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Electronic structure, Fermi surface, and Curie temperature calculations for the Co-Pt system

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Three ordered compounds of the Co-Pt system, namely Co_3Pt, CoPt, and $CoPt_3$, are ferromagnetic in nature. We have performed band-structure calculations for these compounds using the *ab initio* linear muffin-tin orbitals method. Our results are in agreement with the experimentally measured ground-state properties such as density of states, electronic specific-heat coefficient, and magnetic moments. The band-structure results along with the Mohn Wohlfarth theory are used to calculate the Curie temperature of these compounds. Our calculated values of the Curie temperature are in agreement with the experimental data of the Curie temperature. We also report calculations for the Fermi surface of Co_3Pt and $CoPt_3$ with the aim to ascertain how the Fermi surface is altered when Co(Pt) is replaced by Pt(Co), keeping the same crystal structure.
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I. INTRODUCTION

The interplay between magnetic properties and chemical ordering in the $Co_{1-X}Pt_X$ system has been investigated theoretically and experimentally by many workers. Sanchez *et al.*[1] have discussed the experimental results for the Curie temperature, magnetization, and paramagnetic susceptibility in ordered and disordered states of Co-Pt system within the framework of statistical models. Three ordered phases are known to exist in the Co-Pt system at lower temperatures with the stoichiometric concentrations as Co_3Pt, CoPt, and $CoPt_3$. The ordered phases have tetragonal symmetry of $L1_0$ type for CoPt and cubic symmetry of $L1_2$ type for Co_3Pt and $CoPt_3$. The phase diagram of the Co-Pt system shows a fcc structure with a degree of atomic disorder which increases with the increasing temperature.[1–3]

Zeper *et al.*[4] performed magnetic anisotropy and magneto-optical Kerr effect measurements on vapor-deposited Co/Pt multilayers. These Co/Pt layered structures are promising candidates for reversible information storage based on magneto-optical technology. The ordered CoPt phase, with Co on the corners and Pt in the center of the tetragonal unit cell has alternating planes of Co and Pt in the [001] direction and thus this phase can be considered as a (1:1) multilayer structure of Co and Pt. This ordered CoPt phase is one of the hardest permanent magnets known,[5] especially with respect to coercivity H_C which can reach values up to 5000 Oe depending on the aging process. The chemical ordering and magnetic properties of the Co-Pt system have been extensively studied by Leroux[2] and Sanchez *et al.*[1] At temperatures above 1400 K, the paramagnetic A1 phase is stable for all concentrations. For temperatures around 1400 K and on the Co-rich side, the system orders ferromagnetically but stays atomically disordered. An ordered Co_3Pt phase ($L1_2$) has been reported[6,7] to occur with a congruent temperature of approximately 840 K. At $x=0.5$, a CoPt phase ($L1_0$) is observed with a maximum ordering temperature of 1100 K. Furthermore, a $CoPt_3$ phase ($L1_2$) occurs with a maximum ordering temperature of 1000 K. $CoPt_3$ has a Curie temperature of approximately 290 K.[3] The magnetic moments on Co and Pt sites in $CoPt_3$, determined by Menzinger and Paoletti[8] using neutron-diffraction measurements, are $\mu(\mathrm{Co})=1.64\mu_B$ and $\mu(\mathrm{Pt})=0.26\mu_B$. The saturation magnetization, as determined from bulk magnetization measurements, is $M_s=2.43\mu_B$ per unit cell. Ordered CoPt has a Curie temperature of 710 K.[2] The saturation magnetization, as determined by van Laar (reported in Ref. 9) is $M_s=1.90\mu_B$ per unit cell. Neutron-diffraction measurements show a magnetic moment on both types of atoms. Van Laar assumed the moment on the Pt atoms to be larger than $0.3\mu_B$ and the moment on the Co atoms to be smaller than $1.6\mu_B$, however, the measurements of Cable (reported in Ref. 9) give a moment of $0.25\mu_B$ on Pt and about $1.7\mu_B$ on Co.

Tohyama, Ohta, and Shimizu[10] have studied the electronic and magnetic properties of ordered TPt_3 compounds ($T=$Ti, V, Cr, Mn, Fe, and Co) using tight-binding-type self-consistent spin-polarized band calculations. They have reported a large value of charge transfer induced by spin polarization for $CoPt_3$ along with their results for density of states (DOS), magnetic moment, and electronic specific-heat coefficient, etc. For CoPt, calculations are reported by Ohta, Miyauchi, and Shimizu[11] where they have discussed the ground-state properties such as the magnetic phase stability and the local moments in TPt ($T=3d$ transition metals) compounds. A systematic study of Co-Pt system by linearized spin-wave (LSW) method has been done by Kootte, Haas, and Degroot.[9] They have reported important quantitative differences with the results from previous calculations.[10,11] Their calculations reveal that there is an appreciable spin polarization of the Pt atoms in all three ordered compounds (

Co_3Pt, CoPt, $CoPt_3$) which cannot be explained by the simple hybridization of nonmagnetic Pt states with magnetic Co states.

In this paper a detailed and systematic study of the ordered intermetallic compounds Co_3Pt, CoPt, and $CoPt_3$ is presented. The band-structure (BS) calculations along with the Fermi surface (FS) studies are reported. The effect of chemical environment on FS of Co-Pt system is studied. Following our success in studying the Curie temperature (T_C) and its pressure variation for Fe_3Pt,[12] we have also calculated T_C and reported the calculations of the same for the ordered compounds Co_3Pt, CoPt, and $CoPt_3$. We are also concerned with the FS topology and how the FS alters when Co and Pt are interchanged keeping the crystal structure to be same. In the next section, the method of calculation is described. Section III deals with results and discussions, and main conclusions are given in Sec. IV.

II. METHOD OF CALCULATIONS

The linear muffin-tin orbitals (LMTO) method within atomic sphere approximation (ASA) has been used along with combined correction terms.[13] The calculations are semirelativistic in nature and are performed within frozen-core approximation. The von Barth–Hedin exchange-correlation (XC) potential[14] is used. Within spheres around each atomic center the wave function is expanded in muffin-tin orbitals. The basis set includes $s,p,$ and d orbitals at each site. The one-electron self-consistent potentials are obtained by performing iterations on a mesh of 84 k points in the irreducible 1/48th part of the Brillouin zone (BZ). We have used the tetrahedron method[15] to calculate the density of states (DOS).

To calculate T_C, we have used the model proposed by Mohn and Wohlfarth[16] (MW), where they have derived an expression for calculating T_C:

$$\frac{T_C^2}{T_C^{S^2}}+\frac{T_C}{T_{\mathrm{SF}}}-1=0, \tag{1}$$

where T_C^S, the Stoner Curie temperature, is the temperature at which

$$I(E_F)_{-}\int_{-\infty}^{\infty} N(E)dE=1, \tag{2}$$

where $N(E)$ is the DOS per atom per spin[17] and $I(E_F)$ is the Stoner parameter at the Fermi energy (E). T_{SF} is the characteristic temperature describing the influence of spin fluctuations and is given by

$$T_{\mathrm{SF}}=\frac{M_0^2}{10k_B\chi_0}, \tag{3}$$

where M_0 and χ_0 are the equilibrium magnetic moment at $T=0$ and the exchange enhanced susceptibility at equilibrium, respectively, given as

$$M_0^2=\frac{1}{N}\sum_{i=1}^{N} M_i^2 \quad \text{and} \quad \chi_0=\frac{1}{N}\sum_{i=1}^{N}\chi_i; \tag{4}$$

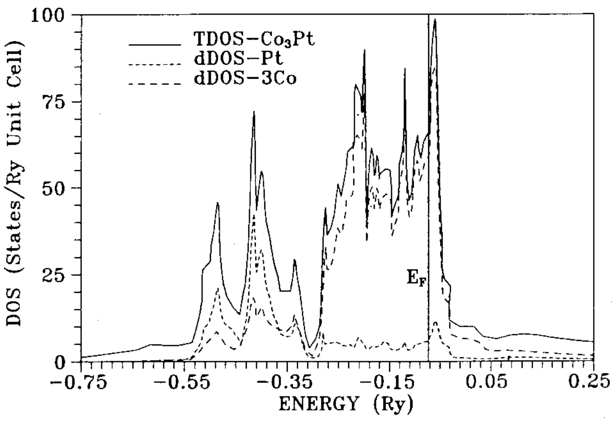

FIG. 1. Total density of states (TDOS) for Co_3Pt in the paramagnetic phase along with density of states at d site (d DOS) for three Co and Pt atoms.

N is the number of atoms in the unit cell. χ_i is calculated using the relation given by Wohlfarth[18] and Gersdorf:[19]

$$\chi_0^{-1}=\frac{1}{2\mu_B^2}\left(\frac{1}{2N^{\uparrow}(E_F)}+\frac{1}{2N^{\downarrow}(E_F)}-I\right); \tag{5}$$

I is the Stoner parameter and $N\!\uparrow\!(E_F)$ and $N\!\downarrow\!(E_F)$ are the spin-down and spin-up DOS per magnetic atom. The Stoner theory, which takes into account only single-particle excitations, is valid for systems where T_{SF} is large compared with T_C. In a pure spin-fluctuation-dependent description of magnetic properties, the Stoner Curie temperature is always assumed to be infinite[20] and T_C is then equal to T_{SF}.

III. CALCULATIONAL DETAILS AND RESULTS

A. Paramagnetic Co_3Pt, CoPt, and $CoPt_3$

Ordered Co_3Pt and $CoPt_3$ has the closely packed Cu_3Au structure with four atoms per unit cell. The atomic position (0 0 0) is occupied by Pt and Co_3Pt and by Co in $CoPt_3$. The three Co (Pt) atoms in Co_3Pt ($CoPt_3$) occupy the sites ($\frac{1}{2}$ $\frac{1}{2}$ 0), ($\frac{1}{2}$ 0 $\frac{1}{2}$), and (0 $\frac{1}{2}$ $\frac{1}{2}$). The (1:1) compound CoPt crystallizes in tetragonal structure with four atoms per unit cell; however, the two Co atoms are not equivalent. In other

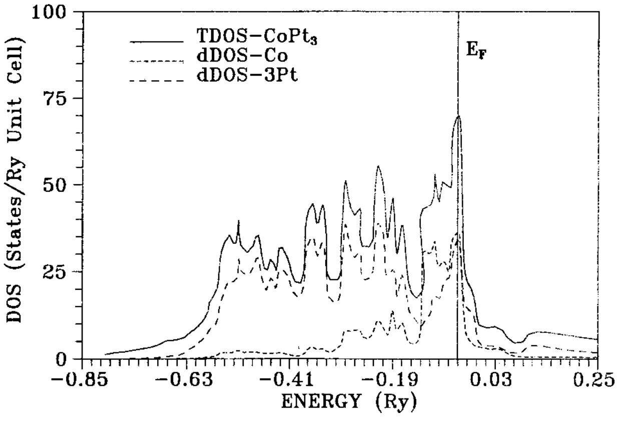

FIG. 2. Total density of states (TDOS) for $CoPt_3$ in the paramagnetic phase along with density of states at d site (d DOS) for Co and three Pt atoms.

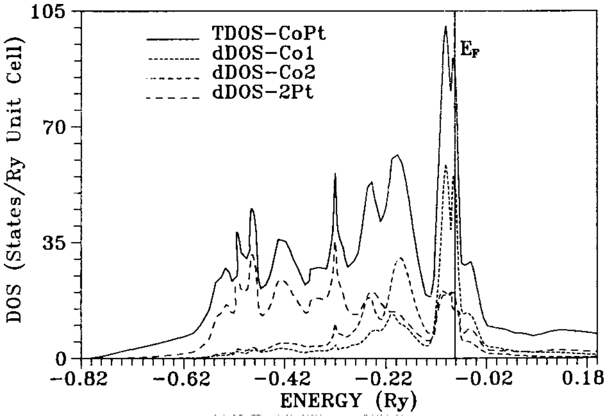

FIG. 3. Total density of states (TDOS) for CoPt in the paramagnetic phase along with density of states at *d* site (*d* DOS) for Co1, Co2, and two Pt atoms.

words, there are three kinds of atoms in the unit cell of CoPt with atomic positions of (0 0 0) for Co(I), ($\frac{1}{2}$ $\frac{1}{2}$ 0) for Co(II), and (0 $\frac{1}{2}$ $\frac{1}{2}$), ($\frac{1}{2}$ 0 $\frac{1}{2}$) for Pt atoms. The experimental lattice parameter for Co_3Pt and $CoPt_3$ are 3.6636 and 3.8310 Å,[21] respectively, which correspond to Wigner-Seitz (WS) radii of 2.7061 and 2.5297 a.u., respectively. For CoPt, the experimental lattice parameters are $a = 3.803$ Å and $c = 3.701$ Å. Corresponding to these parameter the WS radius in case of CoPt is 2.7837 a.u. We have performed our calculations using these values of WS radii. Figures 1, 2, and 3 show the total DOS and *d* DOS at Co and Pt sites for Co_3Pt, $CoPt_3$, and CoPt, respectively. In each case Co-*d* states are contributing significantly at and near E_F. However, at lower energies, contributions from the Pt-*d* states are important. The *l*-decomposed DOS at E_F are displayed in Table I. The total DOS at E_F for Co_3Pt, $CoPt_3$, and CoPt are 64.50, 76.82, and 87.41 states/Ry unit cell. High values of $N(E_F)$ led us to check the stability of this state. We calculated the Stoner product for each compound and found $IN(E_F) > 1$ in each case. This suggests the instability of the paramagnetic (PM) state, in accordance with the experimental evidences. As the PM state is not the stable state for these compounds we did not calculate γ values and also BS's of these compounds are ignored.

TABLE I. Wigner-Seitz radius (SWS), total energy (in mRy), total density of states (TDOS), and *l*-projected density of states at the Fermi energy (in states per Ry unit cell), and the coefficient of electronic specific heat γ (in mJ/mol K^2) for *paramagnetic* Co_3Pt, $CoPt_3$, and CoPt.

	Co_3Pt	$CoPt_3$	CoPt
SWS	2.7061	2.8297	2.7837
Total energy	−236.41	−224.43	−230.39
Total DOS	64.49	76.82	87.41
Co-*s*	0.06	0.07	0.13, 0.12
-*p*	0.23	0.24	0.44, 0.20
-*d*	19.23	39.43	48.96, 16.67
Pt-*s*	0.06	0.11	0.67
-*p*	0.21	0.20	0.32
-*d*	5.65	12.49	10.05
γ (ours)	11.17	13.31	15.25

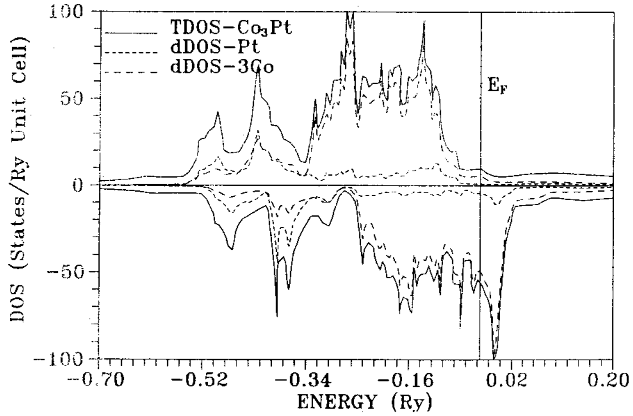

FIG. 4. Total density of states (TDOS) for Co_3Pt in the ferromagnetic phase along with density of states at *d* site (*d* DOS) for three Co and Pt atoms.

B. Ferromagnetic Co_3Pt, CoPt, and $CoPt_3$

As given by Stoner criterion, total energy further confirms the stability of the ferromagnetic (FM) state for all three members of this Co-Pt series. The total energy of the FM state is lower by 41, 100, and 22 mRy than the PM phase of Co_3Pt, CoPt, and $CoPt_3$ compounds, respectively. This is in accordance with other theoretical calculations[9] and experimental findings of Co_3Pt, CoPt, and $CoPt_3$ to be ferromagnetic.

In Figs. 4, 5, and 6 the total DOS and the *d* DOS at the Co and Pt sites in Co_3Pt, $CoPt_3$, and CoPt are shown. Total DOS and *l*-projected DOS at E_F for all the three compounds are given in Table I. For Co_3Pt most of the contribution to DOS at E_F comes from Co atom. As clear in Figs. 4, 5, and 6, there are unfilled spin-down states and filled spin-up states which cause the magnetic moment ($n\uparrow$-$n\downarrow$) in the system. Similarly in $CoPt_3$ and CoPt, Co-*d* states are contributing dominantly at E_F. Using $N(E_F)$ we calculated the electronic specific-heat coefficient γ for Co_3Pt, CoPt, and $CoPt_3$ and found its value equal to 13.93, 10.75, and 14.33 mJ/mol K, respectively. Experimental values for Co_2Pt and $CoPt_3$ are reported to be 24.40 and 20.64 mJ/mol K by Kuentzler and Waterstrat.[22] Koote, Haas, and Degroot[9] have obtained values of 14.36, 10.36, and 12.04 mJ/mol K^2 for the specific-

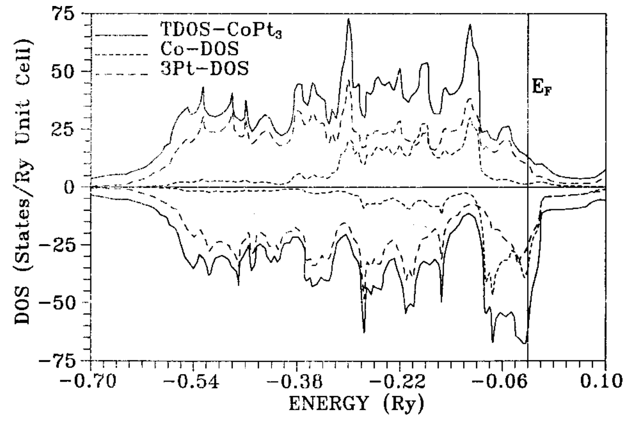

FIG. 5. Total density of states (TDOS) for $CoPt_3$ in the ferromagnetic phase along with density of states at *d* site (*d* DOS) for Co and three Pt atoms.

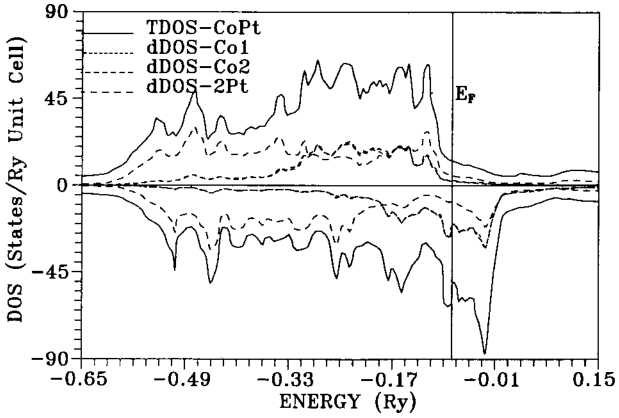

FIG. 6. Total density of states (TDOS) for CoPt in the ferromagnetic phase along with density of states at *d* site (*d* DOS) for Co1, Co2, and two Pt atoms.

heat coefficient of Co_3Pt, CoPt, and $CoPt_3$. Thus both calculations yield values of γ that are less than the experimental values. This is as expected.

In Table II the magnetic moments on the Co and Pt sites (obtained from the difference of spin-up and spin-down charge densities within each WS sphere), together with the value of total magnetization per unit cell, are given for these three compounds. Total moments of 5.54, 4.43, and $2.59\mu_B$ per unit cell is found in Co_3Pt, CoPt, and $CoPt_3$ compounds, respectively. Experimental magnetic moment of Co_3Pt has not been reported, however, for experimental values of magnetic moment at Co and Pt sites are reported to be 1.60 and $0.25\mu_B$, respectively, for the equiatomic compound CoPt by Kren *et al.*[23] For CoPt, experimental ($\sim 1.70\mu_B$ at Co atoms and $\sim 0.25\mu_B$ at Pt atom) and theoretical ($2.88\mu_B$ at Co atom and $0.38\mu_B$ at Pt atom) results are reported by Menzinger and Paoletti[8] and by Tahyama, Ohta, and Shimizu,[10] respectively. Kootte, Haas, and Degroot[9] have performed LSW calculations and reported the magnetic moments of 1.64, 1.69, and $1.69\mu_B$ at Co sites and 0.36, 0.37, and $0.27\mu_B$ at Pt site in case of Co_3Pt, CoPt, and $CoPt_3$, respectively. A comparison of the various results shows that our theoretical results are in better agreement with the experiments as compared to TB calculations of Tohyama, Ohta, and Shimizu.[10] Thus all the three compounds of this Co-Pt system, studied here are found to possess considerable magnetic moment and are strong ferromagnets. For each compound a moment of (0.3–0.4) is seen on Pt site which shows that the Pt atoms are strongly spin polarized by the Co atoms. Thus the moment on Pt atoms is a result of the high magnetic polarizability of the Pt atoms. The Co spins induce magnetic moments on the Pt neighbors.

C. Fermi surface of Co_3Pt and $CoPt_3$

Figures 7(a) and 7(b) and 8(a) and 8(b) show the Fermi surface for majority and minority carriers of compounds Co_3Pt and $CoPt_3$, respectively. For majority spins, six bands

TABLE II. SWS total energy, total density of states (TDOS), and *l*-projected density of states at the Fermi energy (in states per Ry unit cell), the magnetic moment μ for the compound (tot) and for Ni and Pt atoms (in μ_B per unit cell), and the coefficient of electronic specific heat γ (in mJ/mol K^2) for *ferromagnetic* Co_3Pt, $CoPt_3$, and CoPt. In the last column for *l*-projected DOS and magnetic moment the values after ‘‘,’’ are for the second type of Co in CoPt.

	Co_3Pt	$CoPt_3$	CoPt
SWS (a.u.)	2.7061	2.8297	2.7837
Total energy (mRy)	−236.45	−220.45	−230.45
Total DOS ↑	11.97	26.72	12.71
↓	68.42	56.01	49.34
Co-*s*	0.22	0.15	0.21, 0.31
-*p* ↑	0.40	0.20	0.30, 0.29
-*d*	2.38	3.37	2.70, 2.36
Co-*s*	0.14	0.06	0.07, 0.08
-*p* ↓	0.46	0.34	0.31, 0.31
-*d*	20.48	31.64	19.74, 20.22
Pt-*s*	0.17	0.24	0.12
-*p* ↑	0.50	0.49	0.35
-*d*	2.29	6.94	1.70
Pt-*s*	0.03	0.61	0.04
-*p* ↓	0.41	0.24	0.25
-*d*	4.71	7.68	4.09
μ_{tot} (ours)	5.54	2.59	4.43
(expt)	-	2.14 [105]	3.90 [83]
$\mu_{Co, Pt}$ (ours)	1.39, 0.38	1.85, 0.25	~1.85, 0.38
(expt)	-	1.64, 0.26	~1.70, 0.25
[83]	1.64, 0.36	1.69, 0.27	1.69, 0.37
γ (ours)	13.93	14.33	10.75
(expt) [92]	-	20.64	24.40

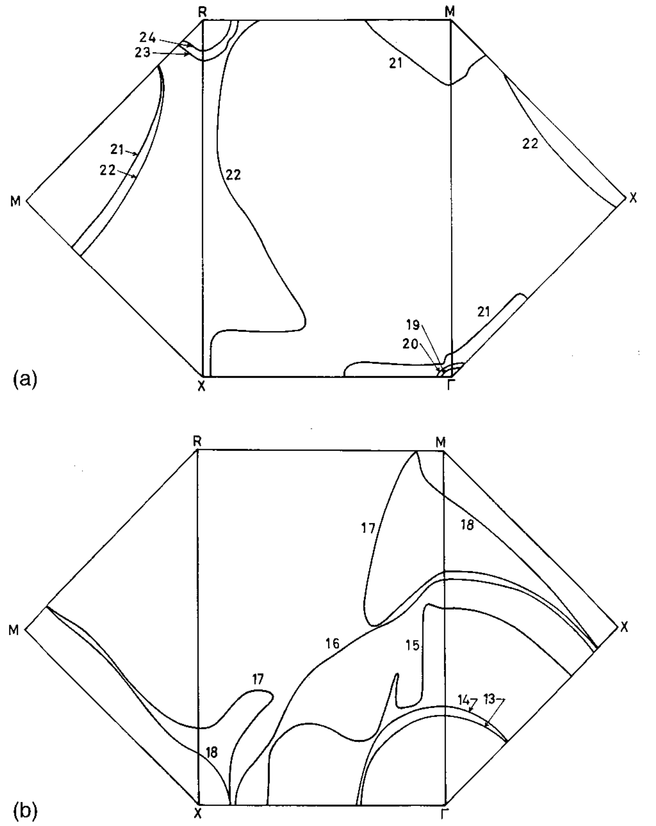

FIG. 7. (a) Fermi surface for majority carriers in Co_3Pt; (b) Fermi surface for minority carriers in Co_3Pt.

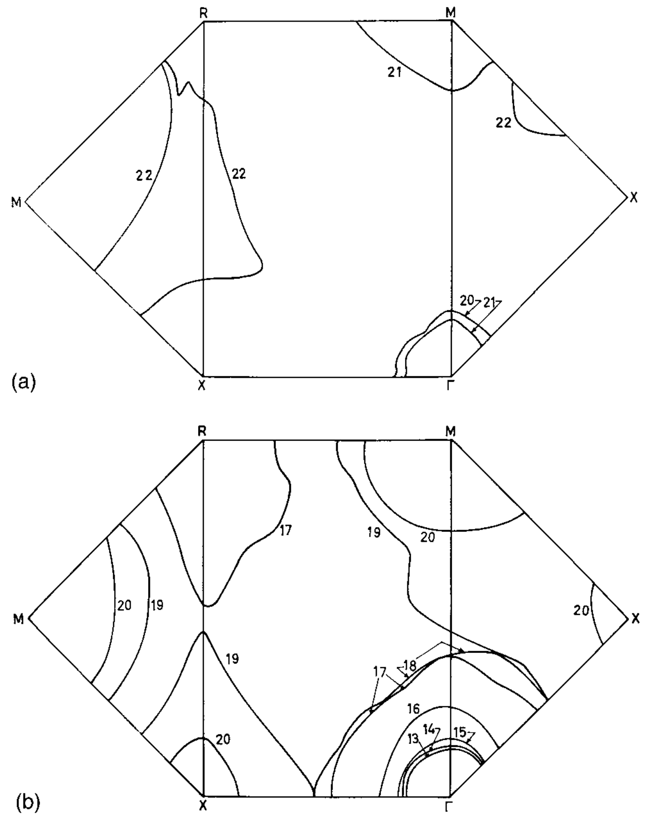

FIG. 8. (a) Fermi surface for majority carriers in $CoPt_3$; (b) Fermi surface for minority carriers in $CoPt_3$.

(19th–24th), in the case of Co_3Pt, and only four bands (19th–22nd) for $CoPt_3$ cut the E_F. The 19th and 20th bands are giving hole orbits around the Γ point in Co_3Pt. The 21st band which is giving hole orbit only around M for $CoPt_3$, is generating hole orbits around Γ, X, and M symmetry points. The 22nd band is giving two hole orbits around the symmetry point X and M in (100) and (110) planes, in the case of Co_3Pt, along with an open orbit in the (110) plane. In $CoPt_3$, the 22nd band is giving a large electron orbit along the XR direction around the center (1 0.5 0.5) and a smaller electron orbit in the XM direction around the same center. The 23rd and 24th bands in Co_3Pt are giving nearly spherical electron orbits around R in (100) and (110) planes. On comparing the Fermi-surface sheets of minority carriers in the two compounds we notice that in $CoPt_3$, eight bands (13th–20th), are cutting the E_F while in Co_3Pt only six bands (13th–18th) bands are doing so. Similar to the previous case, hole orbits are formed due to 13th to 16th bands around the symmetry point Γ. The 17th and 18th bands in $CoPt_3$, also give hole orbits around Γ, however, in Co_3Pt the 17th band is giving an irregular shaped hole orbit around X. A flat electron orbit due to the 18th band is also seen around X. In Co_3Pt open orbits due to the 17th and 18th bands are also noticed in (100) and (110) planes. In the case of $CoPt_3$, the 17th band gives a large hole orbit around R, in addition to the hole orbit around Γ. The 19th and 20th bands are giving closed electron orbits around points X and M. Further, an open orbit due to the 19th band is also seen here.

In Table II, the masses and areas of some electron and hole orbits in (100) and (110) planes are given. However, as there is no experimental data to compare with, we hope that our work will provoke experimentalists to do FS measurements on these compounds.

D. Curie temperature of Co_3Pt, CoPt, and $CoPt_3$

Recently, there have been many attempts to calculate T_C of rare earth metals and compounds.[24–26] Jaswal[25] calculated the spin-polarized electronic structure for the rare-earth compounds $R_2Fe_{17}N_\xi$ ($R=$rare-earth metal) and demonstrated its relationship to site-dependent magnetic moments using the model of MW. Their calculation showed an increase in T_C for the nitrogenated materials in agreement with experiments. Brooks *et al.*[24] have done calculations for the T_C of rare-earth metals. They demonstrated the importance of including the exchange splitting of the $5d$ states in the treatment of magnetic properties under mean-field theory (Stoner model) and obtained comparatively better values for T_C, although still off from experimental values. Using this theory, Severin *et al.*[26] have calculated T_C for $GdCo_2$ and its hydride $GdCo_2H_4$. By simple scaling, they calculated T_C of these two materials with the deGennes factor, they estimated the T_C for other heavy rare-earth cobalt compounds and their hydrides, and obtained good agreement with experiment. But there have been fewer attempts to calculate T_C for transition metals and their compounds. MW's model of spin fluctuations could give value of T_C for Fe, Co, and Ni close to experimental values. The calculated T_C for some transition-metal compounds (Y-Fe and Y-Co) were also found to be in agreement with experiment. Further, our earlier work on

Fe_3Pt[12] showed the pressure dependence of T_C using the same MW model and could obtain a fair agreement to the available experimental data.

Solving the integral given in Eq. (2) we obtained Stoner Curie temperature T_C^S for Co_3Pt, CoPt, and $CoPt_3$ as 4086, 9380, and 4830 K, respectively. According to MW theory, T_C with the help of Eq. (1) is found to be 2239, 2054, and 242 K, respectively. Further, T_{SF}, M_0, and χ_0 are calculated using Eqs. (3), (4), and (5). Using these calculated values of M_0, χ_0, T_{SF}, and T_C^S, we obtained T_C as 1803, 1964, and 242 K for Co_3Pt, CoPt, and $CoPt_3$, respectively. Table III lists the values of T_{SF}, T_C^S and T_C (theoretical), and T_C (experimental) for all the three compounds. Our values are in fair agreement with experiment for Co_3Pt and CoPt. In the case of $CoPt_3$, we considered, according to MW model, our T_{SF} as T_C. Our value of 242 K is quite close to the experimental value of 290 K.

TABLE III. Stoner Curie temperature (T_C^S) in K, spin-fluctuation temperature in K, and Curie temperature (T_C) in K, from our calculation and the experimental values of T_C in K for Co_3Pt, $CoPt_3$, and CoPt.

	Co_3Pt	$CoPt_3$	CoPt
T_C^S	4086	4830	9380
T_{SF}	2239	242	2054
T_C	1803	242	1964
T_C (expt)	1000	290	710

IV. CONCLUSIONS

The three ordered compounds of the Co-Pt system, namely Co_3Pt, $CoPt_3$, and CoPt, are studied. These compounds are FM in nature. Our magnetic moments are in fair agreement with experimental data. We have studied ground-state properties and FS of each of these compounds in detail. The BS results are then used to calculate T_C of these compounds. No theoretical calculations are reported yet for T_C of these compounds. Our results are in good agreement with the experimental values of T_C. This shows that the model we have chosen (MW model) can be successfully applied to calculate T_C of transition-metal compounds.

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