

## **Electronic Occupancy of S and D Shells in Nickel**

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### **Abstract**

In this paper we have calculated the electronic structure of Ni<sup>28</sup> by adopting the RFA model and compared with recent available measured data. It is found that 3d<sup>8.3</sup>4s<sup>1.7</sup> is the best fractional electronic configuration for Nickel.

### **Introduction**

Nickel belongs to group (2) body center cubic (B.C.C) metal with atomic mass=58.693 amu (Pearson, 1964) its electronic structure (Ni) is 3d<sup>8</sup>4s<sup>2</sup> (Kittle, 1996). The First experimental Compton profile for (Ni) reported by Paakkaire et al (Patterson, 1974), It includes atomic weight 58.693 g/mol, atomic number 28, boiling point 2732 °C, melting point 1453 °C and density 8.902 g/ml (chemistry, 2002). For the last decade there has been interest in the study of the energy broadening of Compton scattering  $\gamma$ -ray or x-ray for probing the behaviour of the slowly moving valence electron in solids this broadened line -shape referred to as the Compton profile  $J(\vec{P}_z)$  which is given as:

$$J(\vec{P}_z) = \iint \rho(\vec{P}) dp_x dp_y \quad \dots(1)$$

Where  $\rho(\vec{P})$  is the electron momentum density. Provides a useful test of initial electronic structure theory a general review of this topic has been published by Cooper (Cooper, 1985). In our endeavor to extend the Compton scattering of 3d transition metals, we referred to Compton profile polycrystalline Ni (Taylor, 2001; Furness, 1973; Tomk, 1981 and Terasak, 1972). Since new measured data were reported for Ni (Singh, 1998). It was thought to re-establish and hold new study. In this paper we reported the theoretical Compton profile results of Iron by using the reformulations of free atom (RFA) model which is known to be a reasonable compromise between elaborate band structure and simple atomic calculation (Farid, 1988). We have also attempted to interpret the experimental results in terms of this model.

### **RFA model**

Chodorow (Chodorow, 1939) was the first to use this theoretical model. Later on it was extended for Cu by Segal (Segall, 1962). This approach

simply considers that the atom is not free but confined to particular cell in the solid. The calculation start from Hartree–fock wave function which is truncated at the Winger–Seitz radius ( $R_o$ ) and re–normalized to unity within this sphere to preserve the charge neutrality the new wave function  $R_{n1}(r)$  is given by.

$$R_{n1}(r) = \begin{cases} N_{n1} R_{n1}^{atomic}(r) & r \leq R_o \\ 0 & r > R_o \end{cases} \quad \dots (2)$$

Here  $R_{n1}^{atomic}(r)$  is the atomic radial wave function for the state with quantum number (n) 1 and  $N_{n1}$  is defined by

$$N_{n1}^{-2} = \int_0^{R_o} |R_{n1}^{atomic}(r)|^2 r^2 dr \quad \dots (3)$$

This new function is then used in further computations. In this way the solid is constructed from individual atoms approximately in the same form in which they actually enter the solid before being bound together. As from the successes of this simple model, besides Compton work (Berggren,1972) has shown that this model gives quantitatively correct estimates of the important band structure characteristics and also exolanation of cohesion in the transition metal series. Later (Gellat, 1977) used the RFA model for the determination of cohesive energies for several 3d and 4d metals even in complicated band theoretical calculation, RFA model is invoked to obtain the one electronic potential (Bendick, 1985).Berggren has studed overall behaviour of the RFA wave function (4s electron in vanadium) and has followed it to be a good represented of the true crystal wave function at  $K = 0$ .

### **Theoretical Calculations**

The Compton profile  $J(\vec{P}_z)$  for pollycrstalline sample is related to spherical average of  $\rho(\vec{p})$  by :

$$J(P_z) = \int dp p \langle \rho(\vec{p}) \rangle_{\vec{P}_z} \quad \dots(4)$$

To compute  $\langle \rho(\vec{p}) \rangle_{\vec{P}_z}$  the technique developed by Berggern (Berggren,1972) based on RFA model has been used. We start with the free atom wave function, truncate them at Winger– Seitz radius and re– normalized the wave function to one within (W-S) sphere to preserve charge neutrality.  $J(P_z)$  due to (4s) electrons of Fe were computed for  $(3d^{8+x}4s^{2-x})$  .Where  $(x = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6... \text{ ets})$ , We used the following equation:

$$J_{4s}(P_z) = 4\pi \sum_n \int_0^\infty |\psi_o^c(K_n)|^2 G_n(P_z) \quad \dots(5)$$

$$\mathbf{n} = 0$$

where  $\psi_o^c(\vec{K}_n)$  : - is the fourier transform of the RFA wave function  $G_n(P_z)$  is an auxiliary function depends on  $K_n$  ,  $N_n$  and  $P_f$  .Where  $K_n$  : reciprocal lattice vector.  $N_n$ : number of lattice point . $P_f$ : Fermi momentum .

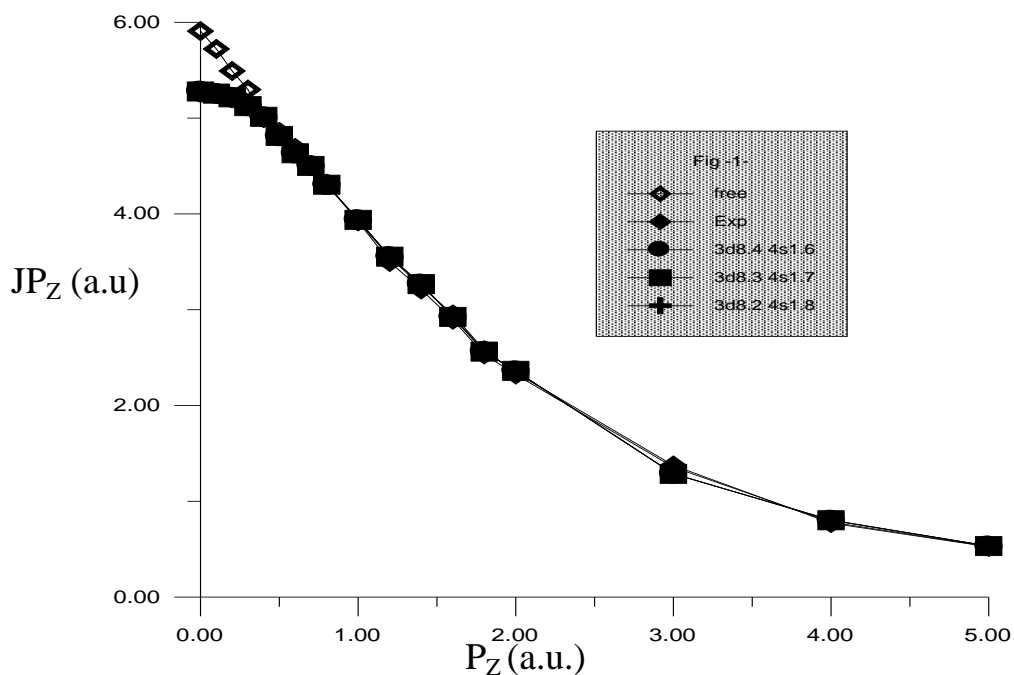
In the calcution free atom Hartree-Fock function were taken from the tables of Clement and Roetti (Clementi, 1974). For  $x =0$  to  $x = 1.5$  the wave function for  $3d^8 4s^2$  was used and for  $x = 1.5$  to  $2$  the wave function for the  $3d^9 4s^1$ . Were used for the rest including  $3d$  electronic values were taken from the tables of the Biggs (Biggs, 1975). Several combination of  $3d$   $4s$  configuration were computed. The Winger– Seitzr radius is  $2.67$  a.u (Kittle, 1996). All these theoretical values were finally convoluted with RFA (residual instrumental function) to make them comparable with experimantal values which have been de–convolution using the known instrumental function (Pattero, 1974).

## **Results and discussion**

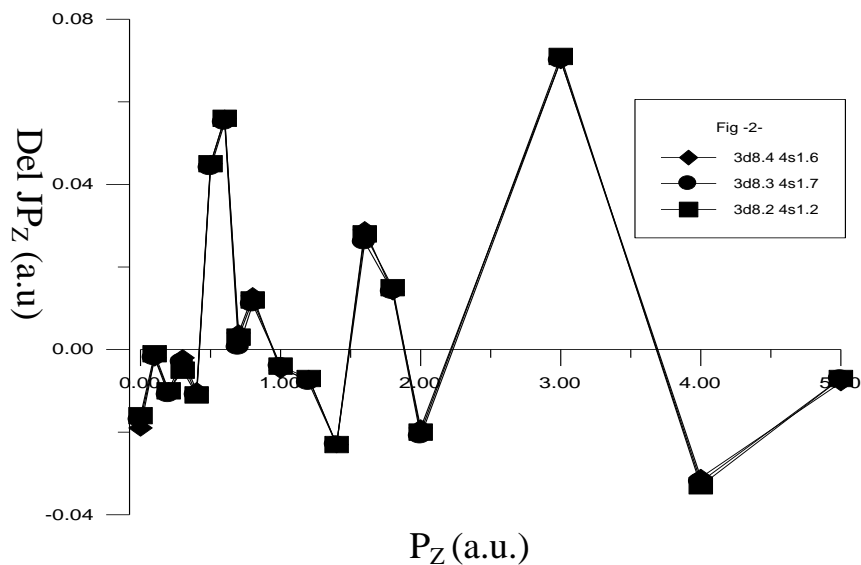
Table (1) shows the different measured and calculated Compton profiles values, all values were normalized to the value ( $13.92a.u$ ) which represents the area under the curve for free atom profile. Fig (1) shows some of the curves given in table (1) and it is observed that the momentum region between  $0$  to  $3a.u$ . the RFA values for  $3d^{8.2}4s^{1.8}$  and  $3d^{8.4}4s^{1.6}$  are closer to the experiment while beyond  $3a.u$  all theoretical values are nearly equal and agree very well with the experimental results. At  $J(0)$  the experiment as well as (RFA)  $3d^{8.2}4s^{1.8}$  almost the same. To show the comparison more clearly, Fig (2) the differences between theory and experiment are plotted for the  $3d^{8.4}4s^{1.6}$ ,  $3d^{8.3}4s^{1.7}$  and  $3d^{8.2}4s^{1.8}$  cases in order to determine the involution in the total square deviation  $\Sigma(\Delta J)^2$  was obtained for each case . The values found were  $0.05336$ ,  $0.06190$  and  $0.04195$  for the (RFA)  $3d^{8.4}4s^{1.6}$ ,  $3d^{8.3}4s^{1.7}$  and  $3d^{8.2}4s^{1.8}$ . Same procedures were done but after convoluting the RFA values and found changed in the favoured configuration.

**Table 1: Shows the present calculation of  $J(P_z)$  compared with measured values of**

$P_z$	$J(P_z)$ a.u Free	$J(P_z)$ a.u Exp	$J(P_z)$ a.u (Core + RFA)		
			$3d^{8.4}4s^{1.6}$ 6	$3d^{8.3}4s^{1.7}$ 7	$3d^{8.2}4s^{1.8}$ 8
0	5.909	5.262	5.281	5.279	5.274
0.1	5.722	5.254	5.256	5.256	5.259
0.2	5.492	5.207	5.217	5.218	5.219
0.3	5.299	5.122	5.124	5.125	5.127
0.4	5.001	5.004	5.014	5.015	5.015
0.5	4.823	4.857	4.712	4.713	4.714
0.6	4.677	4.688	4.532	4.533	4.563
0.7	4.500	4.506	4.494	4.496	4.498
0.8	4.312	4.316	4.303	4.305	4.305
1	3.921	3.933	3.938	3.937	3.937
1.2	3.498	3.546	3.553	3.554	3.555
1.4	3.211	3.244	3.267	3.267	3.267
1.6	2.894	2.951	2.922	2.925	2.927
1.8	2.532	2.577	2.463	2.461	2.461
2	2.323	2.341	2.360	2.360	2.357
3	1.355	1.375	1.287	1.286	1.287
4	0.781	0.771	0.802	0.807	0.805
5	0.529	0.525	0.533	0.532	0.531



**Fig. (1): calculated of measured values of  $J(P_z)$**



**Fig. (2): the differences between theory and experiment**

### **Conclusion**

This paper demonstrates the study on (Ni) to investigate its electronic structure, theoretical calculation by applying RFA model and compared with recent measured data of Compton profile. It shows that best electron configuration for (Ni) is  $3d^{8.2}4s^{1.8}$  before convolution while it turned out to be  $3d^{8.7}4s^{1.3}$  after convolution which demonstrates the effect of the convolution on the results.

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## الأشغال الإلكترونية للغلافين (s, d) لعنصر النيكل

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### الخلاصة

في هذا البحث تم حساب الترتيب الإلكتروني لعنصر النيكل (Ni) بتبني نموذج إعادة المعايير للذرة الحرة والمقارنة مع آخر البيانات المقاسة والمتوفرة . ولقد وجد بان احسن ترتيب إلكتروني للنيكل (Ni) هو  $3d^8 4s^2$  . الترتيب القديم أو الأصلي  $3d^8 4s^{1.3}$ .