

EFFECT OF SUBSTITUTING Pt WITH X (X = Mg, V, Ni, Cr, Ti) ON ELASTIC AND ELECTRONIC PROPERTIES OF Pt₃Al AND Pt₃Sc ALLOYS

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ABSTRACT

Structural materials for airplanes and other space bound turbines are of lower weight ($\approx 4\text{g.cm}^{-3}$). Both $L1_2$ -Pt₃Al and $L1_2$ -Pt₃Sc are good high temperature structural materials. The use of these materials to manufacture space based turbine components has been limited by their weight, which is well above 10g.cm^{-3} . The density functional theory calculation method have been performed to investigate the mechanical and electronic properties of $L1_2$ -Pt₃Al and $L1_2$ -Pt₃Sc in which Pt has been substituted with light weight elements such as Mg, V, Ni, Cr or Ti. The element with highest weight reduction prediction is Ti, followed by Mg, V, Ni and Cr respectively. Both $L1_2$ -Pt₃Al and $L1_2$ -Pt₃Sc would become elastically unstable when about 66% of Pt is substituted with Cr or Ti. All the elements (Mg, Ti, V, Cr, Ni) would lead to strength reduction in $L1_2$ -Pt₃Al and $L1_2$ -Pt₃Sc. Anisotropy is predicted in $L1_2$ -Pt₃Al but not in $L1_2$ -Pt₃Sc when about 33% of Pt is replaced with Ti and at about 66% of Pt replaced with Cr. Overall, substituting Pt with Ti and V should lead to ductility improvements in $L1_2$ -Pt₃Al and $L1_2$ -Pt₃Sc.

Keywords: density functional theory; anisotropy; ductility; strength; phase stability

INTRODUCTION

In the last thirty to forty years, intermetallic compounds with the $L1_2$ structure have received considerable attention. They have shown to be an invaluable intermetallic compounds, due to their strengthening phase capability for high temperature materials, especially the Ni-based superalloys. Greater efforts had been devoted on $L1_2$ compounds that exhibit high temperatures anomalous positive temperature dependence of yield stress. A classical representative of the $L1_2$ compound with positive anomalous temperature dependence of yield stress is Ni₃Al. Unfortunately, Ni-based superalloys are presently used near their melting temperature capabilities (Rytvin, 1987; Whalen, 1988). The Platinum Group Metals (PGMs) are alternative candidates for developing ultra-high temperature alloys that can at least

withstand temperature in excess of 200°C above the existing Ni-based alloys. The interest in PGM based alloys are due to their high melting point, high strength and exceptional environmental stability (Lupton, 1990; Yamabe-Mitarai *et al.*, 1996; Ira *et al.*, 2000; Yamabe-Mitarai *et al.*, 2004). They have found applications as high temperature structural materials in glass-making, catalysts, shape memory alloys and special solder. Pt₃Al and Pt₃Sc are important materials in this class and they have received considerable attention. While there are agreements regarding the low-temperature Cu₃Au/ $L1_2$ form of Pt₃Al (Bronger and Klemm, 1962; Huch, 1964; Chattopadhyay, and Schubert, 1975), other studies showed that Pt₃Al will exhibit the Cu₃Au/ $L1_2$ phase only at high temperature, with a transformation to tetragonal structures at lower

temperatures (McAlister and Kahan 1986; Oya *et al.*, 1987; Massalski, 1990; Cornish *et al.*, 2003). The confusion surrounding the ground state structure of Pt₃Al had been addressed through the Density Functional Theory (DFT) calculation method, where the ground state structure of stoichiometric Pt₃Al was found to be *t*P16-Pt₃Ga (Chauke *et al.*, 2010). The plastic deformation behavior of single crystals of L1₂-Pt₃Al from 77 to 1073K had been studied. Its cubic structure was found to be more stable than the tetragonal structure up to about 100 GPa with excellent resistance to volume deformation under high pressure (Savitskii and Gribulye, 1970; Okamoto *et al.*, 2012).

The crystal structure of Pt₃Sc is also Cu₃Au/L1₂ (Dwight and Conner, 1970). The alloy (Pt₃Sc), is also a strong intermetallic compound, with larger negative enthalpy of formation than Pt₃Al and remains ordered up to its melting point of 1850°C (Massalski, 1990). Despite these investigations and the appealing properties, wide use of Pt₃Al and Pt₃Sc is limited due to their weight and cost. Cost is not much an issue because platinum is recyclable. Also, any gain in materials performance, be it strength, melting temperature or service life, can easily discount cost and invariably push up the performance curve of Pt₃Al and Pt₃Sc as high-temperature materials. In view of this, any attempt to extend the application area of Pt₃Al and Pt₃Sc as performance-critical components by lowering their weight without much compromise on their mechanical properties should be a reasonable venture. The main goal of this work therefore, is to investigate the electronic and elastic properties of Pt₃Al and Pt₃Sc in which up to 66% atom of Pt has been substituted with either a 3s element (Mg) or 3d elements (Ti, V, Cr, Ni). The choice of these elements is due to their much lower weight and other favorable properties including high melting points and good ductility. Many properties including the formation energy, elastic moduli, density, anisotropy, bonding are investigated.

CALCULATION METHODS

The present electronic structure calculations are based on density functional theory (DFT) (Hohenberg and Kohn, 1964; Kohn and Sham, 1965) and have been performed using the Quantum Espresso computer code (Giannozzi *et al.*, 2009). The DFT prescribed total energy for any quantum mechanical system is as given in (1).

$$E[n] = T_s[n] + \int \frac{n(r)n(r')}{r-r'} drdr' + \int n(r)V_{ext}(r)dr + \mu_{xc}(n) \quad (1)$$

$$\text{with } T_s[n] = \frac{\hbar^2}{2m} \sum_i \int \psi_i^*(r) \nabla^2 \psi_i(r) dr \quad (2)$$

where $E[n]$ is the density (n) dependent ground state total energy, $T_s[n]$ is the kinetic energy, the second and third expressions on the right of (1) are the Hartree energy and energy due to the external potentials respectively, while $\mu_{xc}(n)$ is the exchange and correlation energy. $\mu_{xc}(n)$ is an approximation, which in this present calculation was treated using the generalized gradient approximation (GGA) (Perdew *et al.*, 1996). Integration for the total energy over the Brillouin zone was done according to the Monkhorst–Pack scheme (Monkhorst and Pack, 1976). All core states were treated using the Vanderbilt-type ultrasoft pseudopotential (Vanderbilt, 1990). The format for calculating the elastic properties are as follows. A uniform distortion was imposed on the lattice, such that it transforms its set of primitive vectors, \mathbf{a}_i , to a set of new vectors \mathbf{a}'_i , using a strain tensor $\boldsymbol{\varepsilon}$ as given in (3):

$$\begin{pmatrix} \mathbf{a}'_1 \\ \mathbf{a}'_2 \\ \mathbf{a}'_3 \end{pmatrix} = (I + \boldsymbol{\varepsilon}) \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}, \quad (3)$$

where I is the 3×3 identity matrix.

Usually, 21 independent c_{ij} elastic constants are obtained, but the cubic structure symmetry would reduce the number to only three independent constants (c_{11} , c_{12} , and c_{44}). To determine all the three cubic elastic constants, two types of lattice strain are imposed. The first was a volume-conserving orthorhombic strain of the form:

$$\varepsilon = \begin{pmatrix} x & 0 & 0 \\ 0 & -x & 0 \\ 0 & 0 & \frac{x^2}{1-x^2} \end{pmatrix}, \quad (4)$$

whose total energy is an even function of distortion x :

$$\Delta E(x) = \Delta E(-x) = V(C_{11} - C_{12})x^2 + \theta[x^4] \quad (5)$$

and a monoclinic volume-conserving strain of the

$$\text{form: } \varepsilon = \begin{pmatrix} 0 & \frac{x}{2} & 0 \\ \frac{x}{2} & 0 & 0 \\ 0 & 0 & \frac{x^2}{4-x^2} \end{pmatrix} \quad (6)$$

whose total energy dependence is of the form:

$$\Delta E(x) = \Delta E(-x) = \frac{1}{2}VC_{44}x^2 + \theta[x^4] \quad (7)$$

The value of distortion x was varied from zero (for the equilibrium state) to 10%. The elastic constant values were obtained from the derivatives of ΔE with respect to x^2 . For a cubic crystal, mechanical stability requires that:

$$c_{11} - c_{12} > 0; c_{11} + 2c_{12} > 0; c_{11} > 0; c_{44} > 0 \quad (8)$$

The other properties related to the elastic constants include the bulk and shear moduli. There are no exact expressions for the polycrystal-averaged bulk and shear moduli. Approximate averages given by the low and upper bounds of different theories (Voigt, 1928; Reuss, 1929) were used. The bulk modulus B and shear modulus G , for a cubic crystal, are expressed as:

$$B_V = \frac{c_{11} + 2c_{12}}{3} \quad (9)$$

$$G_V = \frac{c_{11} - c_{12} + 3c_{44}}{5} \quad (10)$$

or

$$B_R = \frac{c_{11} + 2c_{12}}{3} \quad (11)$$

$$G_R = \frac{5(c_{11} - c_{12})c_{44}}{[4c_{44} + 3(c_{11} - c_{12})]} \quad (12)$$

Equations (9) – (12), represents the upper and lower limits of a true polycrystalline modulus. The arithmetic mean of these moduli is believed to give a better modulus (Hill, 1952). The Young's modulus E and the Poisson's ratio ν can be evaluated (Green, 1993) from (13) and (14).

$$E = \frac{9BG}{3B+G} \quad (13)$$

$$\nu = \frac{3B-2G}{2(3B+G)} \quad (14)$$

Other important parameters like the Cauchy pressure constant (C'), the anisotropy constant (A), can be evaluated according to (15) and (16).

$$C' = c_{12} - c_{44} \quad (15)$$

$$A = \frac{2c_{44}}{c_{11} - c_{12}} \quad (16)$$

RESULTS AND DISCUSSION

All calculated results are given in Table 1. Instructively, the results on $L1_2$ -Pt₃Al and $L1_2$ -Pt₃Sc are compared with available results. The calculated elastic constants result for $L1_2$ -Pt₃Al is relatively lower compared with the ones given in Chauke et al. (2010); Fu and Yoo (1988). It is to be noted however, that wide variation also exists between these earlier reported theoretical results. Moreover, our calculated c_{11} , c_{12} and subsequently the bulk modulus is found to show close correlation with the results in Razumovskiy et al. (2008). The seemingly wide variation between the other calculated results and the compared ones are so due to the fact that all the expression used are c_{44} dependent. It is important however, to note that the trend between all results on $L1_2$ -Pt₃Al and $L1_2$ -Pt₃Sc is such that $c_{11} > c_{12} > c_{44}$, which is necessary for lattice stability. Using the conditions highlighted in (8), it can be concluded that substituting about 66% at. of Pt with Cr or Ti in Pt₃Al will lead to elastically unstable structures. The formation energy E_F , is negative for a thermodynamically stable material. For unstable/metastable materials, E_F is positive. The E_F results in Table 1, predicts that replacing about 33% at. Pt with Ti in Pt₃Sc and about 66% at. Pt with Ti in Pt₃Al would lead to structures that are thermodynamically unstable. Thermodynamic instability is predicted to increase with Pt substitution with Mg, Cr, Ti and V. Better thermodynamic stability (as shown by increase in

E_F) is predicted in Pt_3Al but not in Pt_3Sc beyond 33% at. Pt replaced with Ni.

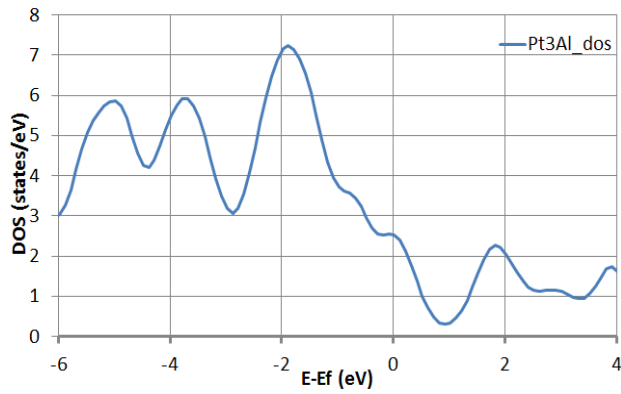
The calculated weight for $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$ are $16.88g.cm^{-3}$ and $16.22g.cm^{-3}$ respectively. Weight reduction prospect through Pt substitution with the elements, shows that Ti would give the best reduction, followed by Mg, V, Ni and Cr. The Shear modulus G , correlates with the strength of a material (Chen et al., 2011). The G result, predicts that the substitution of Pt with Ti, Mg, V, Cr or Ni (regardless of the % of Pt replaced) will reduce strength in $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$. Higher values of Young's modulus E correlate with stiffness. Both $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$ will soften when Pt is substituted with Ti, Mg, V, Cr or Ni. The G/B ratio helps to predict ductility in intermetallics. High values of G/B (>1.06) signify brittleness while low value signifies ductility. The substitution of Pt with Mg, Cr or Ni will reduce ductility while Ti or V will increase ductility in $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$. The anisotropy constant (A) result shows that $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$ are anisotropic ($A > 1$). Anisotropy would be maintained in Pt_3Al and Pt_3Sc when 66% at. Pt is replaced with Mg, Ti, Ni, V or Cr. The compounds will almost become isotropic ($A = 1$) when about 33% at. of Pt is replaced with Mg, Ti, Ni, V but not Cr. The Cauchy pressure (C') and the Poisson's ratio (ν) can be used jointly to determine the nature of bond in a substitution disordered intermetallic. While most covalent bonds would show a negative C' , ionic bonds are characterized more by a positive C' (Mikhal, 2003; Ledbetter and Migliori, 2008). In a typical covalent compound, the Poisson's ratio is much less than 0.25 (around 0.1), while a typical ionic compound is characterized by ν near 0.25 or more (Bannikov et al., 2007). From the results, the same trend is seen in C' and ν . While $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$ are characterized by ionic bonds, it can be predicted that covalent bond will dominate when about 33% of Pt is substituted with Mg in Pt_3Al . The ionic

bond will dominate in Pt_3Sc when about 66% at. Pt is substituted with Cr or Mg respectively. All other compositions are predicted to be characterized by ionic bonds.

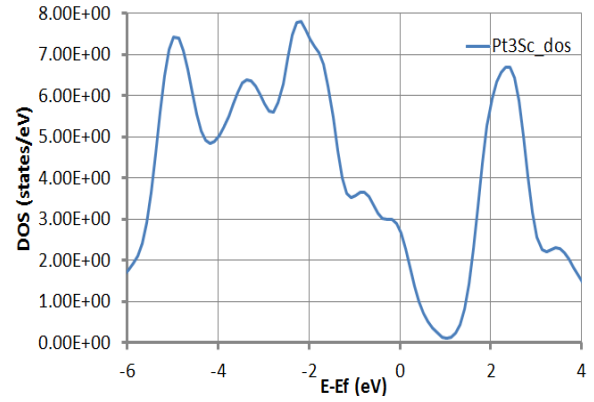
The electronic structure results for $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$ and the other substitution disordered compounds are shown in Figures 1 - 4. The density of states (DOS) at the Fermi level ($E-E_f = 0$ on the plots) for $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$ (shown in Figure 1(a) and (b)), is 2.5states/eV and 2.7states/eV respectively. Any beneficial element addition/substitution into $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$ should lower these DOS values rather than increasing it. A smaller DOS at the Fermi level is observed when $\leq 66\%$ at. Pt is replaced with Mg in Pt_3Al (Fig. 1e and 3c) and Pt_3Sc (Fig. 1f and 3d), when $\leq 66\%$ at. Pt is replaced with Ni in Pt_3Al (Fig. 2a and 3c) and Pt_3Sc (Fig. 2b and 3d) and when about 66% at. Pt is replaced with Cr in Pt_3Al (Fig. 3a) and Pt_3Sc (Fig. 3b) respectively. The varying degree of substitution is beneficial in $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$. Benefits are predicted only when Pt is substituted with Cr at about 66 at. %. A rising DOS is seen around the Fermi level when $\leq 66\%$ at. Pt is replaced with Ti in Pt_3Al (Fig. 2c and 4a) and Pt_3Sc (Fig. 2d and 4b), when $\leq 66\%$ at. Pt is replaced with V in Pt_3Al (Fig. 2e and 4c) and Pt_3Sc (Fig. 2f and 4d), and when $\leq 33\%$ at. Pt is replaced with Cr in Pt_3Al (Fig. 1c) and Pt_3Sc (Fig. 1d) respectively. These substitutions would lead to the creation of increasing instability in $L1_2-Pt_3Al$ and $L1_2-Pt_3Sc$. These may further explain the reason why the formation energy (E_F in Table 1) for $L1_2-Pt_3Al$, $L1_2-Pt_3Sc$, Pt_2NiAl , Pt_2NiSc , $PtNi_2Al$ and $PtNi_2Sc$ are much larger compared with the other compounds. Nickel and chromium are magnetic materials. All compositions containing these elements were examined to ascertain their magnetic state. Only $PtCr_2Al$ (Fig. 3a) showed ferromagnetic character (see the exchange splitting between its up/down spin directions).

Table 1: Calculated Elastic constants (C_{11} , C_{12} , C_{44}), Bulk modulus (B), Shear modulus (G), Young modulus (E), G/B ratio, Poisson's ratio (ν), Density (ρ), Formation energy (E_F), Anisotropy constant (A) and the Cauchy Pressure (C') in $L1_2$ -Pt₃Al, $L1_2$ -Pt₃Sc and their Distorted Structures. Cited result are from *Chauke (2010), #Fu et al. (1988), †Razumovskiy (2008).

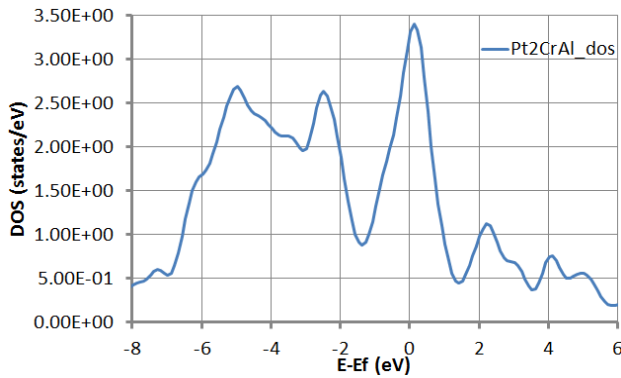
Alloy	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B(GPa)	G(GPa)	E(GPa)	G/B	ν	ρ (g.cm ⁻³)	E_F (Ry)	A	C'
Pt ₃ Al	302.05 (374)* (436) [#]	166.57 (201)* (220) [#]	106.97 (127)* (140) [#]	211.73 (259)* (292) [#]	89.06 (109)* (126) [#]	234.34 (286)* (331) [#]	0.42 (0.42)* (0.43) [#]	0.32 (0.32)* (0.311) [#]	16.88	-479.31	1.58 (1.47)* (1.30) [#]	59.6 (74)* (80) [#]
Pt ₃ Sc	373.53 (379.4) [†]	198.63 (206.9) [†]	144.66 (89.1) [†]	256.93 (264.4) [†]	87.95 (34.49) [†]	237.51 (99.16) [†]	0.33 (0.13) [†]	0.35 (0.44) [†]	16.22	-521.58	1.65 (1.03) [†]	53.97
Pt ₂ CrAl	249.76	142.11	97.26	177.99	76.71	201.21	0.43	0.31	13.51	-321.19	1.81	44.85
Pt ₂ CrSc	220.33	118.36	94.7	152.35	73.86	190.76	0.48	0.29	12.94	-316.2	1.86	23.66
Pt ₂ MgAl	208.14	67.56	84.68	114.42	78.6	191.86	0.69	0.22	11.73	-321.33	1.2	-17.12
Pt ₂ MgSc	168.68	80.83	66.48	110.11	56.31	144.32	0.51	0.28	11.28	-316.32	1.51	14.35
Pt ₂ TiAl	112.99	70.64	8.28	84.76	12.19	34.9	0.14	0.43	10.57	-321.25	0.39	62.36
Pt ₂ TiSc	111.92	63.63	29.23	79.73	27.08	72.97	0.34	0.35	10.18	1005.3	1.21	34.4
Pt ₂ NiAl	255.03	107.32	96.57	156.56	86.74	219.65	0.55	0.27	13.71	-577.05	1.31	10.75
Pt ₂ NiSc	227.65	96.39	89.49	140.14	79.04	199.59	0.56	0.26	13.12	-573.76	1.36	6.9
Pt ₂ Val	187.42	95.35	64.39	126.04	56.29	146.99	0.45	0.31	12.43	-321.24	1.4	30.96
Pt ₂ VSc	163.66	81.31	64.38	108.76	53.82	138.59	0.49	0.29	11.93	-316.24	1.56	16.93
PtCr ₂ Al	36.06	-22.77	91.23	-3.16	58.03	-33.99	-18.37	-1.29	9.39	-163.1	3.1	-114
PtCr ₂ Sc	119.17	62.32	73.52	81.27	50.23	124.95	0.62	0.24	8.44	-250.1	2.59	-11.2
PtMg ₂ Al	111.58	60.73	57.15	77.68	41.29	105.23	0.53	0.27	6.64	-163.21	2.25	3.58
PtMg ₂ Sc	82.82	42.79	48.68	56.13	34.08	85.04	0.61	0.25	6.09	-158.18	2.43	-5.89
PtTi ₂ Al	53.75	43.19	-0.61	46.71	0.32	0.96	0.007	0.5	5.8	851.3	-0.12	43.8
PtTi ₂ Sc	72.82	52.53	19.38	59.29	14.95	41.36	0.25	0.38	6.13	-158.34	1.91	33.15
PtNi ₂ Al	207.54	111.24	97.84	143.34	73.61	188.55	0.51	0.28	10.63	-506.49	2.03	13.4
PtNi ₂ Sc	208.98	110.3	86.24	143.19	68.93	178.2	0.48	0.29	10.3	-501.49	1.75	24.06
PtV ₂ Al	186.67	139.36	78.91	155.13	48.8	132.51	0.31	0.36	9.33	-163.19	3.34	60.45
PtV ₂ Sc	110.73	99.7	20.84	103.38	12.29	35.46	0.12	0.44	8.39	-158.07	3.78	78.86



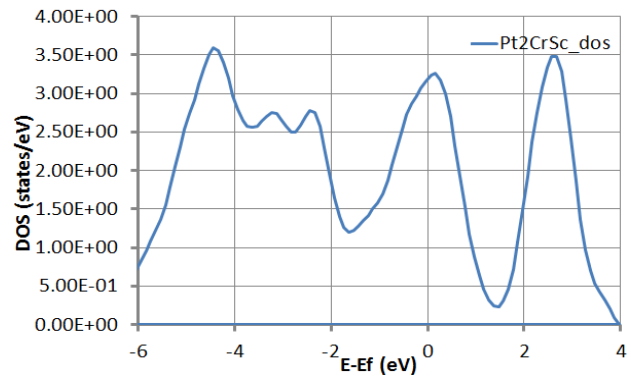
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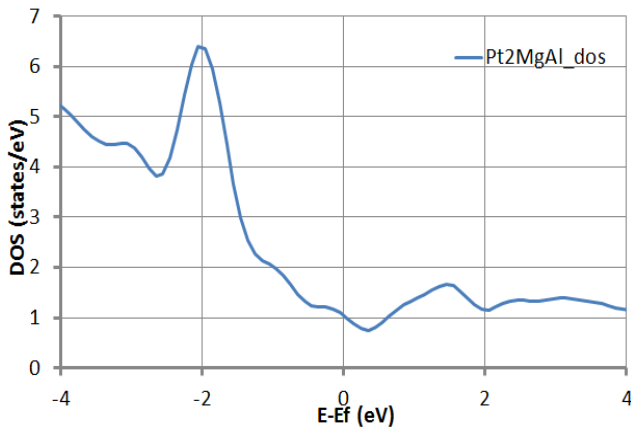
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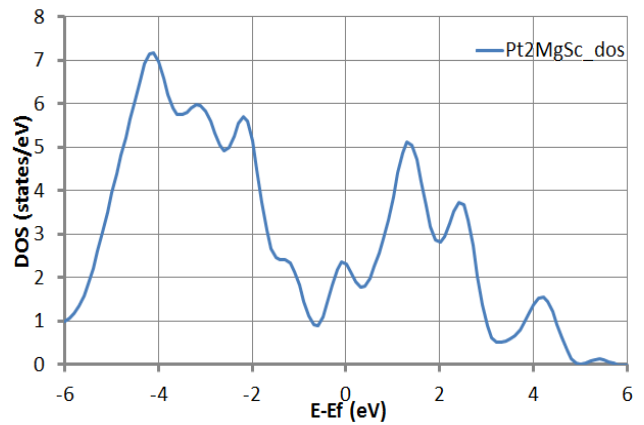
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(d)



(e)



(f)

Figure 1. Total density of states for (a) $L1_2$ -Pt $_3$ Al, (b) $L1_2$ -Pt $_3$ Sc and the substitution disordered (c) Pt $_2$ CrAl, (d) Pt $_2$ CrSc, (e) Pt $_2$ MgAl and (f) Pt $_2$ MgSc.

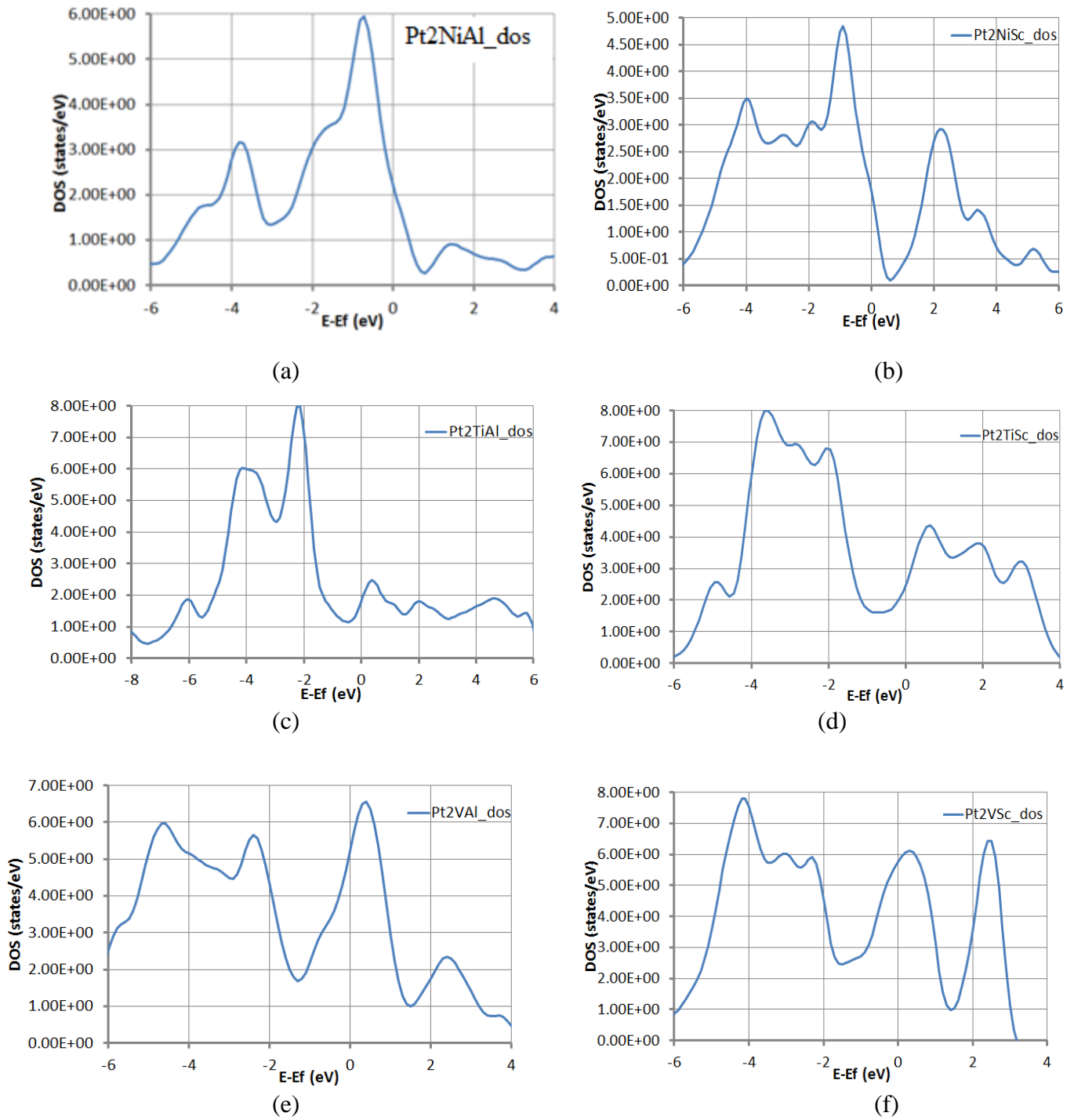
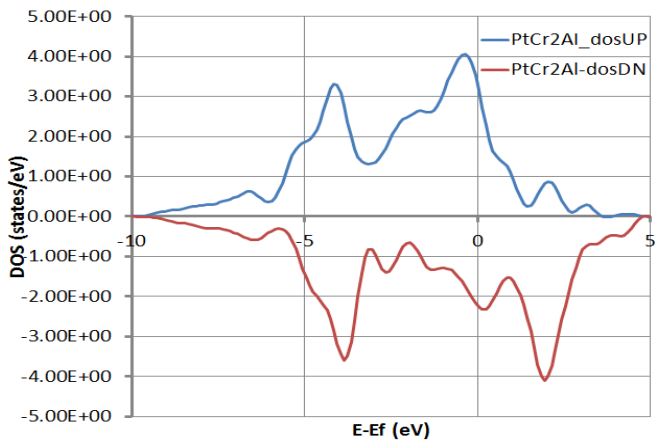
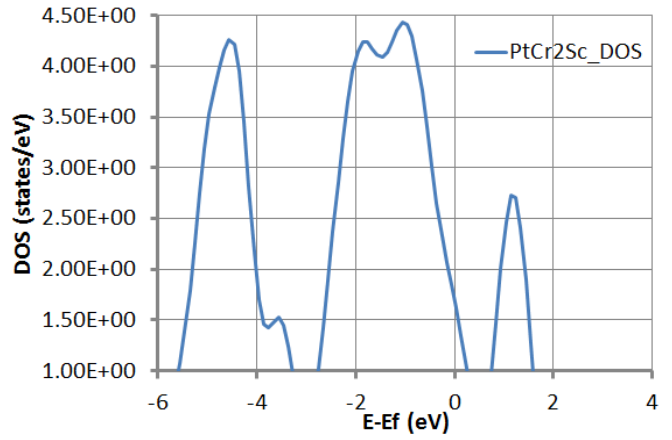


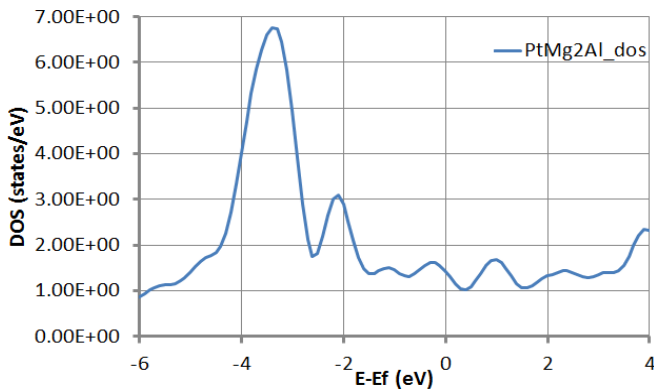
Figure 2. Total density of states for (a) Pt₂NiAl, (b) Pt₂NiSc, (c) Pt₂TiAl, (d) Pt₂TiSc, (e) Pt₂VAl and (f) Pt₂VSc



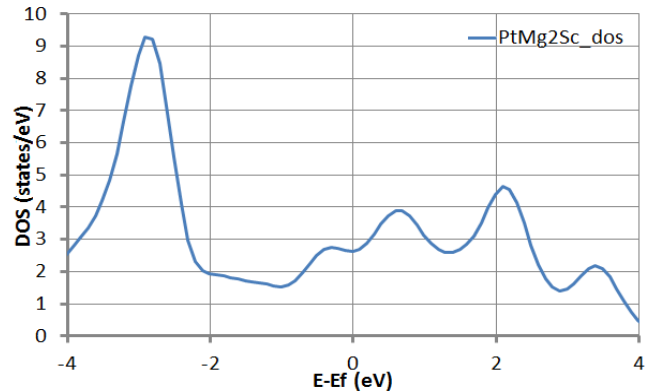
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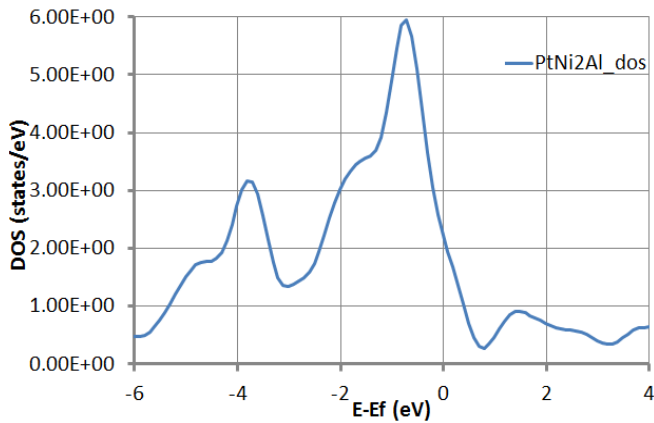
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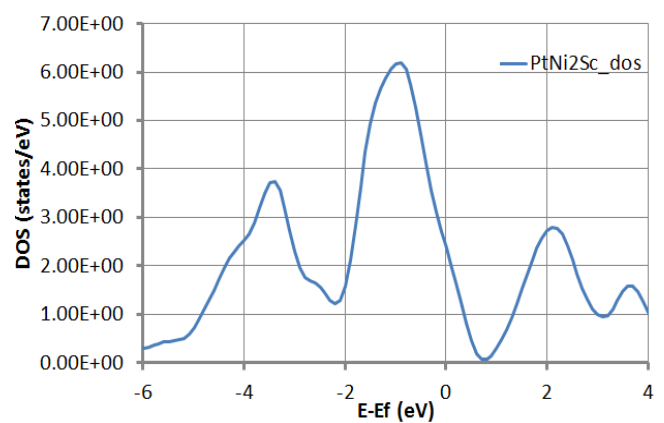
(c)



(d)



(e)



(f)

Figure 3. Total density of states for (a) PtCr₂Al, (b) PtCr₂Sc, (c) PtMg₂Al, (d) PtMg₂Sc, (e) PtNi₂Al and (f) PtNi₂Sc

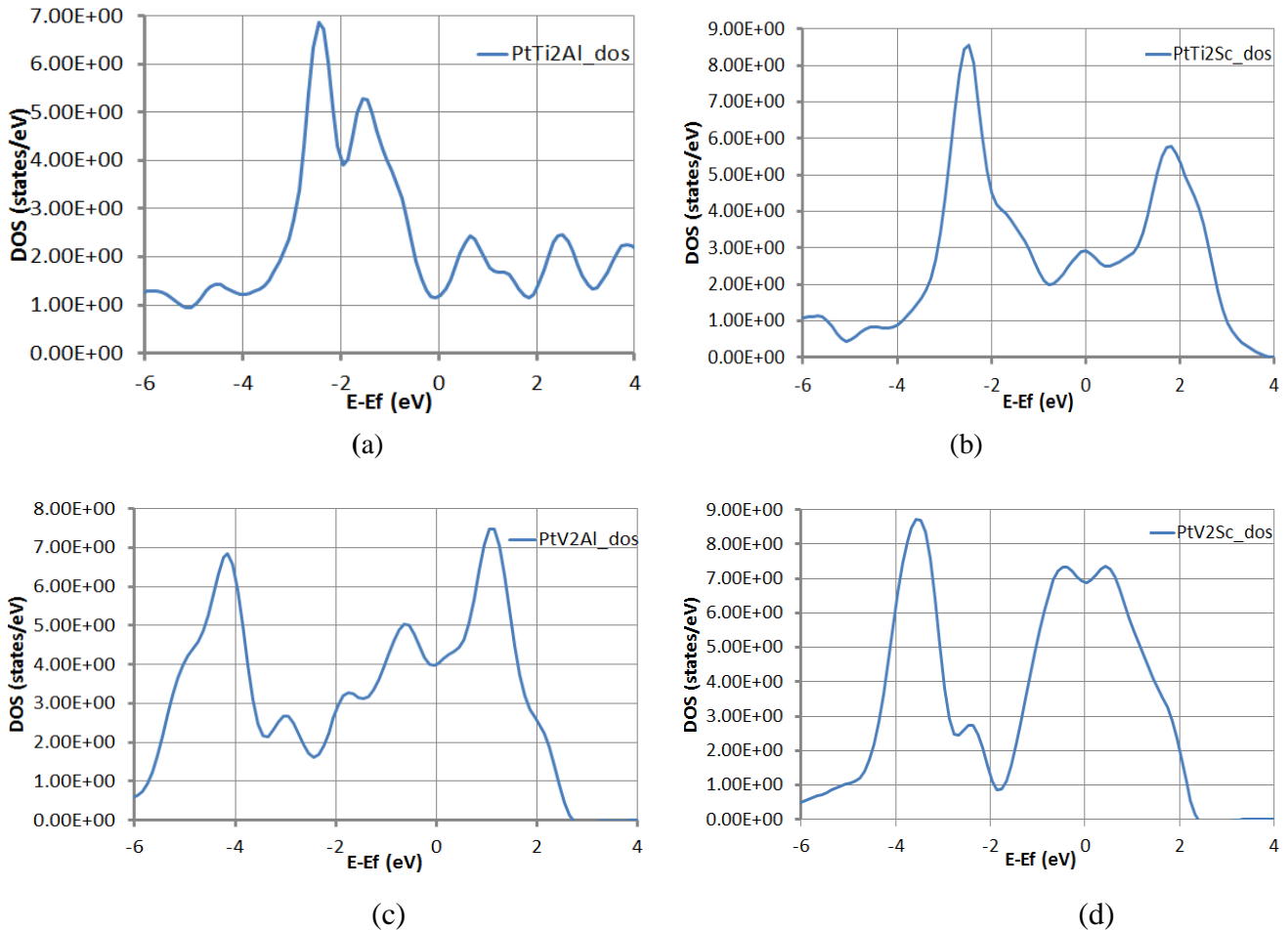


Figure 4. Total density of states for (a) PtTi₂Al, (b) PtTi₂Sc, (c) PtV₂Al (d) PtV₂Sc

CONCLUSION

To extend the application domain of *L*₁₂-Pt₃Al and *L*₁₂-Pt₃Sc, weight lowering is expedient. The DFT has been applied in this study to understand the effect of weight lowering on the electronic and mechanical properties of *L*₁₂-Pt₃Al and *L*₁₂-Pt₃Sc. A tremendous impact will occur on the electronic and mechanical properties of *L*₁₂-Pt₃Al and *L*₁₂-Pt₃Sc when Pt is substituted with Mg, V, Ti, Ni or Cr. The results show that Pt₃Al and Pt₃Sc would attain better structure stability when ≤ 66% at. Pt is substituted with Mg, Ni or Cr. Conversely, tendency for instability is imminent when ≤ 66% at. Pt is substituted with Ti or V and when ≤ 33% at. Pt is replaced with Cr in Pt₃Al. Ferromagnetism is predicted to occur at about 66% at. Pt substituted with Cr (in PtCr₂Al) but not in other compositions. Overall, the substitution of Pt with Mg, Ti, V, Cr or

Ni would lead to strength reduction, while Pt substitution with Ti or V would improve ductility and thus the machinability of *L*₁₂-Pt₃Al and *L*₁₂-Pt₃Sc.

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