Magnetic properties of X-Pt (X=Fe,Co,Ni) alloy systems

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Abstract. We have studied the electronic and magnetic properties of Fe-Pt, Co-Pt and Ni-Pt alloy systems in ordered and disordered phases. The influence of various exchange-correlation functionals on values of equilibrium lattice parameters and magnetic moments in ordered Fe-Pt, Co-Pt and Ni-Pt alloys have been studied using linearized muffin-tin orbital method. The electronic structure calculations for the disordered alloys have been carried out using augmented space recursion technique in the framework of tight binding linearized muffin-tin orbital method. The effect of short range order has also been studied in the disordered phase of these systems. The results show good agreements with available experimental values.

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1. Introduction

The magnetic and chemical interactions in solid solutions, their interdependence and the role they play in determining the electronic and magnetic properties of transition metal alloys have been the subject of extensive research since many years. The interplay between magnetism and spatial order in transition metal alloy systems has been extensively studied both experimentally [1],[2]-[5] and using phenomenological models based on statistical thermodynamics [6]-[12],[13]-[22].

In this communication, we studied the electronic and magnetic properties of ordered as well as disordered phase of the Fe-Pt, Co-Pt and Ni-Pt. Many studies on optical and magneto-optical characterization of these systems are available in recent literatures [23]. Nevertheless, a systematic first-principles study bringing out the interdependence of the magnetic and chemical ordering and the trend in this alloy series is lacking. The present communication aims at a systematic and comparative first principles study of the electronic structure and magnetism in these systems, using techniques based on the local spin density approximation (LSDA) of the density functional theory.
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Considering the case of ordered alloys, we have carried out a thorough study including careful investigation of the influence of various local as well as non-local exchange correlation functionals on the value of the equilibrium lattice parameters and magnetic moments of ordered Fe-Pt, Co-Pt and Ni-Pt alloy systems.

The calculational scheme used for our calculations of disordered alloys is based on augmented space recursion (ASR) technique. While the majority of the existing electronic structure calculations on disordered alloys have been based on the coherent potential approximation (CPA), the CPA, being a single-site mean-field approximation, cannot take into account the effect, at a site, of its immediate environment. As an alternative approach, Saha et al [24] have introduced the augmented space recursion (ASR) based on the combination of the augmented space formalism (ASF) first suggested by Mookerjee [25] and the recursion method of Haydock et al [26]. In this formalism, the configuration averaging is carried out without having to resort to single-site approximations. The recursion method allows one to take into account the effect of the local environment on electronic properties. Moreover, the convergence of various physical quantities calculated through recursion with the number of recursion steps and subsequent termination has been studied in great detail [27, 28]. Among the various advantages of the ASR in going beyond the single-site approximation is the possibility of inclusion of local lattice distortions [29] which is important in the case of alloys with size mismatch between components as in the case of Fe-Pt, Co-Pt and Ni-Pt.

An important aspect in understanding the interplay between magnetism and ordering in disordered transition metal alloys involves investigation of the influence of local environment, namely the short-range ordering (SRO) effect, on electronic and magnetic properties of these alloys. There have been determination of SRO parameters for different degrees of disorder using first principles techniques [30, 31, 32] or extraction of these parameters from experiments and analysis of their effect on electronic structure and properties [33, 34, 35]. SRO for a disordered binary alloy $A_xB_{1-x}$ is described, for example, by the Warren-Cowley parameter [36] which is defined as:

$$\alpha_r^{AB} = 1 - \frac{P_r^{AB}}{y}$$  \hspace{1cm} (1)

for the B atom occupying the r-th nearest neighbour site of the central A atom. $y = 1 - x$ denotes the macroscopic concentration of species B and $P_r^{AB}$ is the joint probability of finding a B atom anywhere in the r-th shell.

Mookerjee and Prasad [37] introduced a method for calculating the electronic structure of disordered alloys with short range order (SRO) which is based on a generalization of the augmented space theorem [25]. Saha et al [38] implemented this within the framework of recursion method. Later Ghosh et al [39] extended the technique to magnetic Co-Pt and Co-Pd systems. In present paper we have carried out charge-self-consistent calculations based on this generalized ASR technique to examine the short range ordering effect in Fe-Pt, Co-Pt and Ni-Pt systems.
The paper has been organized in the following manner. Section 2 is devoted to theoretical and computational details. The results of our study along-with comparison with existing experimental and theoretical studies have been discussed in section 3. We end the paper with the summary and conclusion in section 4. Some of the relevant equations of generalized augmented space recursion method have been put in the appendix.

2. Theoretical and Computational details

For ordered structures we have performed the total energy density functional calculations. The Kohn-Sham equations were solved in the local spin density approximation (LSDA) with von Barth-Hedin (vBH) [40] and Vosko-Wilk-Nusair (VWN) [41] exchange correlations as well as in the non-local (generalized gradient approximation (GGA)) Langreth-Mehl-Hu (LMH) [42] and Perdew-Wang exchange (PW) [43] correlations. The calculations have been performed in the basis of tight binding linear muffin-tin orbitals in the atomic sphere approximation (TB-LMTO-ASA) [44]-[47] including combined corrections. The calculations are semi-relativistic through inclusion of mass-velocity and Darwin correction terms. The k-space integration was carried out with $32 \times 32 \times 32$ mesh resulting 969 k points for cubic primitive structures and 2601 k points for tetragonal primitive structures in the irreducible part of the corresponding Brillouin zone. The convergence of the magnetic moments with respect to k-points have been checked. To have theoretical estimates of the equilibrium lattice parameters, we have carried out the minimization of the self-consistent TB-LMTO-ASA total energies varying lattice parameters for Fe-Pt, Co-Pt and Ni-Pt alloys at different concentrations.

Our disordered calculations are based on the generalized ASR technique [37]-[39],[48]-[49]. The Hamiltonian in the TB-LMTO minimal basis is sparse and therefore suitable for the application of the recursion method introduced by Haydock et al [26]. The ASR allows us to calculate the configuration averaged Green functions. It does so by augmenting the Hilbert space spanned by the TB-LMTO basis by the configuration space of the random Hamiltonian parameters. The configuration average is expressed exactly as a matrix element in the augmented space. A generalized form of this methodology is capable of taking into account the effect of short range order. Please see appendix for relevant equations. The initial guess TB-LMTO potential parameters for the self-consistency iterations for disordered alloy calculations are taken to be the potential parameters of pure constituents. In subsequent iterations the potential parameters are obtained from the solution of the Kohn-Sham equation

$$\left\{-\frac{\hbar^2}{2m} \nabla^2 + V^{\nu\sigma} - E\right\} \phi_{\nu}^\sigma(r_R, E) = 0$$ (2)
where,

\[ V^{\lambda\sigma}(r_R) = V^{\lambda\sigma}_{\text{core}}(r_R) + V^{\lambda\sigma}_{\text{har}}(r_R) + V^{\lambda\sigma}_{\text{xc}}(r_R) + V_{\text{mad}} \]  

(3)

The electronic position within the atomic sphere centered at \( R \) is given by \( r_R = r - R \). \( \sigma \) is the spin component. The core potentials are obtained from atomic calculations and are available for most atoms. For the treatment of the Madelung potential, we follow the procedure suggested by Kudrnovský et al [50] and use an extension of the procedure proposed by Andersen et al [44]. We choose the atomic sphere radii of the components in such a way that they preserve the total volume on the average and the individual atomic spheres are almost charge neutral. This ensures that total charge is conserved, but each atomic sphere carries no excess charge. In doing so, one needs to be careful about the sphere overlap which should be under certain limit so as to not violate the atomic sphere approximation.

In these calculations one also needs to be very careful about the convergence of Fermi energy as well as that of magnetic moments. In fact, errors can arise in the augmented space recursion because one can carry out only finite number of recursion steps and then terminate the continued fraction using available terminators. Also one chooses a large but finite part of the augmented space nearest neighbour map and ignores the part of the augmented space very far from the starting state. This is also a source of error.

The formulation of the augmented space recursion as described in appendix and used for the calculation in the present paper is the energy dependent augmented space recursion in which the disordered Hamiltonian with diagonal as well as off-diagonal disorder is recast into an energy dependent Hamiltonian having only diagonal disorder. We have chosen a few seed points across the energy spectrum uniformly, carried out recursion on those points and spline fit the coefficients of recursion throughout the whole spectrum. This enabled us to carry out large number of recursion steps since the configuration space grows significantly less faster for diagonal as compared with off diagonal disorder. Convergence of physical quantities with recursion steps have been discussed in detail earlier by Ghosh et al [51, 52].

We have checked the convergence of Fermi energy and magnetic moments with respect to recursion steps and the number of seed energy points for the case of NiPt\(_3\) system. We have found that the Fermi energy and magnetic moments converge beyond seven recursion steps and thirty five seed energy points. In our all calculations reported in the following have been carried out with eight recursion steps and thirty five seed energy points.
Table 1. The equilibrium lattice parameters in a.u. of FePt, CoPt and NiPt systems in ordered structures with various choices of exchange correlation functionals. See text for various abbreviations.

| x   | vBH | VWN | LMH | PW | Expt. |
|-----|-----|-----|-----|----|-------|
| Fe$_{1-x}$Pt$_x$ |     |     |     |    |       |
| 0.00 (BCC) | 5.28 | 5.30 | 5.36 | 5.54 | 5.406 [53] |
| (FCC) | 6.47 | 6.47 | 6.53 | 6.63 | 6.877 [53] |
| 0.25(L1$_2$) | 6.71 | 6.91 | 6.99 | 7.21 | 7.049 [54] |
| 0.50(L1$_0$) | a = 7.16 | a = 7.18 | a = 7.22 | a = 7.46 | a = 7.253 [53] |
|       | c = 6.94 | c = 6.94 | c = 7.02 | c = 7.26 | c = 7.020 [53] |
| 0.75(L1$_2$) | 7.25 | 7.27 | 7.30 | 7.54 | 7.313 [55] |
| Co$_{1-x}$Pt$_x$ |     |     |     |    |       |
| 0.00 (hex) | a = 4.65 | a = 4.66 | a = 4.70 | 4.83 | 4.728 [53] |
| (FCC) | 6.55 | 6.56 | 6.63 | 6.81 | 6.684 [53] |
| 0.25(L1$_2$) | 6.78 | 6.80 | 6.86 | 7.06 | 6.923 [54] |
| 0.50(L1$_0$) | a = 7.14 | a = 7.14 | a = 7.18 | a = 7.40 | a = 7.204 [53] |
|       | c = 6.78 | c = 6.78 | c = 6.86 | c = 7.08 | c = 7.007 [53] |
| 0.75(L1$_2$) | 7.21 | 7.22 | 7.25 | 7.50 | 7.240 [53] |
| Ni$_{1-x}$Pt$_x$ |     |     |     |    |       |
| 0.00 (FCC) | 6.54 | 6.55 | 6.61 | 6.80 | 6.646 [53] |
| 0.25(L1$_2$) | 6.77 | 6.78 | 6.84 | 7.05 | 6.890 [56] |
| 0.50(L1$_0$) | a = 7.16 | a = 7.16 | a = 7.18 | a = 7.42 | a = 7.209 [53] |
|       | c = 6.63 | c = 6.64 | c = 6.74 | c = 6.96 | c = 6.769 [53] |
| 0.75(L1$_2$) | 7.20 | 7.21 | 7.24 | 7.49 | 7.251 [56] |
| 1.00 (FCC) | 7.37 | 7.38 | 7.40 | 7.66 | 7.400 [53] |

3. Results and discussions

3.1. Lattice Parameters

In Table 1, we quote the values of equilibrium lattice parameters, obtained by minimizing the total energy with respect to the lattice parameters for L1$_2$ superstructures at 25 and 75% and L1$_0$ superstructure at 50% concentration of Pt in Fe-Pt, Co-Pt and Ni-Pt alloy systems with different choice of local as well as non-local exchange correlation potentials. The first comment is that non-local exchange correlation potentials seem to decrease overbinding and predict larger equilibrium lattice parameters than the local ones. The
PW seems to go overboard and give estimates of the equilibrium lattice parameters which are larger than the experimental values. The best agreement with experiment is found to be LMH.

3.2. Magnetism of Fe-Pt Alloys

3.2.1. Ordered Alloys: In Table 2, we show two sets of calculations for magnetic moments in ordered Fe-Pt alloys. In first set of calculations, we have calculated local as well as average magnetic moments corresponding to the theoretically estimated lattice parameters obtained via energy minimization procedure. In second set, calculations were done using experimental lattice parameters.

For Fe<sub>3</sub>Pt alloy in L<sub>12</sub> super-structure the use of non-local exchange correlation functionals LMH appear to give better agreement with experimental values [54] for local and average magnetic moments as compared to local exchange correlation functionals. This holds good for both the choices of lattice parameters. The results for average and local magnetic moments from previous works by Auluck <i>et al</i> [54] and Podgorny [55], both using TB-LMTO, are in agreement with our corresponding results as can be seen from Table 2. The differences seen with these results are primarily due to different computational details. Auluck <i>et al</i> [54] and Podgorny [55] have used frozen core approximation in their calculations without taking into account of f states for Pt. Podgorny and Auluck <i>et al</i> in their calculations used 286 and 84 k points in the irreducible part of the Brillouin Zone (BZ) respectively. On the other hand, our calculations are all electron calculations taking a spdf minimal basis for Pt and using 969 k points in irreducible part of BZ. The local magnetic moment on Pt sites obtained by Hasegawa <i>et al</i> [16] using augmented plane wave (APW) method is in exact agreement to the corresponding experimental value though their average magnetic moment and local magnetic moment on Fe sites are lower (by 0.20 \(\mu_B\) for average and 0.15 \(\mu_B\) for Fe sites) than the corresponding experimental estimates [54]. Our calculation using the vBH functional for the exchange correlation potential and theoretically estimated lattice parameter leads to the conclusion of a non-magnetic ground state which is in agreement with that found in a previous study by Kubler <i>et al</i> [61]. This once again emphasizes that magnetic moments are very sensitively dependent on the particular exchange-correlation functional used and the detailed accuracy of the numerical calculations.

For FePt alloys the local magnetic moment of Fe site in L<sub>10</sub> superstructure calculated using vBH exchange correlation potential and experimental lattice parameter shows closest agreement with experimental value [58]. The LMH based estimates of the local magnetic moment on Fe sites are rather large as compared with the one experimental datum available [58]. The experimental value for local magnetic moment of Pt in this concentration is not available. The experimentally estimated average magnetic moment is significantly lower than that of the calculated values using both local as well as non local exchange correlations. However all the available theoretical
Table 2. The local and average magnetic moments of Fe-Pt system in ordered structures with various choices of exchange correlation functionals.

| concentration of Pt | XC used/Expt/Ref. | magnetic moment ($\mu_B$/atom) of Fe | with eq. lat. par. | with expt. lat. par. |
|---------------------|-------------------|-------------------------------------|-------------------|---------------------|
|                     |                   | average | Pt | average | Fe | Pt | average |
| 0.00(BCC)           | vBH(this work)    | 2.15     | 2.25 |          |          |          |          |
|                     | VWN(this work)    | 2.21     | 2.30 |          |          |          |          |
|                     | LMH(this work)    | 2.29     | 2.33 |          |          |          |          |
|                     | PW(this work)     | 2.55     | 2.35 |          |          |          |          |
|                     | Expt. [57]        |          |      |          |          |          |          |
| 0.25(L12)           | vBH(this work)    | 0.00     | 0.00 | 0.00     | 2.57     | 0.32 | 2.01 |
|                     | VWN(this work)    | 2.46     | 0.29 | 1.92     | 2.64     | 0.34 | 2.06 |
|                     | LMH(this work)    | 2.63     | 0.33 | 2.06     | 2.70     | 0.35 | 2.11 |
|                     | PW(this work)     | 2.78     | 0.35 | 2.17     | 2.68     | 0.37 | 2.10 |
|                     | Auluck et al (vBH) [54] |          |      |          |          | 2.56 | 0.26 | 1.99 |
|                     | Podgorny (VWN) [55] | 2.51     | 0.26 | 1.95     |          |          |          |
|                     | Hasegawa [16]     |          |      |          | 2.50     | 0.50 | 2.0  |
|                     | Expt. [54]        |          |      |          | 2.70     | 0.50 | 2.15 |
| 0.50(L10)           | vBH(this work)    | 2.73     | 0.35 | 1.54     | 2.81     | 0.35 | 1.58 |
|                     | VWN(this work)    | 2.79     | 0.35 | 1.57     | 2.85     | 0.35 | 1.60 |
|                     | LMH(this work)    | 2.88     | 0.35 | 1.61     | 2.90     | 0.35 | 1.63 |
|                     | PW(this work)     | 3.01     | 0.36 | 1.69     | 2.86     | 0.36 | 1.61 |
|                     | Osterloh et al [58] |          |      |          | 2.92     | 0.38 |      |
|                     | Podgorny (VWN) [55] | 2.85     | 0.30 | 1.57     |          |          |          |
|                     | [Expt.] [58]      |          |      |          | 2.80     | 0.77 |      |
| 0.75(L12)           | Ferromagnetic calculation | vBH(this work)    | 2.99     | 0.31 | 0.98     | 3.10     | 0.32 | 1.02 |
|                     | VWN(this work)    | 3.12     | 0.32 | 1.02     | 3.15     | 0.33 | 1.03 |
|                     | LMH(this work)    | 3.19     | 0.34 | 1.05     | 3.20     | 0.34 | 1.06 |
|                     | PW(this work)     | 3.24     | 0.39 | 1.11     | 3.12     | 0.37 | 1.06 |
|                     | Podgorny [55]     | 3.22     | 0.34 | 1.06     |          |          |          |
|                     | Tohyama et al [59] |          |      |          | 4.21     | 0.33 |      |
|                     | Anti-ferromagnetic calculation | vBH(this work)    | 3.11     | 0.15 |          | 3.16     | 0.15 |      |
|                     | VWN(this work)    | 3.17     | 0.15 |          | 3.20     | 0.15 |      |
|                     | LMH(this work)    | 3.24     | 0.15 |          | 3.25     | 0.16 |      |
|                     | PW(this work)     | 3.31     | 0.17 |          | 3.18     | 0.16 |      |
|                     | Podgorny [55]     | 3.46     | 0.16 |          |          |          |      |
|                     | Tohyama et al [59] |          |      |          | 4.13     | 0.00 |      |
|                     | [Expt.][60]       |          |      |          | 3.3      |      |      |
estimates by different groups [55, 58] are significantly high, just like ours as compared
to the experimental estimate quoted by Osterloh [58]. The experimental result may
be interpreted assuming the magnetic moment at the Fe and Pt sites to be arranged
antiparallely giving rise to ferri-magnetic ground state. However, we were unable to show
any theoretical evidence for this and our calculations do predict a stable ferromagnetic
alignment as pointed out by Osterloh et al [58]. As in the case of Fe₃Pt, the slight
difference between the values obtained by Podgorny [55] and by us is again due to the
difference in the calculational details. In addition to using frozen core approximation
and neglect of f states in Pt site, Podgorny has assumed the cubic crystal structure
for FePt in L1₀ structure while in reality it is tetragonal. In our calculations, we have
assumed the experimentally observed tetragonal structure. The local magnetic moments
obtained by Osterloh et al [58] using augmented spherical wave method are higher than
ours as well as calculations by Podgorny [55].

The experimental ground state ordered magnetic phase FePt₃ is antiferromagnetic. We
have carried out calculations on this alloy both in the ferromagnetic as well as
the antiferromagnetic structures. We have found the total energy in the case of
antiferromagnetic structure is indeed lower than that of ferromagnetic structure. In
the ferromagnetic calculation, the local as well as average magnetic moment obtained
by Podgorny [55] using VWN exchange correlation potential with theoretical estimates
of lattice parameter is in close agreement with our corresponding value. The calculated
local magnetic moment on Fe sites by Tohyama et al [59] using an empirical tight
binding model is significantly higher than both ours and that of Podgorny [55]. Our
calculated magnetic moment on Fe site for the antiferromagnetic structure using PW
non local exchange correlation with theoretically estimated lattice parameter is in
closest agreement with the experimental value [60]. This is the one case where LMH
underestimates the staggered magnetization.

3.2.2. Disordered Alloys : In Figure 1, we compare our calculated disordered magnetic
moments using augmented space recursion with the available experimental values
taken from Landoldt series [62] as well as with CPA calculations. The average
magnetic moments agree quite well with the corresponding experimental values in all
concentrations. The numerical values of local as well as average magnetic moments
calculated using LMTO-CPA are in agreement with those obtained using the ASR. This
shows that the single site approximation like CPA works well for the Fe-Pt disordered
alloys. The average magnetic moments obtained by Drchal et al [63] using CPA matches
well for most concentrations though they deviate a bit at low concentrations of Pt. Our
calculations uses charge neutral spheres to reduce the effect of Madelung whereas Drchal
et al [63] have used equal Weigner Seitz radii of both constituents and the effect of
Madelung due to charge transfer was taken into account using screened impurity model
[63]. The local moment on the Fe sites increases towards the isolated Fe moment as the
concentration of Pt increases. This is an indication of the fact that local environmental
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**Figure 1.** Magnetic moments in disordered Fe-Pt alloy systems using two different configuration averaging methods namely augmented space recursion (ASR) and coherent potential approximation (CPA) as compared to available experimental values given in Landoldt series [62].

**Figure 2.** Magnetic moments as a function of lattice parameters for 25\% concentration of Pt in disordered Fe-Pt alloy. Circles, squares and diamonds denote local magnetic moment Fe site, local magnetic moment on Pt site and average magnetic moment respectively.
Table 3. Various estimates of the local and averaged magnetic moments in Bohr-magnetons for disordered Fe\textsubscript{75}Pt\textsubscript{25} alloy.

| Author               | Fe     | Pt     | Average |
|----------------------|--------|--------|---------|
| Expt. [64]           | 2.03±0.02 | 0.34±0.08 | 1.61±0.03 |
| Expt. [65]           | 2.75   | 0.45   | 2.20    |
| Expt. (a) [62]       | 2.02   |        |         |
| Expt. (b) [62]       |        |        | 2.27    |
| LMTO-CPA [63]        |        |        | 1.81    |
| KKR-CPA [66]         | 2.80   | 0.23   | 2.16    |
| LCAO-CPA [67]        |        |        | 2.17    |
| ASR (this work)      | 2.44   | 0.24   | 1.89    |

Effects are unimportant and consequently the CPA and ASR results agree closely.

In 25% concentration of Pt there is invar effect which shows anomalies in the thermal expansion. We have observed two minima of total energy one with a high moment and a large lattice constant 6.93 au and the other with a zero moment and small lattice constant 6.71 au. The total energy difference between the magnetic and non magnetic states is 2.4 mRyd/atom which is higher than the calculations by Drchal et al (0.7 mRyd/atom) and lower than that of Staunton et al (15.7 mRyd/atom). In Figure 2, we show the behaviour of magnetic moment as a function of lattice parameter which shows non magnetic to ferromagnetic transition at 6.71 a.u. Our calculated average as well as local magnetic moment on Fe and Pt sites corresponding to theoretically estimated lattice parameter 6.93 a.u. via total energy minimization on magnetic state are respectively 1.89, 2.44 and 0.24 \( \mu_B \).

Table 3 summarizes the known experimental and earlier theoretical results on disordered FePt with 25% Pt. The reported experimental results in this case differ to each other. The localized components of the magnetic moments for Fe (2.03 ± 0.02 \( \mu_B \)) and Pt (0.34±0.08 \( \mu_B \)) were estimated from spin polarized neutron diffraction measurements by Ito et al [64], while the magnetization measurements of Caporaletti and Graham [65] indicated moments of 2.75 and 0.45 \( \mu_B \) for Fe and Pt respectively. The values of average magnetic moments quoted in Landoldt series for different experiments are 2.02 and 2.27 \( \mu_B \). The theoretical estimates based on different methods also differ from one another. These differences are mainly due to the differences in the computational details chosen in each framework and also the approximations being used in each method.

For the 75% concentration of Pt our estimate of the magnetic moment on Fe sites...
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is higher than that measured by Kulikov et al [60] (which is about $2\mu_B$). In order to check the possible short range order effect, we have checked the variation of total energy as a function of short range order and found that the total energy decreases as short range order goes from positive (segregation side) to negative (ordering side) confirming this system as an ordering system. We have also checked the variation of the magnetic moments as functions of the SRO parameter. We find that both the local and average magnetic moments increase as the SRO parameter goes from the segregating to the ordering side. This is justified by the fact that the magnetic moment of Fe is enhanced when it is surrounded by Pt as we have seen in the ordered alloys. We therefore conclude that the discrepancy with the experimental data of Kulikov et al [60] cannot be due to the short range ordering effect, probably the other possible factors influencing the experimental results need to be considered.

3.3. Magnetism in Co-Pt Alloys

3.3.1. Ordered Alloys: Table 4 shows the calculated and experimental magnetic moments for ordered Co-Pt alloys. No experimental result is available for 25% of concentration of Pt in ordered case. The local as well as average magnetic moments obtained by Auluck et al [54] using vBH exchange correlation potential with experimental lattice parameter are lower (by 0.30 $\mu_B$ for Co site, 0.01 $\mu_B$ for Pt site and 0.23 $\mu_B$ for average) than our corresponding values which could be due to differences in computational details as mentioned in the case of Fe-Pt. The local as well as average magnetic moments obtained by Kootte et al [68] using localized spherical wave method using vBH exchange correlation and experimental lattice parameters are in agreement with our corresponding values.

For 50% concentration of Pt, our results agree well with the previous theoretical results [54, 68, 69] within the errorbars of different calculational schemes and are in reasonable agreement with the observed magnetic moments [68] as summarized in Table 4.

For 75% concentration of Pt, the calculated local magnetic moments on Co site and that of average magnetic moments using possible exchange correlations with both theoretically estimated as well as experimental lattice parameters are on higher side as compared to the experimental estimates [68]. The calculated local moment of Pt using vBH exchange correlation and theoretically estimated lattice parameter is close to the experimental value [68]. The theoretical estimates for local as well as average magnetic moments by Auluck et al [54] and Kootte et al [68] as in 50% concentration of Pt are in agreement with our corresponding estimates as can be seen from Table 4. The slight differences seen are again due to the differences in computational details. The local magnetic moments calculated by Tohyama et al [59] using tight binding method are significantly higher than ours as well as experimental estimates which can be seen from Table 4. The recent work by Lange et al [70] using fully relativistic TB-
Table 4. The local and average magnetic moments of Co-Pt system in ordered structures with various choices of exchange correlation functionals.

| concentration of Pt | XC used/Expt/Ref. | magnetic moment ($\mu_B$/atom) of Co | magnetic moment ($\mu_B$/atom) of Pt | with eq. lat. par. | with expt. lat. par. |
|---------------------|-------------------|------------------------------------|------------------------------------|-------------------|-------------------|
|                     |                   | Co       | Pt       | average | Co       | Pt       | average |
| 0.00(hex)           | vBH(this work)    | 1.55     | 1.60     |         |           |           |         |
|                     | VWN(this work)    | 1.58     | 1.62     |         |           |           |         |
|                     | LMH(this work)    | 1.62     | 1.64     |         |           |           |         |
|                     | PW (this work)    | 1.67     | 1.63     |         |           |           |         |
|                     | Expt. Kootte [68] |         |         | 1.58    |           |           |         |
| (FCC)               | vBH(this work)    | 1.57     | 1.62     |         |           |           |         |
|                     | VWN(this work)    | 1.60     | 1.64     |         |           |           |         |
|                     | LMH(this work)    | 1.65     | 1.67     |         |           |           |         |
|                     | PW (this work)    | 1.70     | 1.66     |         |           |           |         |
|                     | Expt. Kootte [68] |         |         | 1.61    |           |           |         |
| 0.25(L1_2)          | vBH(this work)    | 1.56     | 0.35     | 1.26    | 1.69     | 0.39     | 1.37    |
|                     | VWN(this work)    | 1.63     | 0.37     | 1.32    | 1.73     | 0.40     | 1.40    |
|                     | LMH(this work)    | 1.73     | 0.40     | 1.40    | 1.76     | 0.39     | 1.42    |
|                     | PW (this work)    | 1.80     | 0.39     | 1.45    | 1.74     | 0.41     | 1.41    |
|                     | Auluck et al [54] |         |         | 1.39    | 0.38     | 1.14    |
|                     | Kootte [68]       |         |         | 1.64    | 0.36     | 1.32    |
| 0.50(L1_0)          | vBH(this work)    | 1.69     | 0.38     | 1.03    | 1.79     | 0.38     | 1.09    |
|                     | VWN(this work)    | 1.74     | 0.39     | 1.07    | 1.83     | 0.39     | 1.11    |
|                     | LMH(this work)    | 1.82     | 0.40     | 1.11    | 1.87     | 0.39     | 1.13    |
|                     | PW (this work)    | 1.91     | 0.42     | 1.16    | 1.83     | 0.40     | 1.12    |
|                     | Auluck et al [54] |         |         | 1.85    | 0.38     | 1.12    |
|                     | Kootte [68]       |         |         | 1.69    | 0.37     | 1.03    |
|                     | Uba [69]          |         |         | 1.60    | 0.30     |         |
|                     | Expt. Cable [68]  |         |         |         | 1.70    | 0.25     | 0.98    |
|                     | Expt. van Laar[68]|         |         |         | 1.60    | 0.30     | 0.95    |
| 0.75(L1_2)          | vBH(this work)    | 1.71     | 0.25     | 0.62    | 1.74     | 0.26     | 0.64    |
|                     | VWN(this work)    | 1.75     | 0.26     | 0.63    | 1.82     | 0.27     | 0.65    |
|                     | LMH(this work)    | 1.83     | 0.28     | 0.67    | 1.87     | 0.28     | 0.68    |
|                     | PW (this work)    | 1.95     | 0.36     | 0.76    | 1.82     | 0.31     | 0.69    |
|                     | Auluck et al [54] |         |         | 1.85    | 0.25     | 0.65    |
|                     | Kootte et al [68] |         |         | 1.69    | 0.27     | 0.63    |
|                     | Tohyama et al [59]|         |         | 2.88    | 0.38     |         |
|                     | Lange et al [70]  |         |         | 1.72    | 0.25     | 0.62    |
|                     | Uba et al [69]    |         |         | 1.74    | 0.24     |         |
|                     | Expt. Menginger [68]|     |         | 1.64    | 0.26     | 0.61    |
|                     | Expt. Lange et al [70]| |         |         | 1.60    | 0.30     | 0.70    |
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LMTO with vBH exchange correlation and theoretically estimated lattice parameter report the local as well as average magnetic moment close to our corresponding values. Their experimental value for average magnetic moment matches with our corresponding calculated value using non local exchange correlation potentials and experimentally estimated lattice parameter. The supercell calculation of Uba et al [69] with LMTO using vBH exchange correlation potential and experimental lattice parameter matches well with our corresponding value.

3.3.2. Disordered Alloys: In Figure 3, we have shown the comparison of local magnetic moments of Co and Pt as well as average magnetic moment of disordered Co-Pt system. Calculations have been done both within ASR and CPA schemes using vBH exchange correlations. The comparison with experimental results for average magnetic moment taken from Landoldt series [62] matches well with our calculations. The calculated magnetic moments with augmented space recursion method are in better agreement with experimental results than that of coherent potential approximation method. From this Figure we can see that the local moment of Co obtained by ASR calculation is almost constant with the increase of concentration of Pt which is the signature of weak local environmental effect on Co site. This finding is in agreement with that of Sanchez et al [71] who also pointed out almost constant magnetic moment at Co site as a function of Pt concentration. The average magnetic moments obtained by Koepernik et al [67] using linear combination of atomic orbitals combined with coherent potential approximation (LCAO-CPA) method taking into account both diagonal and off diagonal disorder effects show close agreement with our results (except 20% concentration of Pt where the value obtained by Koepernik et al [67] is in higher side than ours) using augmented space recursion (ASR).

The results obtained by Ebert et al [72] using Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) are higher than ours as well as experimental values. The calculations by Ebert et al [72] using KKR-CPA with single site approximation were though fully relativistic did not take into account lattice relaxation and off diagonal disorder effects. Therefore it is not surprising that our calculations show better agreement with experiments. According to the calculation of Shick et al [73] using fully relativistic linearized muffin-tin orbital based coherent potential approximation (LMTO-CPA) method the average and partial magnetic moments of Co and Pt in Co\textsubscript{50}Pt\textsubscript{50} are 1.07, 1.79 and 0.35 \(\mu_B\) respectively while the value of Ghosh et al [39] using ASR are 1.05, 1.85 and 0.24 \(\mu_B\) for the same. Our values in this case are 1.05, 1.80 and 0.29. The reason behind the differences seen in between LMTO-CPA of Shick et al [73] and ASR is again same as explained above in the connection with KKR-CPA and ASR. Though the calculations by Ghosh et al [39] (using theoretically estimated lattice parameter) and ours (using experimental lattice parameter) used same ASR method, ours being charge neutral and self consistent show better agreement for local magnetic moments with corresponding charge neutral and self consistent calculations.
In order to investigate the possible influence of short range order on the disordered magnetic moments, we have performed a complete investigation in terms of the total energy calculations as a function of short range order parameter. Like Fe-Pt, Co-Pt also shows a tendency to order. We have also checked the variation of magnetic moments as a function of SRO parameter and find almost constant local as well as average magnetic moments as SRO parameter goes from segregating side to ordering side confirming the very little effect of short range order on magnetism of Co-Pt alloy system.

3.4. Magnetism in Ni-Pt Alloys

3.4.1. Ordered Alloys: In Table 5, we show two sets of ordered calculations in Ni-Pt alloys using possible local as well as non local exchange correlation potentials one with theoretically calculated lattice constants via energy minimization procedure and other using experimental lattice parameters.

For 25% concentration of Pt, the calculated local as well as average magnetic
Table 5. The local and average magnetic moments of Ni-Pt system in ordered structures with various choices of exchange correlation functionals.

| Concentration of Pt | XC used/Expt/Ref. | magnetic moment (\(\mu_B/\text{atom}\)) of Ni | Pt | average | Ni | Pt | average |
|---------------------|-------------------|---------------------------------------------|-----|---------|-----|-----|---------|
| 0.00(FCC)           | vBH(this work)    | 0.61                                        |     | 0.62    |     |     |         |
|                     | VWN(this work)    | 0.62                                        |     | 0.64    |     |     |         |
|                     | LMH(this work)    | 0.64                                        |     | 0.65    |     |     |         |
|                     | PW(this work)     | 0.66                                        |     | 0.64    |     |     |         |
|                     | Expt. [57]        | 0.62                                        |     |         |     |     |         |
| 0.25(L1₂)           | vBH(this work)    | 0.50                                        | 0.24| 0.43    | 0.57| 0.27| 0.49    |
|                     | VWN(this work)    | 0.54                                        | 0.26| 0.47    | 0.60| 0.29| 0.52    |
|                     | LMH(this work)    | 0.62                                        | 0.29| 0.53    | 0.65| 0.30| 0.56    |
|                     | PW(this work)     | 0.71                                        | 0.36| 0.63    | 0.63| 0.32| 0.56    |
|                     | Singh [74]        | 0.58                                        | 0.27| 0.50    |     |     |         |
| [Expt. Parra et al] | [75]              |                                             | 0.49| 0.25    | 0.43|     |         |
| 0.50(L1₀)           | vBH(this work)    | 0.00                                        | 0.00| 0.00    | 0.33| 0.17| 0.25    |
|                     | VWN(this work)    | 0.06                                        | 0.03| 0.05    | 0.46| 0.23| 0.34    |
|                     | LMH(this work)    | 0.55                                        | 0.27| 0.41    | 0.65| 0.31| 0.48    |
|                     | PW(this work)     | 0.72                                        | 0.34| 0.53    | 0.63| 0.32| 0.48    |
|                     | Singh [74]        | 0.60                                        | 0.27| 0.44    |     |     |         |
| [Expt (Parra et al)]| [75]              |                                             | 0.28| 0.17    | 0.22|     |         |
| 0.75(L1₂)           | vBH(this work)    | 0.47                                        | 0.09| 0.18    | 0.55| 0.10| 0.21    |
|                     | VWN(this work)    | 0.50                                        | 0.09| 0.20    | 0.57| 0.11| 0.22    |
|                     | LMH(this work)    | 0.55                                        | 0.11| 0.22    | 0.61| 0.12| 0.24    |
|                     | PW(this work)     | 0.65                                        | 0.16| 0.28    | 0.58| 0.12| 0.24    |
|                     | Singh [74]        | 0.58                                        | 0.10| 0.22    |     |     |         |

Moments in ordered Ni-Pt alloys obtained using vBH local exchange correlation potential in theoretically calculated lattice parameter show very good agreement with experimental values [75]. The values obtained by Singh [74] in the same case are higher in comparison to ours and experimental estimate [75]. Singh's [74] calculations seemingly did not include the \(f\) states in Pt in the TB-LMTO basis. Our test calculations without including \(f\) states of Pt also show higher values of magnetic moments for this concentration of Ni-Pt alloy.

For 50% concentration of Pt in L1₀ structure calculated local as well as average magnetic moments using vBH exchange correlation potential with the use
of experimental lattice parameter is closest to the experimental estimate \cite{75}. Our calculations with the use of local exchange correlations and theoretically estimated lattice parameters lead to non magnetic ground state which is in agreement with that found in previous study by Dahmani et al \cite{76}. In our calculations we have taken into account the tetragonal distortion as in the case of Fe-Pt and Co-Pt alloys in L1\textsubscript{0} structure.

For 75% concentration of Pt, for NiPt\textsubscript{3} alloy in L1\textsubscript{2} structure there is no experimental result available. For this concentration we have got higher local magnetic moment of Ni than at the 50% concentration of Pt. This was obtained while using local exchange correlations. In this case if we use non local exchange correlations then we get the decrease of local magnetic moment of Ni on going from 50% to 75% concentration of Pt. The average as well as local magnetic moments on Pt sites show the decreasing tendency using both local as well as non local exchange correlations with theoretically as well as experimentally estimated lattice constants.

The calculations by Singh \cite{74} using vBH exchange correlations and theoretically estimated lattice parameters show that the local magnetic moment of Ni increases while going from 25% to 50% and decreases while going from 50% to 75% concentration of Pt. The calculations by Singh \cite{74} did not take into account the tetragonal distortion for 50% concentration of Pt which means putting lattice parameters $a = c$ which is not the right ground state structure. For a test we also repeated our calculation without taking into account the tetragonal distortion for 50% concentration of Pt using vBH local exchange correlation potentials and theoretically estimated lattice constants and we also observed same trend as Singh obtained. However, for the calculation taking into account the degrees of freedom for tetragonal distortion we found that the magnetic moments vanish with the use of local exchange correlation potentials in theoretically estimated lattice parameters.

3.4.2. Disordered Alloys: We have plotted the local and average magnetic moments of disordered Ni-Pt system in Figure 4. The comparison of calculated disordered magnetic moments using augmented space recursion (ASR) method with vBH exchange correlation potentials and experimental lattice parameter matches well with experimental values \cite{75} in all concentrations except 55% and 57% of Pt. Our calculations of magnetic moments using coherent potential approximation (CPA) method using vBH exchange correlation potential and experimental lattice parameters are very different than the calculations using ASR method and experimental estimates \cite{75}. Using CPA the local magnetic moments of Ni donot even follow the trend of corresponding experimental estimates. ASR being capable to go beyond single site approximation taking into account lattice relaxation and off diagonal disorder effect which is very important in NiPt alloys as was shown in our previous paper \cite{77} provides better agreement with experiment than CPA. Our calculated values for 55% and 57% concentration of Pt using ASR method are in higher side in comparison to the
experimental estimates which leads us to suspect the presence of short range ordering effect. We performed calculations incorporating short range order for all concentration of Pt in this system and found that the magnetic moments of Ni decreases by appreciable fraction for 55% and 57% concentration of Pt. The moment of Pt increases slightly. These give rise to the decrease of average magnetic moment in these concentrations. Calculations incorporating the effect of short range order agrees well with experimental estimate of Parra et al [75].

4. Summary and conclusions

To summarize, our study for ordered alloys to investigate the role played by different possible exchange correlation functionals shows that choice of the exchange-correlation potential has considerable effect on the values of the equilibrium lattice constants as well as magnetic moments

The present study on disordered alloys shows that the single site approximation based methods work reasonably well for Fe-Pt systems and is in close agreement with our ASR predictions. For the Co-Pt system, the CPA begins to deviate from the ASR. CPA based calculations show slight increase in the local magnetic moment of Co with increasing Pt concentration, while the ASR shows almost constant behaviour. This indicates the signature of weak local environmental effect on Co sites.

It is in the Ni-Pt alloy that CPA shows the largest deviation from the ASR. The CPA estimates of the magnetic moments are quite different from the experimental values. It predicts increase of the local magnetic moment on Ni with increasing Pt
concentration, whereas experimentally the reverse behaviour is observed. In the absence of local environment effects, increase of Pt concentration in Ni-Pt should lead to increase in the local Ni moment, since isolated clusters of Ni in Pt become more probable. This leads to narrowing of the local density of states on Ni and consequently according to the Stoner picture, an increase in the local Ni moment. Finally in the dilute limit, this local moment should approach the moment of an isolated Ni atom. This behaviour is certainly seen in Fe-Pt alloys. However, the fragile moment on Ni seems to need at least 50% Ni atoms in its nearest neighbour environment, otherwise it loses its local moment. This is indeed what one sees in experiment and is a strong indicator of large local environmental effect in Ni-Pt. The CPA predicts increase of the local magnetic moment on Ni with increasing Pt concentration. This is expected, since the CPA does not take into account the effect of local environment. The ASR, however, predicts the correct trend with increasing Pt concentration. The estimates of the actual value of the local magnetic moments are also much better.

Our total energy calculation as a function of short range order confirms the ordering tendency in these systems. The calculation of magnetic moments as a function of short range order shows that its effect is small on the magnetism in Fe-Pt and Co-Pt disordered alloys but significant on the magnetism of disordered Ni-Pt.

Finally, the numerical details of calculations, convergence with the number of k-points in the Brillouin zone integrations, choice of atomic sphere radii, proper convergences in the CPA and the ASR, the proper choice of the minimal basis set in the TB-LMTO, all of these affect the actual values of the estimated magnetic moments.

Appendix A.

Details of the methodology of augmented space recursion has been presented in an earlier papers referred in the text. Here we shall quote the key results of TBLMTO-ASR generalized to take in account the short-range ordering effect. The augmented space Hamiltonian including short range order can be written as

\[
\hat{H} = H_1 + H_2 \sum_R P_R \otimes P_R^R + H_3 \sum_R P_R \otimes (T_{\uparrow\uparrow}^R + T_{\downarrow\downarrow}^R) \\
+ H_4 \sum_{R,R'} T_{RR'} \otimes I + \alpha H_2 \sum_{R,R'} P_{R'} \otimes P_1 \otimes (P_{R''} - P_{R''}^\uparrow) \\
+ H_5 \sum_{R'} P_{R'} \otimes P_1 \otimes (T_{\uparrow\downarrow}^{R'} + T_{\downarrow\uparrow}^{R'}) \\
+ H_6 \sum_{R'} P_{R'} \otimes P_1 \otimes (T_{\uparrow\uparrow}^{R'} + T_{\downarrow\downarrow}^{R'}) \\
+ \alpha H_2 \sum_{R'} P_{R'} \otimes (T_{\uparrow\downarrow} + T_{\downarrow\uparrow}) \otimes (P_{R''} - P_{R''}^\uparrow) \\
+ H_7 \sum_{R'} P_{R'} \otimes (T_{\uparrow\downarrow} + T_{\downarrow\uparrow}) \otimes (T_{\uparrow\uparrow}^{R''} + T_{\downarrow\downarrow}^{R''})
\] (A.1)
where $R''$ belong to the set of nearest neighbours of the site labeled $R$, at which the local density of states will be calculated. $P$'s and $T$'s are the projection and transfer operators either in the space spanned by the tight-binding basis $\{|R\rangle\}$ or the configuration space associated with the sites $R$ spanned by $\{|\uparrow R\rangle, |\downarrow R\rangle\}$ as described in [49].

\[ |\uparrow R\rangle = \sqrt{x}|A_R\rangle + \sqrt{y}|B_R\rangle \quad |\downarrow R\rangle = \sqrt{y}|A_R\rangle - \sqrt{x}|B_R\rangle \]

The different terms of the Hamiltonian are given below.

\[
H_1 = A(C/\Delta)\Delta_{\lambda} - (EA(1/\Delta)\Delta_{\lambda} - 1) \\
H_2 = B(C/\Delta)\Delta_{\lambda} - EB(1/\Delta)\Delta_{\lambda} \\
H_3 = F(C/\Delta)\Delta_{\lambda} - EF(1/\Delta)\Delta_{\lambda} \\
H_4 = (\Delta_{\lambda})^{-1/2}S_{RR'}(\Delta_{\lambda})^{-1/2} \\
H_5 = F(C/\Delta)\Delta_{\lambda}[(1-\alpha)(x+y) + \sqrt{(1-\alpha)y(x+y)} - 1] \\
H_6 = F(C/\Delta)\Delta_{\lambda}[(1-\alpha)(x+y)/x + x(1-\alpha)(y+\alpha x)/y - 1] \\
H_7 = F(C\Delta)\Delta_{\lambda}[(1-\alpha)y(x+y) - \sqrt{(1-\alpha)x(y+\alpha x)}] \\
\]

where
\[
A(Z) = xZ_A + yZ_B \\
B(Z) = (y-x)(Z_A - Z_B) \\
F(Z) = \sqrt{xy}(Z_A - Z_B) \\
\]

$\alpha$ is the nearest neighbour Warren-Cowley parameter described earlier. $\lambda$ labels the constituents A or B in case of binary AB alloy. $C$'s and $\Delta$'s are the potential parameters describing the atomic scattering properties of the constituents and $S$ is the screened structure constant describing the underlying lattice which is face-centered cubic (FCC) in the present case. For convenience, all the angular momentum labels have been suppressed, with the understanding that all potential parameters are 9\times9 matrices (for an spd minimal basis set). We note that in absence of short-ranged order ($\alpha = 0$), the terms $H_5$ to $H_7$ disappear and the Hamiltonian reduces to the standard one described earlier [49].

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