International Research Journal of Pure & Applied Chemistry
10(3): 1-9, 2016, Article no.IRJPAC.20030
ISSN: 2231-3443, NLM ID: 101647669

SCIENCEDOMAIN *international*
www.sciencedomain.org

An Investigation of Atomic Short Range Order (SRO) in Binary $Ni_{20}Pd_{80}$ and $Au_{25}Pd_{75}$ Alloy

Syed Kamran Ajmal[1*], Amer Bashir Ziya[2], Ramiza[3], Nausheen Syed[4], Saleem Akhter[2] and Tahir Bashir[2]

[1] Department of Physics, University of Sargodha, Women Campus, Faisalabad, Pakistan.
[2] Department of Physics, Bahauddin Zakariya University, Multan-60800, Pakistan.
[3] Department of Physics, University of Agriculture, Faisalabad, Pakistan.
[4] Department of Business Administration, G. C. Women University, Faisalabad, Pakistan.

Authors' contributions

This work was carried out in collaboration between the given authors. Author SKA performed the experiments. Author ABZ wrote the paper. Authors Ramiza, NS, SA and TB performed the detail analysis, literature survey. All the authors read and approved the final manuscript.

Article Information

DOI: 10.9734/IRJPAC/2016/20030
Editor(s):
(1) Martin Kröger, Department of Materials, Computational Polymer Physics, Swiss Federal Institute of Technology (ETH Zürich), Switzerland.
Reviewers:
(1) Yong Gan, California State Polytechnic University, Pomona USA.
(2) Subramaniam Jahanadan, Kolej Matrikulasi Labuan (KML), Malaysia.
(3) Chun-Ching Hsiao, National Formosa University, Taiwan.
(4) Azuddin Mamat, University of Malaya, Malaysia.
Complete Peer review History: http://sciencedomain.org/review-history/11960

Original Research Article

Received 7th July 2015
Accepted 9th September 2015
Published 24th October 2015

ABSTRACT

The atomic short range order (SRO) parameters (α_i) have been investigated in polycrystalline alloys i.e., $Ni_{20}Pd_{80}$ and $Au_{25}Pd_{75}$. The $Ni_{20}Pd_{80}$ alloy was annealed at different temperatures (100 to 600℃) then studied with X-ray diffraction (XRD). The electronic theory of atomic short range order (SRO) was utilized to determine the ordering energies and SRO-parameters (α_i) for $Ni_{20}Pd_{80}$ and $Au_{25}Pd_{75}$ alloy using the pseudo-potential approximation technique. The obtained experimental results of the atomic SRO-parameters (α_i) were compared with theoretical results. The intensity distribution pattern of $Ni_{20}Pd_{80}$ alloy obtained through XRD depicts a deviation from random structure at different annealing temperatures. We make an analysis using the prior obtained X-ray intensities of $Ni_{20}Pd_{80}$ and calculated the atomic short range order-function (SROF) g(r) as a

---

*Corresponding author: E-mail: kamranajmalcn@gmail.com;

function of annealing temperatures. Some of the values of α_i calculated by using SROF appear as negative, indicating the existence of SRO in $Ni_{20}Pd_{80}$ alloy. We have obtained the parameters for second and third nearest neighbors, which turned out to be positive. It was found that this theory predicts the same sign of α_1 for selected alloy as observed from the experiment. The results can be further improved by considering the order of perturbation and the atomic size effect for the studied alloys. The α_1 were studied in $Au_{25}Pd_{75}$ alloy using the frame work of the transition metal model pseudo-potential (TMMP). Electronic theory of alloys in the pseudo-potential approximation was employed to calculate the ordering energies and the values of α_1. It was found that this theory predicts the same sign of α_1 for selected alloys.

Keywords: $Au_{25}Pd_{75}$ alloy; $Ni_{20}Pd_{80}$ alloy; short range order (SRO); SRO parameters (α_i); pseudo-potential approximation technique; X-ray diffraction (XRD); short range order-function (SROF).

1. INTRODUCTION

X-ray scattering intensity measurement of alloys reveals the information about the degree of atomic SRO and has been immensely used by many authors to establish the presence of ordering in various binary and multi-component alloys [1]. The presence of the atomic SRO in the disordered solid solutions influences on the physical properties of the alloys significantly. A recent study of the electronic theory of alloys based on the pseudo-potential approximation has appeared successful to predict the ordering in transition metal alloys [2-4]. Lin et al. [5] have shown the formation of clusters in the samples with Pd concentration of 25-75 at.%. Our study shows that beyond 75 at.% Pd, Ni-Pd alloy has a tendency to form SRO.

Shamah et al. [6] studied the atomic SRO in Pd alloys by using XRD in order to make quantitative measurements The Ni-Pd and Au-Pd alloys are actually dental based alloys [7]. The success of the pseudo-potential approximation in explaining and predicting the physical properties of alloys lies infact that this theory yields a central pair wise (CPW) character in the interaction of atomic nuclei, bound electrons and the cloud of conduction electrons with other atoms of the same or different kinds.

Therefore, it encourages us to investigate the atomic SRO in $Ni_{20}Pd_{80}$ and $Au_{25}Pd_{75}$ alloys. This work has been undertaken to study the atomic SRO parameters (α_i) of the $Ni_{20}Pd_{80}$ and $Au_{25}Pd_{75}$ alloys. In the present paper, not only, we establish the atomic SRO in $Ni_{20}Pd_{80}$ but also in an $Au_{25}Pd_{75}$ alloy to check the validity of the theoretical frame work by comparing with the theoretical results. We have carried out the ordering energies for the values of α_i of $Ni_{20}Pd_{80}$ and $Au_{25}Pd_{75}$ alloys. The given samples have been examined and finally the results have been discussed by comparing with those given in literature. The calculation of ordering energies was undertaken using the electronic theory of alloys in the pseudo-potential approximation techniques.

2. MATERIALS AND METHODS

2.1 Experimental Technique

For experimental work XRD technique was employed. The round-shaped master ingot (~10 g) of polycrystalline $Ni_{20}Pd_{80}$ alloy was gratefully supplied by Degussa (Germany). These pellets were cut into two halves, surface-ground and polished to produce a mirror surface suitable for XRD study. Chemical analysis carried out by electron probe micro-analyzer gave nearly the starting compositions. $Ni_{20}Pd_{80}$ alloy was annealed at $600^\circ C$ for 5 hrs in a vacuum better than 10^{-5} mbar and quenched. The X-ray experiments were performed on a diffractometer (Shimadzu XD-5A) in the reflection mode, using line-focused Cu-Kα radiation [7]. The intensity measurements were carried out in the angle range $30^\circ < 2\theta < 130^\circ$ with a step of 0.2 and all measurements were made in the fixed time mode with counting time of 100 sec per angle.

2.2 Theoretical Calculations

The electronic theory of alloys gives the following expression for the ordering energy of binary AB alloy [8]. The electronic theory of alloys in the 2^{nd} order perturbation theory gives the ordering energy of binary alloy corresponding to the i_{th} coordination sphere as given below:

$$E_{AB}(R_i) = \frac{\overline{\Omega_0}}{\pi^2}\int_0^\infty F_{AB}(q)\frac{\sin qR_i}{qR_i}q^2\,dq \qquad (1)$$

Where, $\overline{\Omega_o}$ is the average atomic volume of the alloy and R_i is the radius of i_{th} coordination sphere in the particular crystal structure. The factor $F_{AB}(q)$ represents the energy-wave number characteristics of the alloy [9].

The electronic theory of alloys in 2nd order perturbation theory gives the ordering energy of a binary alloy corresponding to the i_{th} coordination sphere [10].

$$F_{AB}(q) = \frac{\overline{\Omega}_0}{8\pi}\left|\Delta\omega^0(q)\right|^2 q^2\frac{\varepsilon(q)-1}{\varepsilon^*(q)} + \frac{2\pi\left|\Delta z\right|^2}{\overline{\overline{\Omega}}_0 q^2}\exp\left(\frac{-q^2}{4\eta}\right) \qquad (2)$$

Where, $\overline{\Omega_o} = \Omega/N$ is the volume per atom, N is the number of atoms in the crystal of volume Ω, Δw^O_{AB} is the difference of the unscreened pseudo-potential form factors of the alloy constituents [11], $\varepsilon(q)$ and $\varepsilon^*(q)$ are the dielectric and modified screening factors which include the effect of exchange and correlation and η is the Ewald's parameter. Animalu [11] formulated the TMMP on the basis of quantum defect law (QDL) and the generalized quantum defect law (GQDL). The first term in Eq. (2) gives the contribution of the band structure and this second term is of the electro static energy.

$$E(R_1) = \frac{\overline{\Omega_0}}{N\pi^2}\int_0^\infty\left[\frac{\overline{\Omega_0}}{8\pi}\left|\Delta\omega^0(q)\right|^2 q^2\frac{\varepsilon(q)-1}{\varepsilon^*(q)-1} + \frac{2\pi\left|\Delta z\right|^2}{\overline{\overline{\Omega}}_0 q^2}\exp\left(\frac{-q^2}{4\eta}\right)\right]q^2\frac{\sin qR_1}{qR_1}dq \qquad (3)$$

In 3rd order perturbation theory, the ordering energy is given by [6]:

$$E(R_1) = \frac{\overline{\Omega_0}}{N\pi^2}\int_0^\infty\left[\frac{\overline{\Omega_0}}{8\pi}\left|\Delta\omega^0(q)\right|^2 q^2\frac{\varepsilon(q)-1}{\varepsilon^*(q)-1} + \frac{2\pi\left|\Delta z\right|^2}{\overline{\overline{\Omega}}_0 q^2}\exp\left(\frac{-q^2}{4\eta}\right) + T(q)\right]q^2\frac{\sin qR_1}{qR_1}dq \qquad (4)$$

Here,

$$T(q) = 3\overline{\Omega}_0\frac{\Delta w^0(q)}{\varepsilon^*(q)}\sum_{2\pi\overline{H}}\frac{\overline{w^0(2\pi\mathbf{H})}}{\overline{\overline{\varepsilon}}^*(2\pi\mathbf{H})}\frac{\Delta w^0\left(\left|\overline{q+2\pi\mathbf{H}}\right|\right)}{\varepsilon^*\left(\left|q^- + 2\pi\mathbf{H}\right|\right)}\times\lambda^{(3)}\left[q,-(q+2\pi\mathbf{H}),2\pi\mathbf{H}\right] \qquad (5)$$

The term T(q) is the effective pair corrections to the ordering potential. This correction arises in the 3rd order perturbation theory due to double scattering process of conduction electrons from the ion pairs. The term responsible for the effects connected with the presence of three body interaction are not taken into consideration.

In disordered binary solid solutions, if two different atoms A and B have size difference they exhibit static displacements from exact lattice positions. For close neighbors, there can be three different distances depending on whether it is an AA-, BB- or AB-pairs.

$$B(R_1) = \frac{\overline{\Omega}_0}{\pi^2 N}\int_0^\infty\left[\begin{array}{l}\frac{\overline{\Omega_0}}{8\pi}q^2\frac{1-\varepsilon(q)}{\varepsilon^*(q)}\Delta\omega^0(q)\left(\overset{0}{\omega}_A(q)\Delta_{1A} - \overset{0}{\omega}_B(q)\Delta_{1B}\right)+\\ \frac{2\pi}{\overline{\overline{\Omega}}_0}\frac{e^{-(q^2/4\eta)}}{q^2}\Delta Z^*(Z^*_A\Delta_{1A} - Z^*_B\Delta_{1B})\end{array}\right]\times q^2\left[CosqR - \frac{SinqR}{qR}\right]dq \qquad (6)$$

In case of two atoms, that is no close neighbor and the variation in distance results from the variations in the composition of the region between them. The variation in close neighbor distances attributes to the kind of atoms making up the pair [6]. The ordering potential is modified by incorporating the atomic size effect and is given by:

$$E(R_1) = A(R_1) - B(R_1)$$

Where, $A(R_1)$ and $B(R_1)$ are the first nearest neighbor distances of A- and B-atom. Here, the factor $B(R_1)$ is given by:

$$B(R_1) = B_{1A}\Delta_{1A} + B_{1B}\Delta_{1B}$$

Here,

$$B_{1A} = \frac{\overline{\Omega_0}}{N\pi^2}\int_0^\infty \left[-\frac{\Omega_0}{8\pi}\left(\Delta\omega^0(q)\Delta\omega_A{}^0\right)\frac{\varepsilon(q)-1}{\varepsilon^*(q)} + \frac{2\pi}{\Omega_0 q^2}e^{-(-q^2/4\eta)}(\Delta Z^* Z_A \Delta_{1A}) \right] \times q^2\left(\cos qR_1 - \frac{\sin(qR_1)}{qR_1}\right)dq \qquad (7)$$

The expression for B_{1B} can be written in a similar manner.

Where,

$$\Delta\omega^0(q)\omega_A^o = \Delta w^0(q)\omega_A^0(q)\Delta_{1A} \qquad (8)$$

&

$$\Delta Z^* Z_A \Delta_{1A} = \Delta Z_A{}^* Z_A^* \Delta_{1A} \qquad (9)$$

Where,

$$\Delta Z^* = Z_A^* - Z_B^*$$

Here,

$$Z_A^* = Z(1+\alpha_{eff}) \qquad (10)$$

$$\Delta_{1A} = \frac{R_{1A}}{\overline{R_1}} - 1$$

&

$$\Delta_{1B} = \frac{R_{1B}}{\overline{R_1}} - 1$$

Where,

R_{1A}=first nearest neighbor distance of A-metal.
R_{1B}= first nearest neighbor distance of B-metal.
Similarly, for R_{iA}, R_{iB} (i=1,2,3,4,……. etc).

Clapp-Moss relation was used to determine the value of SRO-parameter. The values of α_1 were determined from the ordering energy by using the Clapp-Moss expression [12]:

$$\frac{\alpha_1}{(1-\alpha_1)^2} = c_A c_B\left[e^{-\frac{E(R_i)}{k_B T}} - 1\right] \qquad (11)$$

Where, k_B is Boltzmann constant.

$$E(R_i) = \frac{\overline{\Omega_0}}{8\pi}\int dq\ q^2\ F(q)\frac{Sin(qR_i)}{qR_i} \qquad (12)$$

Where, $E(R_i)$ is the local ordering energy and the coordination sphere of radius R_i. In this work, we have also investigated the effect of the exchange and correlation factors on the ordering energies. The expressions to account for the exchange and correlation correction effect f(q) proposed by Kleinmen [13], Singwi [14], Hubbard-Sham [15], SLTS [14] and Lindhard [16] are given below:

Kleinman:

$$f(q) = \frac{1}{4}\left[\frac{q^2}{q^2 + k_F^2 + k_S^2} + \frac{q^2}{q^2 + k_S^2}\right]$$

$$K_S^2 = \frac{2K_F}{\pi}(a.u.)$$

Singwi: $$f(q) = A\left[1 - \exp\left[-B\left(\frac{q}{k_F}\right)^2\right]\right]$$

A=0.8894
&
B=0.3401

Hubbard-Sham: $f(q) = \frac{1}{2}\left(\frac{q^2}{q^2 + k_F^2 + k_0^2}\right)$

SLTS: $f(q) = \frac{9}{32}\left[\frac{2}{105}\left(\frac{24}{x^2} + 44 + x^2\right) - \frac{2}{x}\left(\frac{8}{35x^2} + \frac{4}{15} + \frac{x^2}{16}\right) \times \ln\left|\frac{x+2}{x-2}\right| + x^2\left(\frac{x^2}{210} - \frac{2}{15}\right)\ln\left|1 - \frac{4}{x}\right|\right]$

Lindhard: f (q) =0

3. RESULTS AND DISCUSSION

XRD experiments were performed on the $Ni_{20}Pd_{80}$ alloy to study SRO. Fig. 1 shows the XRD pattern recorded at room temperature obtained for the annealed sample of $Ni_{20}Pd_{80}$ at various temperatures. The patterns were indexed following the procedure mentioned in [17]. Since, all the fundamental reflections (hkl all even or all odd) were present; the patterns were therefore indexed as face centered cubic (FCC). The analysis of the experimental data yields information regarding the SRO.

The sample was single phase and has FCC structure of A1-type structure with lattice parameter *a*=0.382 nm [7]. The lattice parameters were calculated from XRD patterns taken after annealing. The structure of the alloy is FCC over a temperature range of 100-600 °C. The lattice parameter of the alloy increases with temperature clearly shown in Fig. 2.

At various annealing temperatures by the extrapolation of Nelson-Riley function and their values are plotted in Fig. 2. It can be clearly seen that the value of lattice parameter '*a*' increases linearly with temperature. The reason for this increase in '*a*' is the thermal expansion in lattice due to increase of temperature.

Fig. 3 shows the plot of SRO-function g(r) corresponding to temperatures (100, 300 and 600 °C). The SRO-function g(r) was determined from the measured intensities using the following relation [18]:

$$g(r) = \frac{2\pi}{r}\int_0^\infty Q\ j(Q)\ Sin(Qr)\ dQ \qquad (13)$$

Where, *r* is the radial distance, and *Q* is the reciprocal lattice vector

$$j(Q) = \frac{I_{eu}(SRO)}{Nc_A c_B (f_A - f_B)^2} - 1 \qquad (14)$$

Where, *I_{eu}(SRO)* is the observed intensity free from parasitic contributions and is measured in electron units. The procedures for the removal of parasitic contributions and the method to convert the measured intensities into electron units are outlined [19,20]. The radii of the coordination spheres were calculated from the lattice parameters determined from the XRD pattern.

The function g(r) was determined from the intensities measured for each annealing temperature (100-600℃). It is clear from Fig. 3 that the variations in the g(r) with respect to temperature are subjected to the changes in SRO inside the alloy. The first peak in the plot of g(r) is not relevant to the structure but comes from the modification function used in the calculation in order to take into account the infinite limit of the integral in the expression of g(r). This feature is more prominent in the curve corresponding to 100℃ as compared to the other two curves see Fig. 3. The SRO-parameters were determined from the data shown in Fig. 1, using the following expression [18-20]:

$$c_i \alpha_i = \int_{r<R_i}^{r>R_i} g(r)\, dr \qquad (15)$$

Where c_i is the coordination number, α_i is the radius and α_i for the i_{th} coordination sphere. There values are listed in Table 1 for the first, second and third nearest neighboring spheres. The value of α_1 was observed to be negative for all annealing temperatures. The variations in its value are due to the variation in the degree of SRO taking place with a change of temperature. The values of α_2 and α_3 were found to be positive for all investigated temperatures which indicate the formation of clusters in the second and third nearest neighboring spheres.

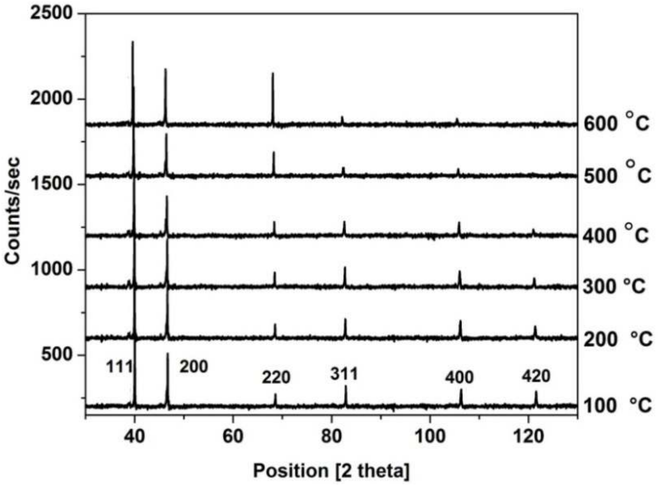

Fig. 1. XRD patterns of $Ni_{20}Pd_{80}$ alloy taken at different annealing temperatures

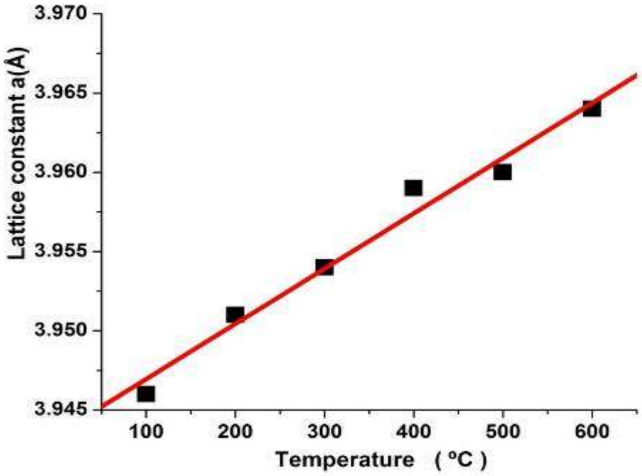

Fig. 2. Temperature dependence of lattice parameter *a*(Å) of $Ni_{20}Pd_{80}$ alloy determined from the Nilson-Riley (N-R) function

Table 1. The SRO-parameters (α_i) for various shells of atoms obtained from experimental diffuse scattering intensities of X-rays for $Ni_{20}Pd_{80}$ alloy

Temperature (℃)	Coordination no. *i*	c_i	α_i
100	1	12	-0.12
	2	6	0.32
	3	24	0.05
300	1	12	-0.14
	2	6	0.37
	3	24	0.07
600	1	12	-0.06
	2	6	0.18
	3	24	0.02

The parameters of TMMP [8] and the lattice parameters determined using the Vegard's rule was used as input for these calculations. The results of these calculations are listed in Table 2. It is seen that the values of α_1 is negative corresponding to different exchange and correlation factors. The values of α_1 were found to be negative from the XRD experiments too. It is therefore concluded that the electronic theory of alloys (2nd order perturbation) yields a good agreement between the experiment and theory as far as sign of the α_1 is concerned. The values of α_1 calculated employing the 3rd order perturbation correction and by taking into account the difference in atomic size of $Ni_{20}Pd_{80}$ are also given in Table 2. The difference in the magnitude of experimental and theoretical values may be attributed to the following reasons, (i) these calculations apply only to the ground state 100 °C where as the experiments have been done at higher temperatures. (ii) The values of lattice parameters used in these calculations were calculated from Vegard's rule.

The results of ordering energy calculated for $Au_{25}Pd_{75}$ alloy are given in Table 3. The pseudo-potential approximation views the matter as a sea of valence electrons moving around in a background composed of rigid ions. Much pseudo-potential has been formulated for simple metals and their alloys. The Pd-Ni and Ag-Ni Alloys nanoparticles were studied at room-temperature and characterized by various analytical characterization techniques [21]. The magnetic properties of disordered Ni-Pd and Ni-Pt alloys, phase stability and magnetism which showed the separation between s–d bands of 5d elements in these alloys [22]. Magnetic Properties of Metals: d-Elements, Alloys and Compounds the magnetic properties of

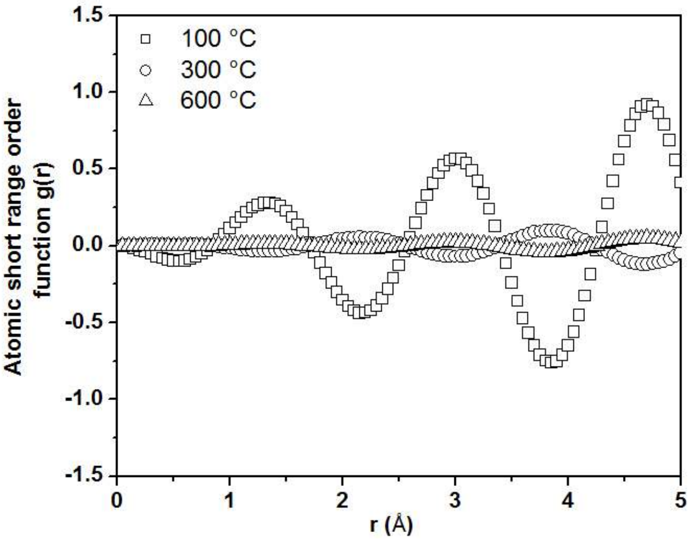

Fig. 3. Temperature dependence of atomic short range order function g(r)

Table 2. The ordering energies for $Ni_{20}Pd_{80}$ alloy calculated by using the electronic theory of alloys in the pseudo-potential approximation techniques

E(R$_i$) (eV) (10^{-2}) Coordination no. *i* 1	2	3	α_i	Order of perturbation	Exchange & correlation factor *f(q)*
1.591	0.433	-0.162	-0.150	II	Kleinman
1.559	0.424	-0.158	-0.148		Singwi et al.
1.504	0.423	-0.158	-0.144		Hubbard-Sham
1.448	0.420	-0.156	-0.140		SLTS
1.453	0.423	-0.157	-0.141		Lindhard
1.588	0.434	-0.163	-0.150	III	Kleinman
1.557	0.424	-0.159	-0.148		Singwi et al.
1.502	0.423	-0.158	-0.144		Hubbard-Sham
1.566	0.433	-0.162	-0.148		SLTS
1.451	0.423	-0.158	-0.141		Lindhard
2.107	0.028	0.081	-0.179	II	Kleinman
2.065	0.027	0.081	-0.177	with size effect	Singwi et al.
2.009	0.039	0.073	-0.174		Hubbard-Sham
1.948	0.050	0.065	-0.171		SLTS
1.956	0.051	0.065	-0.171		Lindhard

Table 3. The ordering energies for $Au_{25}Pd_{75}$ alloy calculated by using transition metal model pseudo-potential (TMMP)

$E(R_i)$ (eV) (10^{-2})			α_i	Order of perturbation	Exchange & correlation factor *f(q)*
Shell no. *i*					
1	2	3			
0.432	-0.411	0.222	-0.060	II	Kleinman
0.417	-0.397	0.216	-0.058		Singwi et al.
0.415	-0.373	0.208	-0.057		Hubbard-Sham
0.408	-0.346	0.199	-0.057		SLTS
0.413	-0.350	0.201	-0.057		Lindhard
0.432	-0.411	0.222	-0.060	III	Kleinman
0.417	-0.397	0.216	-0.058		Singwi et al.
0.415	-0.372	0.208	-0.057		Hubbard-Sham
0.430	-0.404	0.220	-0.060		SLTS
0.413	-0.350	0.201	-0.057		Lindhard
0.442	-0.421	0.242	-0.061	II	Kleinman
0.431	-0.408	0.237	-0.060	with size effect	Singwi et al.
0.437	-0.388	0.234	-0.060		Hubbard-Sham
0.439	-0.367	0.230	-0.061		SLTS
0.442	-0.370	0.231	-0.061		Lindhard

the d transition elements and of their metallic alloys and compounds have increased widely for well-defined substances, the development of sophisticated measuring methods needs in the improvement of preparation techniques [23]. The pseudo-potential approximation relies on the distinction between the core and valence states. In non-simple metals e.g. transition metals, the d-states are not the core states. Therefore, the essential simplification due to pseudo-potential method is thus lost. To rectify this, a method has to be adopted which gives a good description of the outer core and the d-band near the nucleus.

The QDL works well for monovalent atoms, but fails for complex atoms. Abbas & Khalil studied the concentration dependence of atomic SRO in the $Ni_{100-x}Ti_x$ (x =2, 5, 10, 15, 20, 25, 35, 50 at.%) alloys using the framework of the transition metal model pseudo-potential (TMMP) [24].

4. CONCLUSION

The experimental values of α_1 were found to be negative at all investigated temperatures, which indicates formation of SRO in $Ni_{20}Pd_{80}$ alloy. The experimental values of α_2 and α_3 were found to be positive, which indicates formation of clusters in the second and third neighboring spheres. The order of perturbation and size-effect is taken into account in these calculations. The values of α_1 are found to be negative. Theoretical calculations using pseudo-potential approximation were performed on the Au-Pd alloy. Following conclusions can be drawn from the present work. The theoretical values of α_1 were found to be negative at all investigated values, which indicates SRO formation in Au-Pd alloy. The theoretical values of α_1 were found to be -ve, which indicates the clustering behavior in an alloy. The theoretical calculation of ordering energies were undertaken by using the electronic theory of alloys in the pseudo-potential approximation resulted in a correct prediction of the sign of α_1. These results are seen to further improve if the order of perturbation and size-effect are taken into account in these calculations.

ACKNOWLEDGEMENTS

The author Dr. S. K. A. Tirmizi would like to thank Farooq Bashir and Syed Waqas Shah for their helpful discussions in manuscript and technical assistance in XRD.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Iveronova VI, Katsnelson AA. Short range order in metallic solid solutions. Moscow University Press, Nauka; 1977 (in Russian).
2. Pfeiler W. Acta Metallurgy. 1988;36:2417.

3. Abbas T, Khalil RMA, Rana AM, Mahtabullah. Ordering behavior of FCC and HCP alloys in Ni-Hf and Re-Ti systems. Modern Physics Letter B. 2006;20:2425.
4. Akhtar S, Ziya AB, Abbas T. Order-disorder transformation in the binary MPt3 and ternary $CuMPt_6$ (M=3d metals) alloys. Physica B. 2009;404:2241.
5. Lin W, Spruiell JE. The structure of nickel-pallidium solid solutions. Acta Metallurgy. 1971;19:451.
6. Shamah AM, Cowlam N, Carr GE. An investigation of atomic short range order in palladium alloys by diffraction methods. Journal of Materials Science. 1987;22: 2859.
7. Ahmad S, Ziya AB, Aziz A, Zafar ZI. Structure and thermal parameters of $Ni_{20}Pd_{80}$ alloy. Journal of Material Science Technology. 2009;25:208.
8. Katsnelson AA, Silonov VM, Khawaja FA. Electronic theory of short-range order in alloys using the pseudopotential approximation and its comparison with experiments. Physica Status Solidi (b). 1979;91(1):11–33.
9. Rossiter PA. The electrical resistivity of metal and alloys. Cambridge University Press. Cambridge; 1987.
10. Khawaja FA, Katsnelson AA, Silonov VM. Many - electron effects on the characteristics of short - range order in the pseudopotential approximation. Physical State Solution. 1978;88:477.
11. Animalu AOE. Electronic structure of transition metals. I. Quantum defects and model potential. Physical Review B. 1973; 8:3542.
12. Clapp PC, Moss SC. Correlation functions of disordered binary alloys. II. Phys. Rev. 1968;171:754.
13. Kleinman L. New approximation for screened exchange and the dielectric constant of metals. Physical Review. 1967;160:585.
14. Singwi KS, Tosi MP, Sjolander A, Land RH. Electron correlations at metallic densities. Physical Review. 1968;176:589-99.
15. Hubbard J, Sham LJ. Proceedings of Royal Society (London). 1957;A240:359.
16. Lindhard, Langreth D. Approximate screening functions in metals. David C. Langreth. Physical Review. 1969;181:753.
17. Cullity BD. Elements of X-ray diffraction. Addison-Wesley, Philippines; 1978.
18. Warren BE. X-ray diffraction. Dover Publications, New York; 1990.
19. Abbas T, Ziya AB. Evidence of short-range order in the disordered Cu-Ti alloys. Journal of Materials Science. 1993;28(18): 5010-5013.
20. Khawaja FA, Katsnelson AA, Silonov VM, Khrushchov MM. Physical State Solution. 1977;82:70.
21. Zhang ZY, Nenoff TM, Leung K, Summer RF, Jian YH, Donald TB, Paula PP, Roland S. Room-temperature synthesis of Ag-Ni and Pd-Ni alloy nanoparticles. Journal of Physical Chemistry C. 2010;114:14309.
22. Durga P, Abhijit M. Phase stability and magnesium in NiPt and NiPd alloys. Journal of Physics Condensed Matter. 2004;16:5791.
23. Wijn HPJ. Magnetic properties of metals: d - elements, alloys and compounds. Springer Science & Business Media. Technology & Engineering. 2012;190.
24. Abbas T, Khalil RMA, Rana AM, Mehtab U. Calculation of short range ordering in Ni-Ti alloys. Journal of Research (Science) (B.Z.U, Multan). 2005;16(2):87.

Peer-review history:
The peer review history for this paper can be accessed here:
http://sciencedomain.org/review-history/11960