2 that the calculated values of elastic constants of TMAl are in good agreement with the experimental [27, 28] and theoretical data [29].

3.4 Mechanical Properties

Elastic constants are used to determine the mechanical properties such as Young's modulus (*E*), shear modulus (G_H), Poisson's ratio (v), anisotropic ratio (A), for useful applications. The various mechanical properties of these compounds are presented in Table 2 and compared with the experimental [29] and theoretical [30, 31] results. The shear modulus G_H describes the material's response to shearing strain using the 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 monocrystals. The Hill shear modulus G_H is given as:

$$G_H = \frac{G_V + G_R}{2}$$

(10)

where $G_V = \dfrac{C_{11} - C_{12} + 3C_{44}}{5}$ is the Voigt shear modulus (11)

and $G_R = \dfrac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}$ is the Reuss shear modulus (12)

Using the mechanical and physical properties of these compounds based on their elastic properties, we have analyzed their ductility using the (B/G_H) ratio. The shear modulus G_H represents the resistance to plastic deformation while the bulk modulus B represents the resistance to fracture. As suggested by Pugh [35], if $B/G_H > 1.75$ a material behaves in a ductile manner. From this ratio we observed that CoAl and RuAl are brittle while NiAl is ductile.

Ganeshan *et. al.* [36] have established a correlation between the binding properties and ductility. The bond character of cubic compounds is explained with respect to their Cauchy pressure (C_{12}-C_{44}). Compounds having more positive Cauchy pressure tend to form bonds which are primarily metallic in nature, whereas compounds having more negative Cauchy pressure from bonds which are more angular in character [37]. Thus, the ductile nature of the three TMAl compounds, can be correlated to their positive Cauchy pressure and thereby the metallic character in their bonds. The Cauchy pressure is found to be negative for CoAl and RuAl and positive for NiAl. The Young's modulus (E) is important for technological and engineering application. Young's modulus is defined as the ratio of stress and strain, and is used to provide a measure of the stiffness of the solid, i.e., the larger value of E, the stiffer is the material. And the stiffer solids have covalent bonds [38]. Young's Modulus E is given by-

$$E = \frac{9BG_H}{3B + G_H} \tag{13}$$

The Poisson's ratio (σ) is given by eq. (14) as

$$\sigma = \frac{3B - 2G_H}{2(3B - G_H)} \tag{14}$$

It is observed from Table 2 that values of Poisson's ratio lies between 0.22 - 0.29 for the TMAl. Another important parameter is the elastic anisotropic factor A, which gives a measure of the anisotropy of the elastic wave velocity in a crystal and it is given as:

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{15}$$

which is unity for an isotropic material, anisotropy factor (A) is listed in Table 2. For NiAl A (>2) tends to elastically enhance the cross slip [39] that means large value of A can give rise to the driving force (tangential force) acting on screw dislocations to promote the cross-slip pinning across.

Bulk modulus is still used as a preliminary measure of the hardness of material but it is well known that other properties must be taken into account. A high bulk modulus does not mean a material is hard. Elastic characteristics must be considered as well, and shear modulus might even provide a better correlation with hardness than bulk modulus. Covalent materials generally have a high shear modulus. The value of Poisson's ratio, found to be ~ 0.1 in covalent materials and ~ 0.33 in metallic materials. If a material contains highly directional bonds, the shear modulus will increase and give a low Poisson ratio. If a material has short covalent bonds, atomic dislocations that lead to plastic deformation are less likely to occur than in materials with longer, delocalized bonds. If a material contains many delocalized bonds it is likely to be soft [40, 41]. An inspection of Table 2 revels that the shear modulus and Young's modulus of NiAl is lowest amongst the TMAl resulting it the most soft materials. The value of Young's modulus (*E)* is also lowest for NiAl indicating the presence of metallic bonding in it. The highest value of Young's modulus in rest of the TMAl is indicating the presence of covalent bonds along with the metallic bonding [38].

3.4 Thermal properties

Once we have calculated the Young's modulus (E), Bulk modulus (B) and the shear modulus (G_H), we may obtain the Debye temperature (θ_D) as well as the density by using the average sound velocity (v_m). At low temperature the vibrational excitations arise solely from acoustic vibrations. Hence, at low temperature the Debye temperature calculated from elastic constants. We have calculated the average sound velocities and Debye temperatures as well as the densities for TMAl by using the calculated elastic constants which are given in Table 3.

Conclusion

In conclusion we have systematically investigated the structural, electronic, elastic, mechanical and thermal properties of the three B_2-type intermetallics namely CoAl, NiAl and RuAl using ab-initio DFT. The computed electronic band structures and density of states show that studied TMAl are metallic in nature. From the band structure we observe that as one goes from Co to Ru, the '*d'* band becomes systemically filled up. Also, as the number of '*d'* electron increases the number of bands crossing at the Fermi level increases. From DOS it can be observed that the main features around Fermi level in the three TMAl arises from the TM sites. Ductility of these compounds has also been examined using electronic structure. We have also presented the elastic moduli at ambient pressure. Using these elastic constants, the shear modulus (G_H), Young's modulus (E), Poisson's ratio (σ) and anisotropic ratio (A) are also reported. We found that NiAl is ductile having positive Cauchy pressure and B/G_H ratio > 1.75. We also observed that the value of E, G_H and σ is highest for NiAl among the three TMAl reveals that it is the softest one. We also report thermal properties of these compounds.

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Table 1. Calculated ground state properties for TMAl (TM=Co, Ni and Ru)

TMAl	Work	Approximation	a_0 (Å)	B(GPa)	B'	N(E_F)
CoAl	Pre. (Q.E)	LDA	2.78	199	4.13	0.97
	(Wien2k)	LSDA (non- spin)	2.79	198.8	3.31	
		GGA	2.85	181.7	4.48	
	Expt.		2.86[a]			
	O. Theo.	LDA	2.80[b]	207[b]		
NiAl	Pre. (Q.E)	LDA	2.81	180	4.57	1.29
	(Wien2k)	LSDA (non- spin)	2.83	180.5	2.87	
		GGA	2.89	184.6	2.75	
	Expt.		2.88[a]	189[c]		
	O. Theo	LDA	2.84[d]	192[d]		
RuAl	Pre. (Q.E)	LDA	2.99	211	4.49	1.48
	(Wien2k)	LSDA (non- spin)	2.95	202.2	4.8	
		GGA	3.01	221.9	4.12	
	Expt.		3.03[e]	207[f]		
	O. Theo	LDA	3.02[g]	220[g]		

[a]:Ref[19] [b]:Ref[7,23] [c]:Ref[20] [d]:Ref[24] [e]:Ref[21] [f]:Ref[22] [g]:Ref[25]

Pre. = Present, Q. E = Quantum Espresso, Expt. = Experimental, O. Theo. = Other Theoretical

Table 2. Calculated elastic and Mechanical properties for TMAl (TM = Co, Ni and Ru)

TMAl	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	E (GPa)	G_H (GPa)	A	σ	C_{12}- C_{44} (GPa)	B/G_H
CoAl Pre.	297.8	113.45	151.69	303.51	114	1.64	0.21	-52.98	1.46
O. Theo.	251.±4[a]	101. ±3[a]	134. ±1[a]	278[b]	114[b]		0.22[b]		
NiAl Pre.	250.90	151.44	122.59	221.9	85.37	2.46	0.29	28.85	2.16
O. Theo.	237.±10[a]	155. ±8[a]	132.±5[a]						
Expt.	211.5[c]	143.2[c]	112.1[c]	184[c]	70[c]	3.28[c]	0.31[c]		
RuAl Pre.	338.01	143.31	158.14	321.54	130.18	1.62	0.23	-14.83	1.55
O. Theo.	346[d]	162[d]	141[d]	266[e]	104[e]	1.49[e]	0.28[e]		
	308.±6[a]	144.±5[a]	122.±10[a]						

[a]:Ref[27] [b]:Ref[30] [c]:Ref[29] [d]:Ref[28] [e]:Ref[31]

Expt. = Experimental, O. Theo. = Other Theoretical

Table 3. Calculated longitudinal vl, transverse vt , average elastic wave velocities vm, Debye Temperature θ_D for TMAl (TM = Co, Ni and Ru)

TMAl	$\rho*10^3$ (kg/m$^{3)}$	ν_l (ms^{-1})	ν_t (ms^{-1})	ν_m (ms^{-1})	θ_D (K)
CoAl	4744.49	8532.45	5191.74	5730.55	428.81
NiAl	4537.49	8254.74	4538.08	5054.28	372.97
RuAl	6002.63	8025.71	4721.67	5228.75	370.46

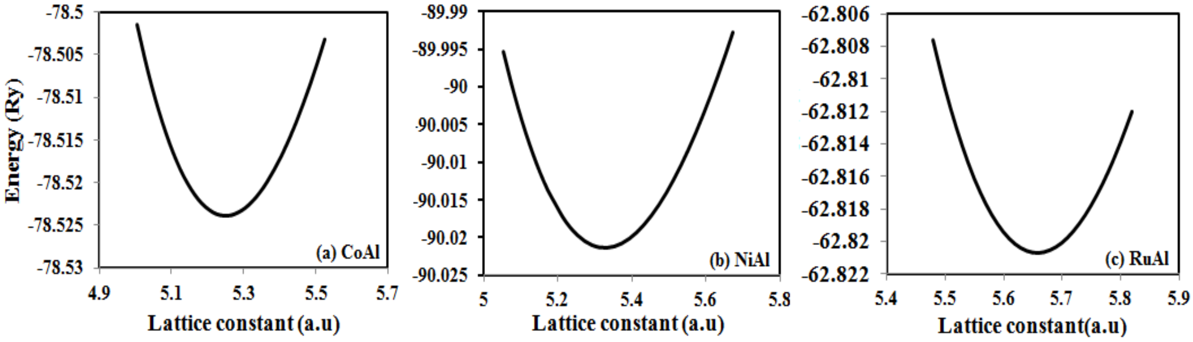

Figure 1. Variation of total energy with lattice constants for (a) CoAl (b) NiAl and (c) RuAl.

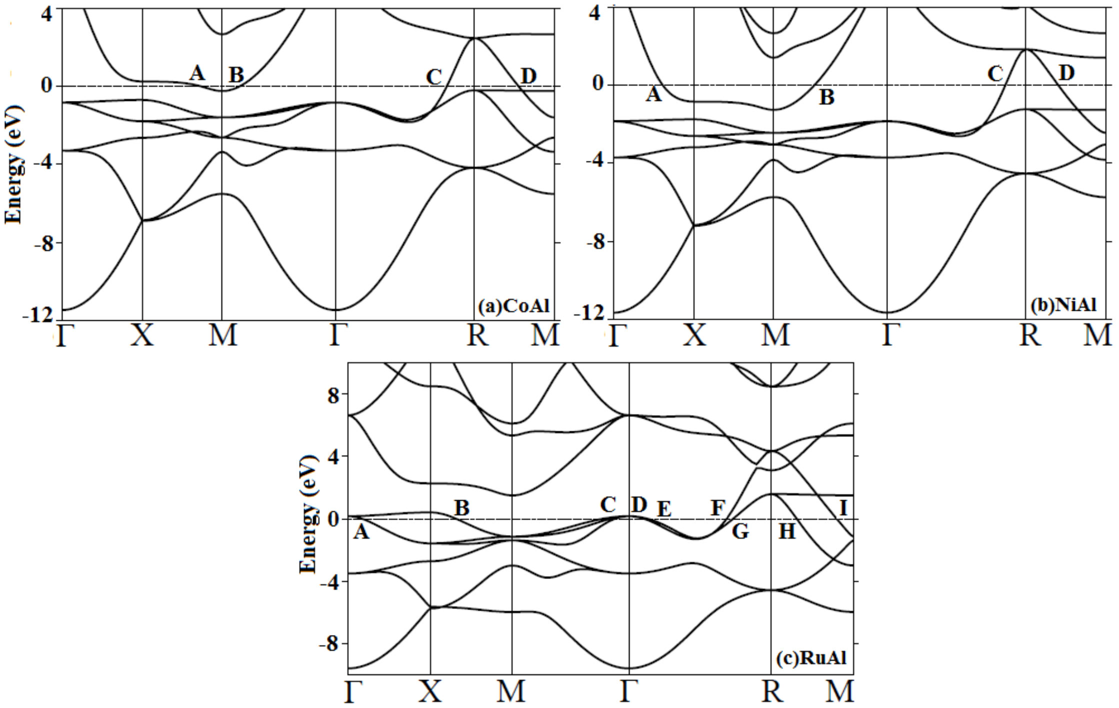

Figure 2. Band Structure of (a) CoAl (b) NiAl (c) RuAl

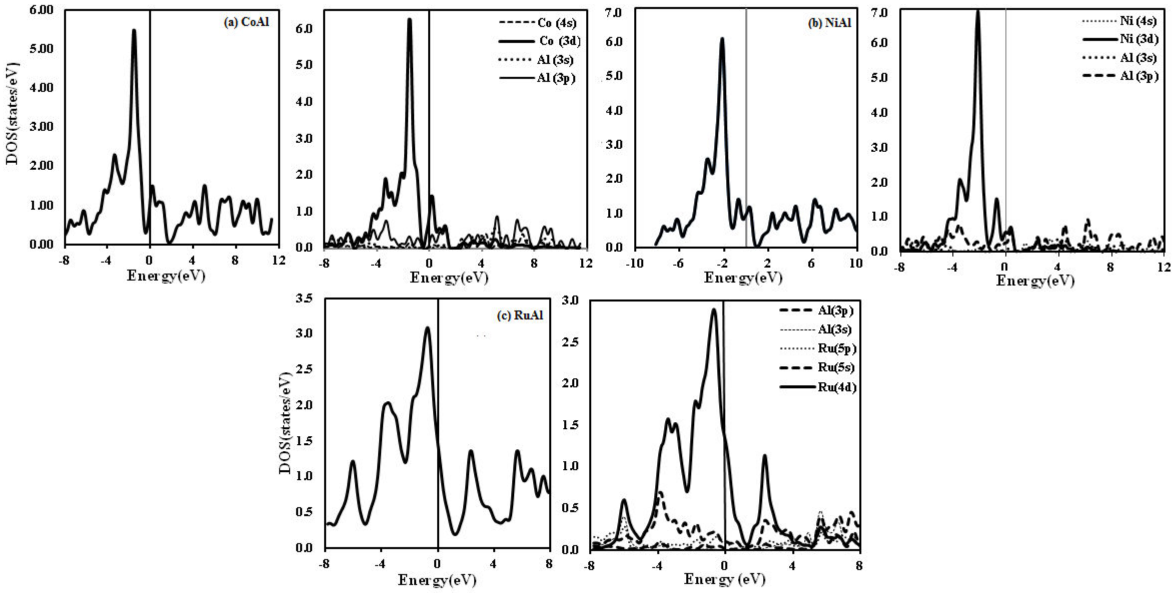

Figure 3. Total and Partial DOS of (a) CoAl (b) NiAl (c) RuAl.

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