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Research Article

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Effect of ternary addition on bonding properties of Rh3V intermetallics: A theoretical study

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ABSTRACT

Structural, Elastic and Electronic properties of Rh_3V and $Rh_3V_x(Ni)_{1-x}$ are studied by Full Potential Linearized Augmented Plane Wave(FP-LAPW) method. The basic physical parameter such as lattice constants, elastic constants, bulk modulus, shear modulus, Young's modulus and Poisson's ratio are reported. Furthermore, the chemical bonding properties of Rh_3V and $Rh_3V_x(Ni)_{1-x}$ discussed using Cauchy's Pressure, Poisson's Ratio, Pugh Rule and charge density plot. A strong directional bonding is seen between V-Rh-V atoms in Rh_3V compound whereas no such directional bonding is seen in $Rh_3V_x(Ni)_{1-x}$ compound.

Keywords: Ternary alloying, Intermetallics, Interatomic bonding, Electronic band structure.

INTRODUCTION

Platinum metal base alloys, such as Ir and Rh- base alloys are base elements for ultra-high temperature applications owing to their high-melting temperatures, good oxidation resistance and good high temperature strengths[1-4]. Among platinum group metals, Rh- base alloys are more promising materials for ultra-high temperature gas turbine applications, due to its high thermal conductivity, lower thermal expansion coefficient, low density and better oxidation resistance[5]. In addition, Rh- based alloys can be prepared with a microstructure similar to that of nickel based alloys with enhanced ductility and workability[6], which is our reason for studying on these compounds. The ductile/brittle nature of Rh- based intermetallic compounds with ternary addition by $Rh_3Tix(V, Hf, Al)_{1-x}$ is reported[7]. In this present study we have considered the more brittle material Rh_3V[20] and for the first time the bonding mechanism and elastic properties of $Rh_3V_{87.5}Ni_{12.5}$ has been analyzed and computed.

COMPUTATIONAL DETAILS

In the present paper, all calculations have been carried out using Full Potential Linearized Augmented Plane Wave (FP-LAPW) method implemented in the WIEN2K code[8]. Generalized Gradient Approximation(PBE-GGA) based on Perdew et al [9] has been used to determine the exchange and correlation energy. The plane wave expansion is taken as Kmax x Rmax equal to 7.0 and lmax=10.. For K-space summation the 14x14x14 for Rh_3V and 10x10x10 for $Rh_3V_{87.5}Ni_{12.5}$ Monkhorst and Pack grid of k-points have been used[17]. The self-consistent calculations are carried out to an accuracy of 0.0001ev for energy and 0.001 for charge.

RESULTS AND DISCUSSION

The optimized lattice parameters for Rh3V $Rh_3V_{87.5}Ni_{12.5}$are presented in the Table1. The calculated lattice constant for Rh_3V correlate very well with the experimental value. For Rh_3V, the percentage error between the calculated and the experimental lattice constant is 0.3.

The calculated values of Bulk modulus(B), Shear modulus(G), Young's modulus (E), Cauchy pressur(C_{12}-C_{44}), G/B, Poisson's ration(ν) and Hv for Rh_3V and $Rh_3V_{87.5}Ni_{12.5}$ are reported in table1. From Table.1, it can be noted that for Rh_3V the computed B,G, E and C_{44} values are 258.646GPa, 165.719GPa, 409.664GPa and 204.005GPa respectively, which are quantitatively higher than the $Rh_3V_{87.5}Ni_{12.5}$ values viz., 252.553GPa, 145.805GPa, 366.823GPa and 168.46GPa1 respectively.

The covalent/ionic nature of the compounds could be predicted by Cauchy pressure (C_{12}-C_{44}), Poisson's ratio(ν), Young's modulus(E) and Pugh criterion G/B. According to Pettifor[10] and Johnson[11], for metallic bonding, Cauchy pressure(C_{12}-C_{44}) is positive; whereas for directional bonding the Cauchy pressure is negative. From Table.1 one can observe that the Rh_3V compound having negative Cauchy pressure(-26.363GPa) represents more directional characteristics and $Rh_3V_{87.5}Ni_{12.5}$ having positive Cauchy pressure(5.773) represents metallic non-directional bonding. For covalent materials, the value of Poisson's ratio is small (ν=0.1), whereas for ionic materials the value of ν is 0.25[12,13]. In the present case, the $Rh_3V_{87.5}Ni_{12.5}$ has the largest Poisson's ratio(0.26) represents ionic contributions to the atomic bonding are dominant and the Rh_3V has the ν value (0.23) which is less than 0.25 represents covalent contribution in inter-atomic bonding are dominant.

Young's modulus(E) is used to provide a measure of the stiffness of the solid and when the value of E is large, the material is stiff. If the value of Young's modulus(E) increases, the covalent nature of the material also increase[12]. From Table.1, it is observed that the value of E, for Rh_3V is 409.664GPa and for $Rh_3V_{87.5}Ni_{12.5}$ is 366.823GPa. Due to the higher value of Young's modulus, Rh_3V is stiffer than $Rh_3V_{87.5}Ni_{12.5}$ and having higher covalent nature.

In covalent and ionic materials, the brittle/ductile behavior are G ~ 1.1B and G ~ 0.6B respectively[12,13]. According to the Pugh criterion[14], if G/B > 0.57, the material behaves in a brittle manner and the stronger the directional bonding character. This ratio for Rh_3V is 0.64 and for $Rh_3V_{87.5}Ni_{12.5}$ is 0.57. Hence Rh_3V will behave as brittle manner(covalent nature) and $Rh_3V_{87.5}Ni_{12.5}$ behave as ductile manner(ionic nature).

Based on charge density plots also we can study the covalent/ionic nature of the materials. Figure 1a&1b and 2a&2b shows that the X-CRYSDEN and charge density plot of cubic Rh_3V and $Rh_3V_{87.5}Ni_{12.5}$ compounds respectively. From Fig. 1a&2a, one can observe that the charge locate between V-Rh-V atoms, suggesting strong covalent bonds between them[15]. One can note that the absence of such charge density contours in Fig.1b&2b. Hence it can be concluded that Rh_3V having higher covalent nature in inter-atomic bonding whereas $Rh_3V_{87.5}Ni_{12.5}$ having ionic nature in inter-atomic bonding.

Figure 3a & 3b represents DOS curves of Rh_3V & $Rh_3V_{87.5}Ni_{12.5}$. In fig.3a, one can notice a pseudogap in Rh_3V intermetallic compound and in fig.3b, there is no noticeable pseudogap in $Rh_3V_{87.5}Ni_{12.5}$ compound. Hence, we conclude that the presence of pseudogap in intermetallic compound Rh_3V is originating from V-Rh-V bond as shown in fig. 1a&2a[16].

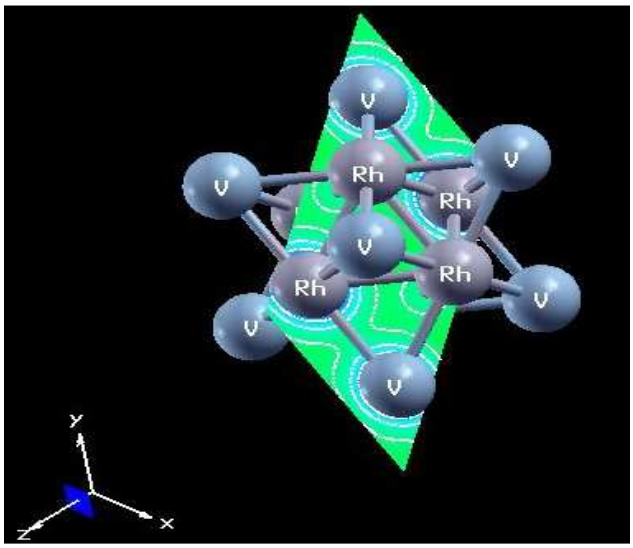

FIGURE 1a. X-CRYSDEN plot of (001) plane of cubic Rh_3V compound

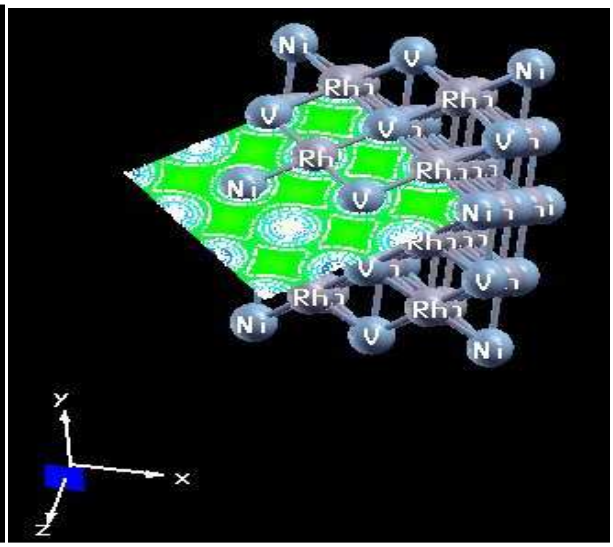

FIGURE 1b. X-CRYSDEN plot of (001) plane $Rh_3V_{87.5}Ni_{12.5}$ compound.

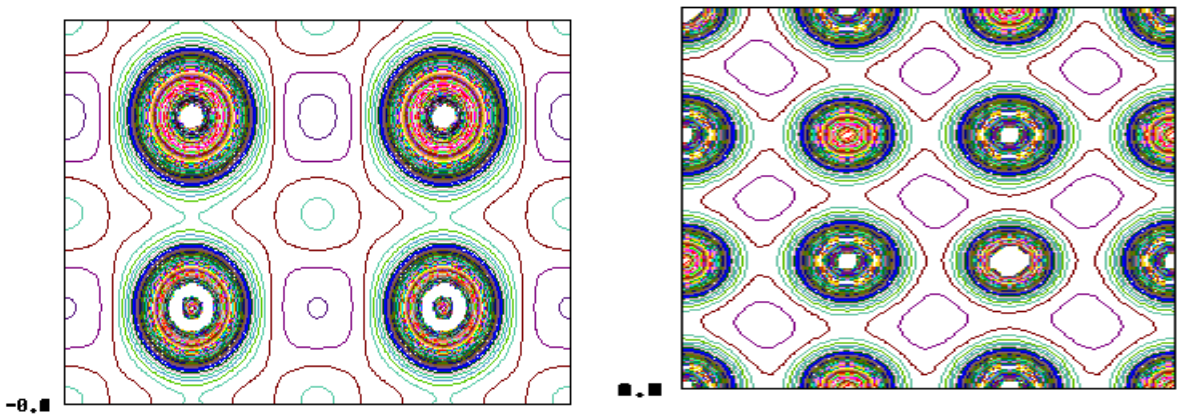

FIGURE 2a&2b. charge density plot of (001)plane of cubic Rh_3V & $Rh_3V_{87.5}Ni_{12.5}$

TABLE 1. The optimized lattice parameter, elastic constants and elastic properties of Rh3Vx(Ni)(1-x) intermetallic compounds

Parameters	Rh_3V	$Rh_3V_{87.5}Ni_{12.5}$
Lattice Constant (a.u.)	a_{exp}=7.17391 a_{cal} =7.2014	a_{opt}=14.4028
Other study[a]	a_{exp}=7.17147 a_{cal} =7.2432	
C_{11}	420.654	409.189
C_{12}	177.642	174.234
C_{44}	204.005	168.461
Cauchy Pressure(C_{12}-C_{44})	-26.363	5.773
Bulk Modulus(B) GPa	258.646 at -0.003 GPa	252.553 at -0.938 GPa
Shear Modulus(G) GPa	165.719	145.805
Young's Modulus(E) GPa	409.664	366.823
G/B	0.64	0.57
Poisson's Ratio(v)	0.24	0.26
Hv	29.167	23.637

a Ref.[5]

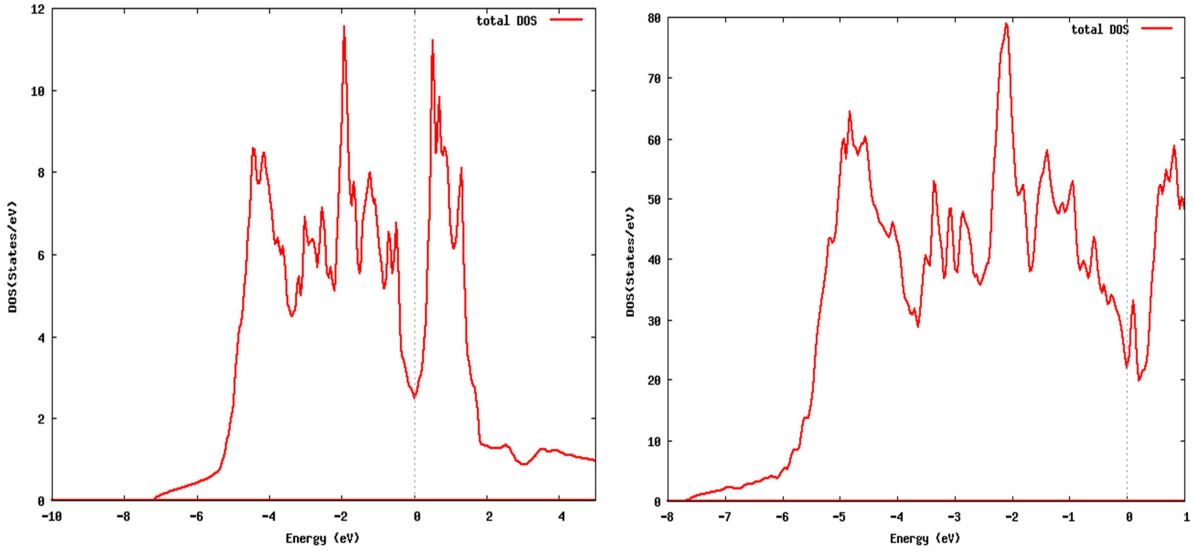

FIGURE 3a&3b. DOS histogram of cubic Rh_3V & $Rh_3V_{87.5}Ni_{12.5}$

CONCLUSION

From this study, we concluded that the covalent contribution in inter-atomic bonding are dominant in Rh_3V compound and the ionic contributions to the atomic bonding are dominant in $Rh_3V_{87.5}Ni_{12.5}$ compound.

REFERENCES

[1] Y. Yamabe, Y. Koizumi , H. Murakami , Y. Ro, H. Maruko, *Scr. Metall. Mater*. 35 (**1996**) 211.
[2] Y. Yamabe , Y. Koizumi, H. Murakami, Y. Ro, H. Maruko, *Scr. Metall. Mater*. 36 (**1997**) 393.

[3] Y. Yamabe - Mitarai, et al., *Scr. Mater*. 36 (**1997**) 393.
[4] S. Miura , et al., *Intermetallics* 8 (**2000**) 785.
[5] K. Chen , L.R. Zhao, J.S. Tse, J.R. Rodgers, *Phys Lett* A **2004**;331:400
[6] M. Rajagopalan, M. Sundareswari, *J Alloys Compd* **2004**;379:8
[7] M. Sundareswari, M. Rajagopalan (**2005**), *Int. J. Modern Physics* B, Vol. 19, No. 31, pp. 4587-4604.
[8] P. Blaha, K. Schwarz, G. K. H. Madsen, D. K. Vasnicka and J. Luitz WIEN2 k (Austria: Vienna University of Technology) (**2001**)
[9] J.P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett*. 777 (**1996**) 386.
[10] D.G. Pettifor, *Mater.Sci.Technol*. 8 (**1992**) 345.
[11] R.A. Johnson, *Phys. Rev*. B 37 (**1988**) 3924.
[12] E. Deligoz, H. Ozisik, K. Colakoglu, G. Surucu, Y.O. Ciftci, *J Alloys Compd* 509 (**2011**) 1711-1715.
[13] G. Surucu ,K. Colakoglu ,E. Deligoz, H. Ozisik . *Intermetallics* 18 (**2010**), 286-291.
[14] S.F. Pugh, *Phil. Mag*. 45 (**1954**) 823.
[15] H. Ozisik, E. Deligoz, K. Colakoglu, E. Ateser, *Intermetallics* 39 (**2013**) 84-88.
[16] P. Vajeeston, P. Ravindran, C. Ravi, R. Asokamani, *Phys Rev B*.63. 045115.
[17] H.J. Monkhorst , J.D. Pack , *Phys Rev B* 13(**1976**)5188.
[18] K.Chen, L.R.J. Zhao, *Applied Phys*, (**2003**),2414-2417.
[19] Y. Oleg, Kontsevoi, N. Yuri, Gornostyrev and Arthur J. Freeman. (**2005**), JOM, 43-47.
[20] M. Sundareswari, M. Rajagopalan, *Eur Phys J B* **2006**;49:67
[21] G. Kresse, *Hafner J. Phys Rev B* **1994**;47:558.
[22] L.Vitos, P.A. Korzhavyi, B. Johansson, *Nature Mater* 2(**2003**)25.