# Structural, Electronic, Thermal and Elastic Properties of Ductile PdSc and PtSc Intermetallic Compounds

Ekta Jain [a], Gitanjali Pagare [a,*], Sunil Singh Chouhan [a] and Sankar P. Sanyal [b]
[a] Department of Physics, Government M. L. B. Girls P. G. Autonomous College, Bhopal 462002, India
[b]Department of Physics, Barkatullah University, Bhopal 462026, India
*Corresponding Author E-mail: gita_pagare@yahoo.co.in

## Abstract

The *ab-initio* calculations were performed to investigate structural, electronic, thermal and elastic properties of the binary ductile intermetallic compounds PdSc and PtSc with $B_2$ (CsCl-type) structure using full potential linear augmented plane wave method (FP-LAPW) on the basis of density functional theory (DFT).The generalized gradient approximation (PBE-GGA and WC-GGA) is applied for PdSc and PtSc. The calculated equilibrium properties such as lattice constant ($a_0$), bulk modulus (B) and its first derivative (B') are in better agreement with experimental and theoretical results. The elastic constants ($C_{11}$, $C_{12}$ and $C_{44}$) of these compounds are reported first time. The value of $B/G_H$ ratio for both the compounds are larger than 1.75, indicating the ductile manner of these materials. From density of states and Band structure, it is observed that these intermetallic compounds are metallic in nature. We report first time mechanical and thermal properties which are predicted from the calculated values of elastic constants.

**Keywords:** Intermetallic compounds, Ab-initio calculations, Thermal properties, Mechanical properties, Density of states, Ductility

## 1. Introduction

The $B_2$ (CsCl-type structure) intermetallic compounds have been extensively studied for several decades due to their high oxidation resistance, high stiffness and high strength for elevated temperature engineering applications [1, 2-4]. The first principles study of structural, electronic and elastic properties of AgX and AuX compounds (X = Mg, Sc, Zn and Cd) was reported by Chouhan *et.al.* [5]. Tianshu *et.al.* [6] presented the ideal tensile strength of $B_2$ transition metal aluminides (FeAl, CoAl and NiAl). The structural stability of many binary intermetallics compounds was studied by Curtarolo *et. al.* [7] using *ab-initio* theory within LDA/GGA (local density approximation/generalized gradient approximation) methods. A comparative study of elastic constant of NiTi and NiAl alloys from first principles calculations was performed by Jianmin *et.al.* [8]. Nguyen *et.al.* [9] studied electronic structure, phase stability and elastic moduli of AB transition metal aluminides. Baranov [10] predicted structural stability of pure elements and binary intermetallics compounds by assuming the density of atoms as stationary and un-deformable in internal and external spherical symmetrical shell. Although there is a lot of work has been done on the structural stability and mechanical properties of $B_2$ (CsCl-type) intermetallic compounds. Again the first principle calculation of ductile CeAg intermetallics compound was studied by Shi *et.al.* [11]. It is found that very scant attention has been paid for electronic and elastic properties of ScPd and ScPt intermetallics compounds. Lack of the study of these properties of ScPd and ScPt intermetallics compounds motivated us to perform systematic study of these compounds. In the present paper a comparative study of electronic structure and elastic properties of ScPd and ScPt is evaluated. The ductile behaviour of these intermetallics compounds is predicted on the basis of the calculated results. The aim of this work is to understand the structural, electronic, thermal and elastic properties of the ScPd and ScPt intermetallic compounds using *ab-initio* method. In Section 2, a brief outline of the method of calculation is presented. In Section 3, the results and discussion are presented.

## 2. Method of calculations

The presented calculations were performed by using the full-potential linearized augmented plane wave method (FP-LAPW) as implemented in the latest WIEN2k code [1]. It is based upon the density functional theory (DFT) within the generalized gradient approximation (GGA) in the scheme of Perdew, Burke and Ernzrhof (PBE), Wu and Cohen (WC) is used for the exchange and correlation effects [12]. 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 [13] have been employed for the Brillouin zone integration. The total energies are fitted to Birch-Murnaghan [14] 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:

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

One of the standard methods to calculate the Debye temperature is from elastic constants data, since $\theta_D$ may be estimated from $v_m$ by the following equation [15, 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 Planck's constant, $k_B$ is Boltzmann's constant; $V_a$ is the average atomic volume.

## 3. Results and Discussion

### 3.1 Structural Properties

The equilibrium lattice parameter has been determined by minimizing the total energy calculated for different values of the lattice parameter. The energy vs. volume curves of PdSc and PtSc are shown in Figure 1. Then, these energy values have been fitted to Birch-Murnaghan equation of state [14]. For the comparison of our results, we have used PBE-GGA and WC-GGA approximations for these compounds as there are very less experimental as well as theoretical results are available.The PdSc and PtSc compounds are found to be stable in $B_2$ Phase at ambient conditions. As a comparative study the bulk modulus of PtSc is the higher, showing that it is harder as compared to PdSc. Our calculated bulk moduli for both the intermetallic compounds do not match with the other theoretical results which may be due to the different exchange correlation approximations. As shown in the table, the calculated lattice constants and equilibrium volumes are in good agreement with those experimental values. Thus, we can conclude that the computation parameters and conditions selected in this calculated work should be suitable.

### 3.2 Electronic Properties

The self consistent band structures along the high symmetry directions for both the compounds are presented in Figure 2.The Fermi level is fixed at the origin. The total and partial densities of states (DOS) for these compounds at ambient pressure are presented in Figure 3. For PdSc the lowest lying bands are due to mainly '*s*' like states of Sc. The bands below the Fermi level between -6 eV to -2 eV are due to '*d*'like states of Pd. The metallic behaviour of PdSc is observed due to hybridization of 'd' like states of Pd and Sc and because of little contribution of '*p*' like state of Pd. For PtSc the lowest lying bands are also due to '*s*' like states of Sc. The bands are due to the '*d*' like states of Pt below the Fermi level between -6 eV and -2 eV. The metallicity in PtSc is observed due to the crossing of '*d*' like states of Pt and Sc along with the '*s*' like state of Pt. Due to the metallic character the finite DOS at fermi level are 1.4514 and 1.3147 states/eV/F.U. for PdSc and PtSc respectively.

### 3.3 Elastic Properties

Elastic properties of solids are closely related to many fundamental solid-state properties, such as Debye temperature, melting point, specific heat, thermal expansion coefficient and etc. Cubic crystals have only three independent elastic constants, namely $C_{11}$, $C_{12}$ and $C_{44}$. These theoretical elastic constants are obtained from the energy variations caused by small strains applied to equilibrium lattice configuration. It can be noted that our calculated elastic constants satisfy the stability criterions: $C_{11} - C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{11} < B < C_{12}$, which clearly indicate the stability of these compounds in $B_2$ phase.

### 3.4 Mechanical Properties

Elastic constants can be used can determine the mechanical properties such as Young's modulus (E), Shear modulus ($G_H$), Poisson's ratio (σ), Anisotropic ratio ($A$), for useful applications. We have calculated these properties of PdSc and PtSc compounds and presented them in Table 2. The shear modulus $G_H$ describes the material's response to shearing strain using the Voigt-Reuss-Hill (VRH) method [18-20]. 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:

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \text{ and } G_H = \frac{\dfrac{C_{11} - C_{12} + 3C_{44}}{5} + \dfrac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}}{2}$$

where Hill shear modulus $G_H$ is the average sum of Voigt shear modulus ($G_V$) and Reuss shear modulus ($G_R$).

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 [21], if $B/G_H > 1.75$; a material behaves in a ductile manner. The ($B/G_H$) ratio for PdSc and PtSc are found to be 2.9418 and 3.5013 respectively, indicating PtSc to be more ductile as compared to PdSc. Ganesham et. al. [22] has 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, where as compounds having more negative Cauchy pressure from bonds which are more angular in character [23]. Thus, the ductile nature of both the PdSc and PtSc compounds, can be correlated to their positive Cauchy pressure and thereby the metallic character in their bonds. The PtSc has higher positive Cauchy pressure; resulting strong metallic bonding (ductility) as compared to PdSc. 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 [24]. Young's Modulus E is given by

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

It can be seen from Table 2 that PtSc have higher value of E implying to be more covalent in nature rather than PdSc. The Poisson's ratio (σ) is given by Eq. (10) as

$$\sigma=\frac{3\mathrm{B}-2\mathrm{G}_H}{2(3\mathrm{B}+G_H)}$$

It is observed from Table 2 that value of Poisson's ratio for PdSc is 0.3473 and for PtSc it is 0.3696. 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:

$$A=\frac{2\mathrm{C}_{44}}{C_{11}-C_{12}}$$

For an ideal isotropic system, A is unity and deviation from unity measures the amount to elastic anisotropy.The calculated anisotropy factor for PdSc and PtSc greater than 1 which shows that these compounds are elastically isotropic.

### *3.5 Thermal Properties*

We have calculated the average sound velocities and Debye temperatures as well as the densities for $B_2$ phase using the calculated elastic constants that are given in Table 2. In the absence of any available measured data in the literature, they could not be compared. Future experimental work will testify our calculated results.

## 4. Summary and Conclusions

The ground state electronic and the elastic properties of PdSc and PtSc in the $B_2$ phase were studied by the *ab-initio* calculations. The total energy is fitted to the Birch-Murnaghan equation of state. The lattice constant obtained in this work accorded well with the experimental value. Three independent elastic constants and the bulk modulus were calculated. The electronic density of states (DOS) was calculated. The electronic band structures of PdSc and PtSc exhibit a metallic character. In present study we found $B/G_H > 1.75$ and $C_{12}$–$C_{44} > 0$; for both the compounds which implies that all these compounds are ductile in nature. PtSc is found to be more ductile as compared to PdSc. We also report mechanical and thermal properties will be tested in the future experimentally and theoretically.

## Acknowledgement

The authors are thankful to UGC (New Delhi) for the financial support for Major Research Project. SPS is thankful to UGC (SAP).

## References

1. Shi, Y. J., Du, Y. L., Chen, G. & Chen, G. L. (2008). *Material Transactions*, 49, 2480-2483
2. Liu, C. T., George, E. P., Maziasz, P. J. & Schneibel, J. H. (1998). *Materials Science and Engineering*, A 258, 84–98.
3. Stoloff, N. S., Liu, C. T. & Deevis, S. C. (2000). *Intermetallics*, 8, 1313– 1320.
4. Miracle, D. B. (1993). *Acta Metallic Material*, 41, 649–684.
5. Chouhan, S.S., Soni, P., Pagare, G., Sanyal, S.P. & Rajagopalan, M. (2012). *Computational Material Science*, 65, 58-65
6. Li, Tianshu, Morris, J. W., Jr. & Chrzan, D.C. (2004). *Physical Review B*, 70
7. Curtarolo, S., Morgan, D., & Ceder, G. (2005). *CALPHAD*, 29, 163–211.
8. Lu, Jianmin, Hu, Qingmiao & Yang, Rui (2009). *Journal Material Science Technology*, 25
9. Nguyen-Manh, D. & Pettifor, D.G. (1999). *Intermetallics*, 7, 1095-1106
10. Baranov, M.A. (2006). *EPhTJ,* 1, 49–62.

11. Yao-jun, SHI, Yu-lie, DU, Guang, CHEN (2012). *Transactions* of *Nonferrous Metals Society of China,*22, 654-660
12. Perdew, J.P.,Burke, K & Ernzerhop, M. (1996). *Physical Review Letters,* 77, 3865–3868.
13. Monkhorst, H.J & Pack, J.D. (1976). *Physical Review B*, 13, 5188–5192.
14. Birch, F. (1938). *Journal Applied Physics*, 9, 279–288.
15. Sun, Z., Li, S., Ahuja, R. and Schneide, J.M. (2004). *Solid State Communication,* 129, 589–592.
16. Wachter, P., Filzmoser, M. & Rebizant, J. (2001). *Physica B,* 293, 199–223 (25).
17. Jansiukiewicz, C. & Karpus, V. (2003). *Solid State Communication,* 128, 167–169.
18. Hill, R. (1952). *Preceeding of Physical Society London*, A 65, 349–354.,
19. Voigt, W. (1889). *Annals of Physics.,* 38, 573–587.
20. Reuss, A. & Angew, Z. (1929). *Journal of Mathematical Physics*, 9, 49–58.
21. Pugh, S.F. (1954). *Philosophical Magazine.* 45, 823–843.
22. Ganeshan, S., Shang, S.L., Zhang, H., Wang, Y., Mantina, M. & Liu, Z.K. (2009). *Intermetallics*, 17, 313–318.
23. Pettifor, D.G. (1992). *Material Science Technology*, 8, 345–349.
24. Jenkins, C.H. & Khanna, S.K. (2005). *Mechanics of Material*, ISBN 0-12-383852-5, 62–72.
25. Elliott, R.P. (1968). *Constitution of binary alloys.* New-York, St. Louis, San Fracisco, Toronto, London, Sydney. McGraw-hill Book company, v. 1-2
26. Shunk, F.A. (1971). *Constitution of binary alloys* New-York, St. Louis, San Fracisco, London, Sydney, Toronto, Mexico, Panama. McGraw-hill Book company, v. 1-2

Table 1 Calculated ground state and elastic properties for PdSc and PtSc.

| Solids | Work | Approximations | $a_o$ (Å) | B (GPa) | B' | N($E_F$) (eV) | $C_{11}$ (GPa) | $C_{12}$ (GPa) | $C_{44}$ (GPa) |
|---|---|---|---|---|---|---|---|---|---|
| PdSc | Pre. | PBE-GGA | 3.3165 | 106.63 | 4.32 | - | 159.78 | 87.59 | 39.51 |
| | | WC-GGA | 3.2695 | 121.99 | 4.72 | 1.45 | 153.39 | 108.68 | 64.00 |
| | Exp. | - | 3.283$^a$ | - | - | - | - | - | - |
| | Oth. The. | - | 3.313$^b$ | 62.70 | - | - | - | - | - |
| PtSc | Pre. | PBE-GGA | 3.3055 | 135.08 | 4.52 | - | 187.38 | 113.31 | 47.11 |
| | | WC-GGA | 3.2647 | 148.28 | 4.95 | 1.31 | 186.80 | 132.75 | 58.85 |
| | Exp. | - | 3.270$^a$ | - | - | - | - | - | - |
| | Oth. The. | - | 3.304$^b$ | 80.26 | - | - | - | - | - |

$^a$Ref [25,26], $^b$Ref [10], Pre.- Present, Exp.- Experimental, Oth. The. - Other Theory

Table 2
The calculated density (ρ), bulk modulus (B), Young's modulus (*E*), Shear modulus ($G_H$), Anisotropy factor (*A*), Poisson's ratio ($\sigma$), (B/$G_H$) ratio , Cauchy's pressure ($C_{12}$ - $C_{44}$), longitudinal ($v_l$), transverse ($v_t$), average elastic wave velocities ($v_m$) and Debye temperature ($\theta_D$) for PdSc and PtSc.

| Solid | $\rho$x10 (kg/m$^3$) | B (GPa) | A | $G_H$ (GPa) | *E* (GPa) | $\sigma$ | B/$G_H$ | $C_{12}$-$C_{44}$ (GPa) | $v_l$ (m/s) | $v_t$ (m/s) | $v_m$ (m/s) | $\theta_D$ (K°) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PdSc | 28.7 | 123.5 | 2.8 | 42.0 | 113.2 | 0.34 | 2.94 | 44.6 | 2549 | 1284 | 1438 | 204 |
| PtSc | 45.7 | 150.7 | 2.1 | 43.0 | 117.9 | 0.36 | 3.50 | 73.9 | 2154 | 1004 | 1130 | 160 |

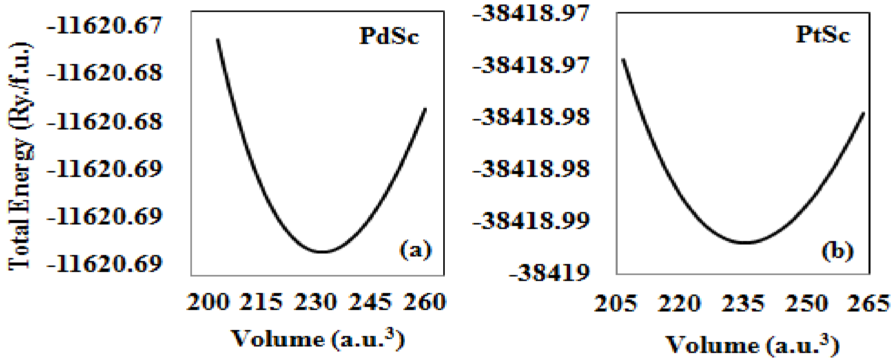

Figure 1. (a) and (b) Variation of total energy with volume in PdSc and PtSc intermetallics.

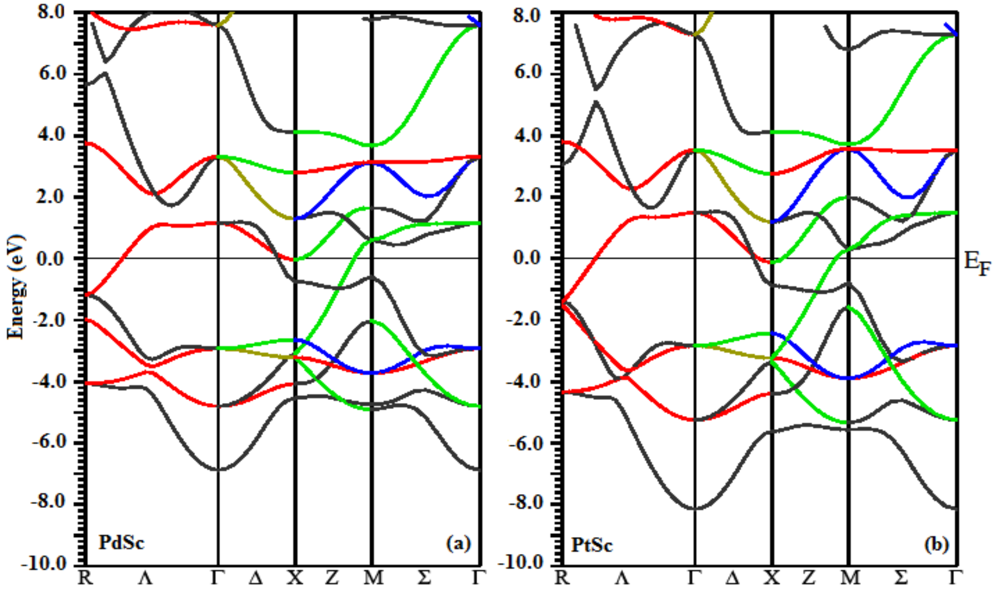

Figure 2. (a) and (b) Density of state of PdSc and PtSc intermetallics.

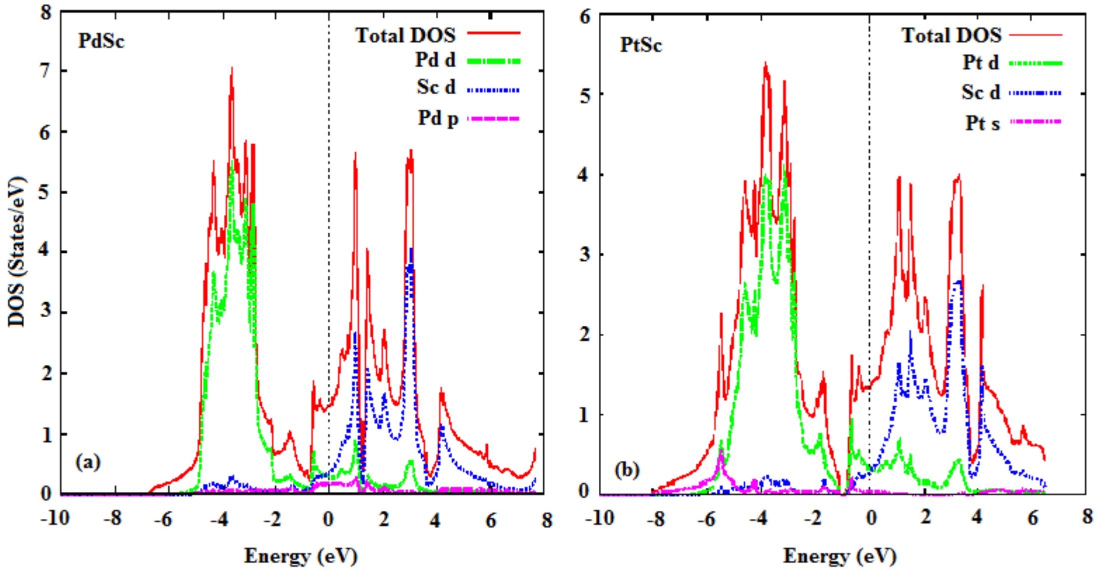

Figure 3. (a) and (b) Band structure of PdSc and PtSc intermetallics.

This academic article was published by The International Institute for Science, Technology and Education (IISTE). The IISTE is a pioneer in the Open Access Publishing service based in the U.S. and Europe. The aim of the institute is Accelerating Global Knowledge Sharing.

More information about the publisher can be found in the IISTE's homepage:
http://www.iiste.org

## CALL FOR PAPERS

The IISTE is currently hosting more than 30 peer-reviewed academic journals and collaborating with academic institutions around the world. There's no deadline for submission. **Prospective authors of IISTE journals can find the submission instruction on the following page:** http://www.iiste.org/Journals/

The IISTE editorial team promises to the review and publish all the qualified submissions in a **fast** manner. All the journals articles are available online to the readers all over the world without financial, legal, or technical barriers other than those inseparable from gaining access to the internet itself. Printed version of the journals is also available upon request of readers and authors.

### IISTE Knowledge Sharing Partners

EBSCO, Index Copernicus, Ulrich's Periodicals Directory, JournalTOCS, PKP Open Archives Harvester, Bielefeld Academic Search Engine, Elektronische Zeitschriftenbibliothek EZB, Open J-Gate, OCLC WorldCat, Universe Digtial Library , NewJour, Google Scholar