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The electronic configuration of Fe-Ni alloy's system by Compton profile probe

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Abstract

The calculated values of Compton profile of Fe,Ni metals and their two alloys namely $Fe_{0.5}$-$Ni_{0.5}$ and $Fe_{0.64}$-$Ni_{0.36}$ are reported. The Renormalized Free Atom(RFA) model are used to determine the most favored electron configurations for the two metals which are found to be Fe($3d^{6.7}$-$4s^{1.3}$) and Ni($3d^{8.8}$-$4s^{1.2}$) respectively ,the values for FREE ELECTRON(FE) model and FREE ATOM(FA) were calculated for the same also. The Super Position model were used to find the Compton profile values for the two alloys .All theoretical values for the two metals as well as their alloys are compared with the recent available experimental and theoretical values and they show a good agreement.

Introduction

Many authors have studied the Fe-Ni alloys due to their important magnetic and other properties. The f.c.c. solid solution lattice spacing's have been measured by[1,2,3]. The lattice spacing's rise to a maximum at -38%Ni [4]. Among the early theoretical research, band structure of transition metals and their alloys were studied by[5], it concludes that First, the 3d wave functions are anisotropic which implied that there may be localized and collective 3d electrons simultaneously present. Secondly, localized electrons obey Hand's rules and may therefore contribute an atomic moment and the corresponding energy levels, or narrow bands are split into discrete sub bands. Thirdly, the nearest neighbor anti-ferromagnetic order can be propagated throughout a lattice and the nearest-neighbor directed 3d orbitals are half or less filled. The collective electrons can be stabilized by bonding-band formation and if the orbitals are more than half filled, the extra
electrons cannot be stabilized by anti-ferromagnetic correlations between nearest neighbours. If anti-ferromagnetic nearest neighbor order is not possible, the electrons form a conventional metallic band. The anomalies of electrical and magnetic properties in Fe-Ni alloys (INVAR) at low temperature were studied and explained in terms of the latent anti ferromagnetism by[6]. The fine structure of the k-absorption edge was studied by[7] and a general shift of the k-absorption structure towards longer wavelengths (at 160^{o}C) was seen for a number of Fe-Ni alloys. An investigation of the temperature dependence of yield point and hardness in Fe-Ni alloys in the annealed and strain hardened was made by[8]. Weiss (1963) attempted to explain the origin of (INVAR) effect on the idea that there are two electronic configurations of iron atoms in a f.c.c. lattice of Fe-Ni alloy system. By a reasonable variation of the energy difference of these two configurations with Ni concentration, it was shown that the (INVAR) effect originated from the thermal excitation of the configuration with lower atomic volume in opposition to the normal an harmonic origin of expansion. It was also shown in this work that this model could explain the anomalous pressure dependence of the Curie temperature and the variation of Curie temperature with concentration. The direction of electron transfer in Fe-Ni alloys was studied by an infrared technique by[9] from which it was suggested that there is an electron transfer from Fe to Ni in the Fe-Ni alloy system in contrast to Co-

Ni alloy system. A recent calculation of the electronic structure of random substitutional alloys Fe-Ni alloy has been reported by [10]. It was found that the average moment varied linearly with concentration of iron atoms and with the increase of iron concentration the iron moment slowly decreases and the nickel moment increases. Hence they concluded that the collapse of the magnetism was precipitated by the collapse of the iron moment.

In this work we have studied two alloys in the f.c.c. Fe-Ni system namely **$Fe_{0.5}$-$Ni_{0.5}$** and **$Fe_{0.64}$-$Ni_{0.36}$** having lattice parameter (a) 6.77476 a.u. and (a) 6.79479 a.u. respectively [4]. Superposition model used in the case of β-aluminides [11] and vanadium silicides [12] is employed in this case also to obtain charge transfer between Fe-Ni atoms. Accordingly, the Compton profile of the two constituent metals i.e. Fe and Ni are also determined experimentally. The results on pure metals have been compared with our **RFA** calculations for different 3d-4s configurations and other available results (theoretical as well as experimental). These measured values are used to obtain the Compton profile for the two alloys by suitably adding their contributions, which are then compared with the measurements on the alloys.

Theoretical Calculations:

In the superposition model [12], the Compton profile for a given alloy $J^{AB}(P_Z)$ is given by the formula.

$$J^{AB}(P_Z) = (1 - x)J^{A}(P_Z) + xJ^{B}(P_Z) \quad \ldots(1)$$

Where x is the (fractional) atomic concentration of B atoms in the AB alloy. $J^{A}(P_Z), J^{B}(P_Z)$ are the experimental Compton profiles of A and B metals respectively. The Compton profiles for **$Fe_{0.5}$-$Ni_{0.5}$** and **$Fe_{0.64}$-$Ni_{0.36}$** were computed using this procedure. For the sake of comparison we also obtained the Compton profiles using the free atom values. Theoretical Compton profiles were obtained for Fe and Ni. They were then convoluted with the RIF of our spectrometer for the purpose of a proper comparison with the experiment, because no deconvolution procedure removes the instrumental broadening completely due to statistical noise ever present in the experiment [13].

The RFA and FE models are adopted to calculate the Compton profiles for the two constituent of the alloys i.e Fe and Ni,the theories and detailes of calculations are given elsewhere[14,15],while the values of FA are taken directly from [16]

Results and Discussion

In tables (1-2) we illustrates all the results of compton profile values for Fe and Ni by applying RFA and FE models as well as FA values[14,15,16],also the results for the two alloys by applying the superposition model, this calculation was based on the f.c.c Ni lattice (Fe is bcc) which was adjusted to have the same lattice parameters as the alloy [13]. The free atom values given in these tables have been convoluted with the residual instrumental function (RIF). And all values were properly normalised to the number of electrons of the respective free atom Compton profiles in 0-5a.u. interval. The contributions of $1S^2$ were taken upto 5a.u. and 4 a.u. for Fe and Ni respectively.

To compare our results on the two alloys with the free atom and superposition model .At the high momentum region (i.e. p_z above 3.5 a.u.) it has been found that the values are very close to the free atom and superposition model. This provides confidence in our results and data analysis because in the superposition model we had used our values for Fe and Ni . These values are close to free atom values in this momentum region and hence it is no surprise that for the two alloys also they agree very well. In fact this comparison only confirms that the inner electron do not undergo any drastic change on alloy formation, for the low momentum region (P_z < 3.5 a.u.) it is obvious that the free atom values for both cases are variant from the experimental data upto 0.4 a.u. The deviations are very obvious and hence we have not considered this model for any analysis of the alloy data. Interestingly, the superposition model agrees quite well with the experiment in both the alloys. In figures I and II , we show the comparison of our results with superposition model for **$Fe_{0.5}$-$Ni_{0.5}$** and **$Fe_{0.64}$-$Ni_{0.36}$** respectively. For **$Fe_{0.5}$-$Ni_{0.5}$** (Fig.I.) it is seen that superposition values are almost equal to the experiment for p_z=0 and 0.1 a.u. Between p_z= 0.2 to 1.4 a.u. the experimental values are a bit higher. For p_z=1.6 a.u. the superposition model is higher but it gets reversed again between p_z= 3.5 to 3.8 a.u. whereas at p_z= 4 a.u. the two values are equal while for p_z=4.5 a.u. the superposition model is slightly higher. However, the overall nature of the two curves is similar. For the case of INVAR (**$Fe_{0.64}$-$Ni_{0.36}$**), this comparison is seen in Fig.II. It is obvious that in this case also the superposition model and the measured values are very close

In order to determine electron configuration and examine any differences in the behavior of two alloys, we have plotted the differences between the superposition model and experimental data for both the cases, the standard deviation $\sum_0^{5a.u}|\Delta j|^2$

i.e. [{free atom, free electron, present work }compton profile(CP) values – Experimental (CP)values]

are obtained for each case ,the values obtained are (4.86479,0.286209,0.3276139) for **$Fe_{0.5}$-$Ni_{0.5}$** and (4.91993,0.2314082,0.252574) for INVAR (**$Fe_{0.64}$-$Ni_{0.36}$**), in Fig.III. It is very obvious from this figure that the differences are very small (already discussed) and the nature of the difference curves is almost identical. At some points between 1.4 and 1.8 a.u. they do show a different behavior and in fact for **$Fe_{0.5}$-$Ni_{0.5}$** alloy one point(p_z=1.9a.u.) is few larger than other points. We could not identify the reason for this sudden behavior but it does point to some systematic change in this region.

It has been noticed that in the case of Ti-Ni alloys the superposition model could reproduce the profile for the alloys[13]. Also in a study on Cu-Ni alloys,[17] had reported similar results. This work also supports

essentially these conclusion. The isotropic Compton profile of **$Fe_{0.5}$-$Ti_{0.5}$** alloy are measured by using 320 KeV γ-ray source and the data interpreted by employing the RFA model and found that the best agreement between theory and experiment could be obtained if the configuration was taken as Fe($3d^6$-$4S^2$) Ti($3d^2$-$4S^2$)[18]. Another work on **$Fe_{0.5}$-$Ti_{0.5}$** alloy was again investigated by [19] using 412 KeV γ-radiation. They used these data to test the prediction of Rigid Band (R.B) model by studying the difference between the CPs of alloy and Cr metal[20]. Interestingly, both these materials possessed identical structures and equal number of valence electrons. The differences were in contrast to the predictions of the R.B. model and this work yielded the configuration as Fe($3d^6$-$4S^2$) Ti($3d^2$-$4S^2$) in agreement with the work of [21].

Thus, this comparison suggests that out of the 36 valence electrons in the unit cell of F.C.C. alloy, about 28 electron belong to the ,d, band and 8 to 4S and 4p band. In our analysis of data on metals (cols.4 and 5.) from table I(1-2) we have observed that favoured configurations as determined in the RFA model are Fe(**$3d^{6.7}$-$4s^{1.3}$**) and Ni(**$3d^{8.8}$-$4s^{1.2}$**) configurations respectively. Considering the agreement with superposition model it means that the electron distribution in the two alloys should be identical and close to the average of Fe(**$3d^{6.7}$-$4s^{1.3}$**) Ni(**$3d^{8.8}$-$4s^{1.2}$**) configuration. For the occupancies of electrons in s-d shells the average are taken for the two alloys as (**$3d^{7.25}$-$4s^{1.75}$**) and (**$3d^{6.90}$-$4s^{1.82}$**) respectively. Both these electron configuration are very similar to Co metal for which (**$3d^7$-$4s^2$**) is considered to be the stable state in the metal. In order to examine the effects of electron transfer on Compton profiles in Fe-Ni alloys observed by[9], we plot in Fig.IV. the Compton profiles for valence electrons (per electron) for Fe and Ni. These values are obtained by subtracting from the data on metal the corresponding core contribution and dividing by the number of valence electrons. The difference is maximum in the J(0) values and that is only 0.046 e/a.u. Thus if we consider a transfer of electrons from Fe to Ni then the J(0) value should decrease in the alloy and for each electrons transferred the change would be about 0.05 from that of the superposition model.

Conclusion

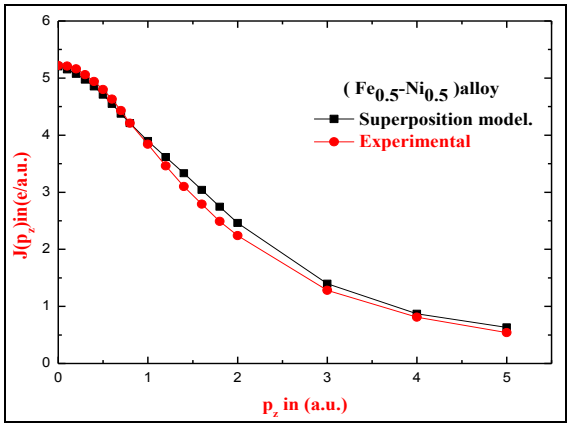
In this work we have calculated the Compton profiles of Fe ,Ni metals and two of their alloys. Our results on metals agree very well with previous results and with superposition calculations. The RFA model also predicts reasonably well the overall nature of Compton profiles. In the case of **$Fe_{0.5}$-$Ni_{0.5}$** and **$Fe_{0.64}$-$Ni_{0.36}$** the measurement is reproduced very well in term of the superposition model. Some indication of charge transfer from Fe to Ni atom are visible but the experimental accuracy needs to be improved by at least a factor 4 or so, to establish conclusively whether there is charge transfer or not.

Table-1: Theoretical results Compton profile of the alloy $Fe_{0.5}$-$Ni_{0.5}$ compared with experimental value [22]. All the quantities in atomic units. All theoretical values have been convoluted with the residual instrumental function (RIF) of 0.6 a.u. These values have been normalized to 11.054 electrons

P_z (a.u.)	J(p_z)(e/a.u.)					
	Free atom ($3d^6$-$4s^2$)	Free electro-n model	Theory(RFA) model			Expt. [22]
			Fe Core+RFA $3d^{6.7}$-$4s^{1.3}$	Ni Core+RFA $3d^{8.8}$-$4s^{1.2}$	$Fe_{0.5}$-$Ni_{0.5}$ Present work.	
0.0	6.78	5.397	5.211	5.192	5.202	5.22
0.1	6.395	5.325	5.159	5.143	5.151	5.21
0.2	5.932	5.22	5.079	5.066	5.073	5.16
0.3	5.512	5.088	4.976	4.969	4.973	5.06
0.4	5.135	4.93	4.851	4.853	4.852	4.94
0.5	4.788	4.749	4.702	4.714	4.708	4.8
0.6	4.479	4.556	4.534	4.558	4.546	4.63
0.7	4.222	4.361	4.356	4.395	4.376	4.43
0.8	4.014	4.177	4.179	4.236	4.208	4.21
1.0	3.702	3.857	3.848	3.948	3.898	3.84
1.2	3.439	3.577	3.543	3.689	3.616	3.46
1.4	3.171	3.299	3.237	3.428	3.333	3.1
1.6	2.891	3.012	2.925	3.153	3.039	2.79
1.8	2.608	2.724	2.617	2.871	2.744	2.49
2	2.335	2.446	2.326	2.594	2.46	2.24
3	1.331	1.392	1.287	1.504	1.396	1.28
4	0.836	0.867	0.81	0.934	0.872	0.81
5	0.609	0.626	0.594	0.667	0.631	0.54

Table-2: Theoretical results Compton profile of the alloy $Fe_{0.64}$-$Ni_{0.36}$ compared with experimental value [22]. All the quantities in atomic units. All theoretical values have been convoluted with the residual instrumental function (RIF) of 0.6 a.u. These values have been normalized to 10.942 electrons

P_z (a.u.)	$J(p_z)$(e/a.u.)					
	Free atom ($3d^6 4s^2$)	Free Electro-n Model	Theory(RFA) model			Expt. [22]
			Fe Core+RFA $3d^{6.7}$-$4s^{1.3}$	Ni Core+RFA $3d^{8.8}$-$4s^{1.2}$	$Fe_{0.64}$-$Ni_{0.36}$ Present work.	
0.0	6.796	5.4	5.211	5.192	5.204	5.19
0.1	6.406	5.328	5.159	5.143	5.153	5.18
0.2	5.936	5.222	5.079	5.066	5.074	5.12
0.3	5.512	5.089	4.976	4.969	4.973	5.02
0.4	5.132	4.93	4.851	4.853	4.852	4.91
0.5	4.783	4.748	4.702	4.714	4.706	4.78
0.6	4.471	4.553	4.534	4.558	4.543	4.61
0.7	4.212	4.357	4.356	4.395	4.37	4.41
0.8	4.003	4.172	4.179	4.236	4.2	4.21
1.0	3.687	3.8847	3.848	3.948	3.884	3.81
1.2	3.419	3.562	3.543	3.689	3.596	3.44
1.4	3.145	3.277	3.237	3.428	3.306	3.1
1.6	2.86	2.984	2.925	3.153	3.007	2.77
1.8	2.573	2.693	2.617	2.871	2.708	2.47
2	2.299	2.412	2.326	2.594	2.422	2.2
3	1.302	1.364	1.287	1.504	1.365	1.25
4	0.82	0.851	0.81	0.934	0.855	0.79
5	0.599	0.616	0.594	0.667	0.62	0.54



Fig(I).Comparison of the experimental Compton profiles of poly- crystalline $Fe_{0.5}$-$Ni_{0.5}$ alloy with that calculated from superposition model

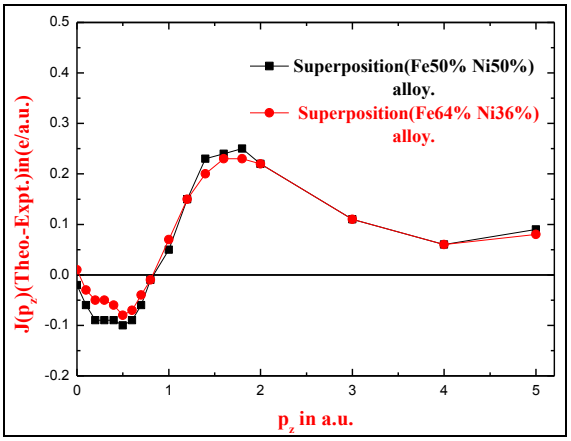
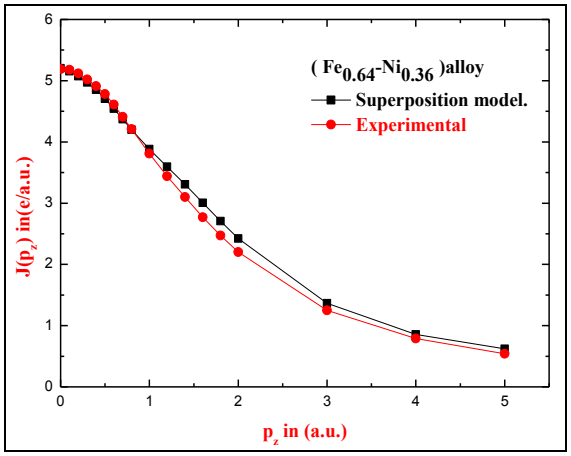


Fig (III). Plot of the differences between superposition model (theory) and experimental Compton profiles of the two alloys ($Fe_{0.5}$-$Ni_{0.5}$ and $Fe_{0.64}$-$Ni_{0.36}$) [18]



Fig(II).Comparison of the experimental Compton profiles of poly- crystalline $Fe_{0.64}$-$Ni_{0.36}$ alloy with that calculated from superposition model.

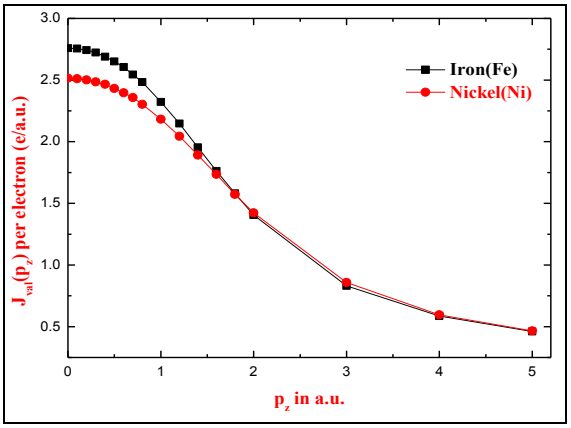


Fig (IV). Experimental Compton profile for each valence electron in polycrystalline Fe and Ni.

Reference

1. Owen, E.A., Yates, E.L. and Sully, A.H. (1937) proc. Phys. Sec. 49,315.
2. Owen, E.A. and Sully, A.H. (1941) Phil. Mag. 31, 314.
3. Bradley, A.J. Jay, A.H. and Taylor, A.(1937) Phil. Mag. 23, 545.
4. Pearson, W.B (1964) "A handbook of lattice spacings and structures of metals and alloys" Pergamon Press Ltd.
5. Goodenough, J.B. (1960), Phys. Rev. Vol. 120(1), PP. 67.
6. Kondorsky, E.I. and Sedov, V.L.(1969) J. Appl. Phys. Vol. 31(5), PP.3315
7. Bally, D. and Meller, L. (1959), C. R. Acad. Sci. (Paris), (13),PP.1099
8. Kardonski, V.M., Kurdymov, V.G., Kurdymov, G.V. and Perkas, M.D. (1961) physics of metals and metallography (GB), Vol. 11 (H), No.4, PP.117.
9. Cho, J.S. and Schulma, J.H. (1964), Surface Sci (Netherlands) Vol.2,PP.245.
10. Johnson, D.D., Finski, F.J. and Staunton, J.B. (1987) J. Appl. Phys. 61 (8),PP.3715.
11. Manninen, S., Sharma, B.K., Paakkari, T., Rundqvist, S. and Richardson, M.W. (1981) Phys. Stat. Sol. (b) 107, 749.
12. Paatero, T., Mannunen, S. and Paakkari, T. (1974) Phil. Mag. 30, 1281.
13. Paatero, T., and Mannunen, S. (1974) J. Phys. F., 4, L133.
14. Fareed M. Mohammed, A. M. Ghaleb, M.A. Majeed, M.N. Mohammed and N,S. Mohammed., Advance in Appl. Sci. Res.,6(8):118-124.(2015).
15. A.M.Ghaleb,FareedM.Mohammed,M.A.Majeed, M.N.Mohammed,N.S.Mohammed Advances in phys. Theo. and Appl.,Vol.46,(2015).
16. Biggs, L. Mendelson, L. Bandmann, J.B (1975) At. Data and nuclear data tables 16,201.
17.Manninen, S., Paakkari, T., Sharma, B.K., Rachardson, M.W. and Rundqvist, S. (1985), India, J. Phys.59A, 889-894.
18. Lasser, R., Lengeler, B. and Arnold, G. (1980), Phys. Rev. B, 22, PP. 663.
19.Ahuja, B.L. (1988), unpublished Ph.D. thesis submitted to the University of Ragjasthan.
20.Ahuja, B.L, Sharma, B.K. and Aikala, O. (1987), Pramana, J. Phys., Vol. 29, No. 3, PP. 313-320 (India).
21.Wakoh,S.,private communication to Cooper, M.J. (1988).
22. B. L. Ahuja, M. D. Sharma, B. K. Sharma, S. Hamouda and M. J. Cooper.(1998)."Compton Study of the Electronic State in Fe–Ni Alloys" Physica Scripta. Vol. 58, 185-188.

الترتيب الالكتروني لسبيكة (Fe-Ni) بواسطة شكل منحنى كومبتون كمجس

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الملخص

قيم شكل منحنى كومبتون لمعدني الحديد والنيكل وسبائكهما تم حسابهم باستخدام نماذج مختلفة هي نموذج اعادة معايرة الذرة الحرة ونموذج الالكترون الحر وقيم الذرة الحرة للمعدنين، والذي تم ايجاد افضل ترتيب الكتروني لكل منهما. لقد استخدم نموذج التركيب الاعظم لايجاد قيم شكل منحنى كومبتون للسبيكتين $Fe_{0.5}$-$Ni_{0.5}$ و $Fe_{0.64}$-$Ni_{0.36}$. جميع القيم المحسوبة تمت مقارنتها مع احدث ما متوفر من قيم تجريبية حيث وجدنا تطابق كبير بينها، تم ايضا دراسة احتمالية انتقال الشحنة بين مكونات السبيكتين من المعدنين.