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A tight-binding calculation of the magnetic properties of TPt (T \equiv 3d transition element) ordered alloys with CuAu structure

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Abstract. A tight-binding-type self-consistent band calculation is performed to study the magnetic properties of the ordered TPt (T \equiv V, Cr, Mn, Fe, Co and Ni) alloys with CuAu structure within the Hartree–Fock approximation of the Hubbard model for their spin polarisation. Global features of their ground-state magnetic properties such as phase stability and local moments are explained successfully. The characteristic tetragonality of the lattice is argued from the calculated uniaxial pressures to be a consequence of the spin polarisation.

1. Introduction

Ordered alloys between a 3d transition element (T) and a group-VIII 4d or 5d element show a number of ordered structures, and their wide variety of magnetic properties has been observed from various viewpoints (see, e.g. Franse and Gersdorf 1986). One such system is TPt (T \equiv V, Cr, Mn, Fe, Co and Ni) which has a tetragonal CuAuI-type crystal structure and whose magnetic ground state is paramagnetic in VPt and NiPt, ferromagnetic in FePt and CoPt and antiferromagnetic in CrPt and MnPt. Such variation in the properties not only induces good motivation for elucidating the relevant mechanism but also makes it suitable to study by a simple model such as the tight-binding (TB) model whereby the global trends of the electronic properties can be examined.

A crystal of the TPt system is characterised by the layer structure where the layer consisting of T atoms and the layer consisting of Pt atoms accumulate alternately along the *c* axis of the tetragonal lattice. This is interesting because we can regard the system as a perfect ‘artificial’ layered superlattice which the molecular beam epitaxy (MBE) technique could produce. From this viewpoint a theoretical study of magnetism of the transition-metal monolayer on bulk Pd with FCC structure is being made (Blügel *et al* 1988). It is experimentally known that the magnetic moments in a TPt system are mainly associated with the layer consisting of T atoms and within each T-atom layer the local moments exhibit ferromagnetic (FePt and CoPt) or antiferromagnetic (CrPt and MnPt) ordering (Krén *et al* 1968). The anomalously large moments on T atoms ($4.3\mu_B$ on a Mn atom in MnPt and $2.8\mu_B$ on a Fe atom in FePt) are also noticeable. For the disordered phase of NiPt alloys, some electronic structure calculations (Staunton *et al* 1983) and studies of magnetic properties (Parra and Medina 1980) have been carried out within

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the magnetic environment model. No theoretical work based on the band calculation, however, has so far been done for the ordered alloy systems as far as we know.

In this paper, we apply the TB method to the TPt system and explain the magnetic ground-state properties such as phase stability and local magnetic moments. The characteristic tetragonality of the lattice is also discussed. The TB calculation adopted here has been performed successfully to explain the magnetism of the Laves phase compounds (Yamada 1988), for example. This method has also been applied to TPt₃ systems, and the results will be published elsewhere (Tohyama *et al* 1988).

In § 2, we outline the method of calculation, and in § 3 we present the calculated results for the total energy, local moments, electronic specific heat coefficient and electronic uniaxial pressure and compare them with experiment. The conclusions are given in § 4.

2. Method of calculation

We start from the Hubbard model whose Hamiltonian is expressed as a sum of the electron hopping term and the orbital-independent Coulomb repulsion term (see, e.g., Yamada and Shimizu 1985). The Hartree–Fock approximation of the Hamiltonian leads to a self-consistent band calculation for which we adopt the TB parametrisation scheme. No constraints for the magnetic structure are given in the self-consistent calculation besides the size of the unit cell. The Hamiltonian H to be diagonalised in k -space may then be written

$$H_{LL'}^{ii'}(\mathbf{k}) = \sum_{\mathbf{R}} \exp(i\mathbf{k} \cdot \mathbf{R}) H_{LL'}^{ii'}(\mathbf{R}) \quad (1)$$

with

$$H_{LL'}^{ii'}(\mathbf{R}) = \int d^3r \psi_L^i(\mathbf{r} - \boldsymbol{\rho}_i)^* H \psi_{L'}^{i'}(\mathbf{r} - \boldsymbol{\rho}_{i'} - \mathbf{R}) \quad (2)$$

where the energy integral $H_{LL'}^{ii'}(\mathbf{R})$ expresses the electron hopping between the L th atomic orbital $\psi_L^i(\mathbf{r} - \boldsymbol{\rho}_i)$ on the t th atom in the zeroth unit cell and the L' th atomic orbital $\psi_{L'}^{i'}(\mathbf{r} - \boldsymbol{\rho}_{i'} - \mathbf{R})$ on the i' th atom in the \mathbf{R} th unit cell. We adopt the two-centre approximation for $H_{LL'}^{ii'}(\mathbf{R})$ whereby all the integrals are written in terms of the hopping integrals such as $dd\sigma$, $dd\pi$ and $dd\delta$ for d electrons and the on-site integrals representing the centres of gravity of the local bands (Slater and Koster 1954). The energy bands thus obtained provide the total and local densities of states (DOSS), magnetic energy, local moments, etc.

Expressing the total electronic energy in terms of the covalent bond energy rather than the usual band energy, we can make a close link to the theory of metallic cohesion developed by Pettifor (1987). The total binding energy due to the cohesion may be obtained as a sum of this bond energy and the repulsive energy E^{rep} . The covalent bond energy in the non-magnetic state E^{p} may be written

$$E^{\text{p}} = \sum_i \int_{\epsilon}^{E_{\text{F}}^{\text{p}}} (\epsilon - V_{\text{pi}}) 2N_{\text{pi}}(\epsilon) d\epsilon \quad (3)$$

where $N_{\text{pi}}(\epsilon)$ is the non-magnetic local DOS per spin on site i , V_{pi} is the non-magnetic self-energy on site i (or the centre of the i th band) and E_{F}^{p} is the non-magnetic Fermi energy

determined by the total number of electrons. In the spin-polarised state the total electronic (or bond) energy E may be expressed as

$$E = E^p + E^{\text{mag}} \quad (4)$$

where the magnetic contribution E^{mag} may be written

$$E^{\text{mag}} = \Delta T - \frac{1}{4} \sum_i U_i m_i^2 + \sum_i V_{pi} q_i + \frac{1}{4} \sum_i U_i q_i^2 \quad (5)$$

with

$$\Delta T = \sum_{i\sigma} \int_{\varepsilon_F}^{\varepsilon_F^f} (\varepsilon - V_{i\sigma}) N_{i\sigma}(\varepsilon) d\varepsilon - E^p. \quad (6)$$

The first term ΔT in (5) is the increase in the kinetic energy due to the spin polarisation where $N_{i\sigma}(\varepsilon)$ is the i -site local DOS with spin σ , $V_{i\sigma}$ is the i -site self-energy with spin σ , and ε_F^f is the Fermi energy in the spin-polarised state. The second term in (5) is the energy gain due to exchange interaction where U_i is the intra-atomic Coulomb integral on site i and m_i is the number of polarised electrons on site i . The last two terms in (5) are the correction coming from the charge transfer due to the spin polarisation where q_i is the increment in electron number on site i with the constraint of total charge conservation $\sum_i q_i = 0$. All the terms are independent of the choice of the energy origin.

We assume the hopping integrals to have the canonical form given by Pettifor (1977) and use the parameters for d-band mass and Wigner-Seitz radius listed by Andersen and Jepsen (1977) for elemental metals. The hopping integrals between different kinds of atom are assumed to be the geometrical means of the two hopping integrals between atoms of the same kind as is justified from the canonical band theory. All the hopping integrals are truncated midway between the second and third neighbours of the FCC lattice. Only the d orbitals are taken into account for simplicity because the sp electrons are not mainly responsible for the magnetism in d-band metals. The unit cell in the spin-polarised cases is taken to be the tetragonal one containing four independent atoms, whereas in the non-magnetic calculations we can use the smallest possible unit cell containing two independent atoms. The k -space integration in the self-consistent band calculation is made by the tetrahedron method (Rath and Freeman 1975), where we check the convergence to confirm that the 196 regular mesh points in the irreducible Brillouin zone are normally sufficient to obtain the total energy within an accuracy of 1 mRyd. We use the values of parameters listed in table 1, where the values of the intra-atomic Coulomb integral U are, by definition, twice the values of I calculated by Janak (1977) within the local spin-density approximation, and the number n of d electrons on each atom is assumed to decrease from 9.4 for Ni metal to 3.9 for V metal keeping the same intervals of 1.1 electrons/atom. Such values of n are chosen not only because they are simple to use but because their variation is consistent with the values obtained (Papaconstantopoulos 1986) through the TB fits of the APW energy bands. For Pt, we simply assume $n = 9.4$ per atom and $U = 46$ mRyd. These values have often been used in the theory of transition-metal magnetism (Shimizu 1981). Fine adjustments of the parameters are not made here since we are interested in the general trends of magnetism in TPt systems. The lattice constants used for calculation are all experimental values except the value of c/a for CrPt for which we assume the ideal ratio $c/a = 1$ because no data are available. The computational procedures written above have been coded as a package program named TBPACK designing wide applications to any covalent-bonded periodic systems (Ohta 1987).

Table 1. Values of the parameters used for calculation. The number n of d electrons on each atom, the intra-atomic Coulomb integral U , the lattice constant a and c/a for the unit cell containing four atoms are listed.

Parameter (units)	V	Cr	Mn	Fe	Co	Ni	Pt
n (atom ⁻¹)	3.9	5.0	6.1	7.2	8.3	9.4	9.4
U (mRyd atom)	52 ^a	56 ^a	60 ^a	68 ^a	72 ^a	74 ^a	46 ^g
a (Å)	3.808 ^b	3.816 ^c	4.00 ^d	3.855 ^e	3.803 ^f	3.8227 ^f	—
c/a	0.986 ^b	1.0 ^g	0.918 ^d	0.963 ^e	0.975 ^f	0.939 ^f	—

^a Janak (1977).

^b Amamou and Kuentzler (1982).

^c Besnus and Meyer (1973).

^d Pál *et al* (1968).

^e Men'shikov *et al* (1974).

^f Pearson (1967).

^g Assumption.

3. Results of calculation

The DOS curves illustrate the electronic structure of the system. In figure 1, we show the calculated total and local DOS curves of the TPt systems corresponding to the respective magnetic orderings observed experimentally. The Fermi level in the paramagnetic state lies somewhere around the large higher-energy peak of the DOS curves coming mainly from the electrons on T atoms. It is well known (see, e.g., Shimizu 1981) that the shape of the non-magnetic DOS curve around the Fermi level substantially explains the magnetism of the system. In the present cases the Fermi level goes over the large peak of the local DOS of T atoms on an increase in the number of electrons on T atoms (or from V to Ni), exhibiting in order paramagnetism, antiferromagnetism, ferromagnetism and again paramagnetism. The local DOS curves for the spin-polarised states indicate that the local DOS of T atoms polarises very strongly while that of Pt atoms shows quite a small spin polarisation. This explains the anomalously large local moments on T atoms in MnPt and FePt alloys. The charge flows q_i due to spin polarisation should be noted; their direction is usually from a T atom to a Pt atom, but their magnitudes are fairly small (at most 0.3 electrons/atom) and thus no large qualitative alterations may be expected to the integrated magnetic properties of the system such as the local moments and total energy although the non-integrated quantities relating to the height of the DOS at the Fermi level can change considerably. We can compare the DOS curve for ordered NiPt (see figure 1(*f*)) with that for disordered NiPt obtained (Staunton *et al* 1983) by the kkr CPA method; it should be pointed out that the curves are very similar to each other.

The total energies are calculated for the paramagnetic, ferromagnetic and antiferromagnetic states of each alloy, and the results are given in figure 2. Stable and/or metastable magnetic orderings are found for all the alloys except NiPt where only the paramagnetic state is stable. No ferromagnetic solution is found for VPt. The most stable magnetic states are obtained by comparing the total energy as shown in table 2. The experimental sequence paramagnetic, antiferromagnetic, ferromagnetic and paramagnetic running from VPt to NiPt along the series is reproduced successfully except for a small difference in VPt where the energy of the antiferromagnetic state is a little lower than the energy of the paramagnetic state. In MnPt the ferromagnetic state has

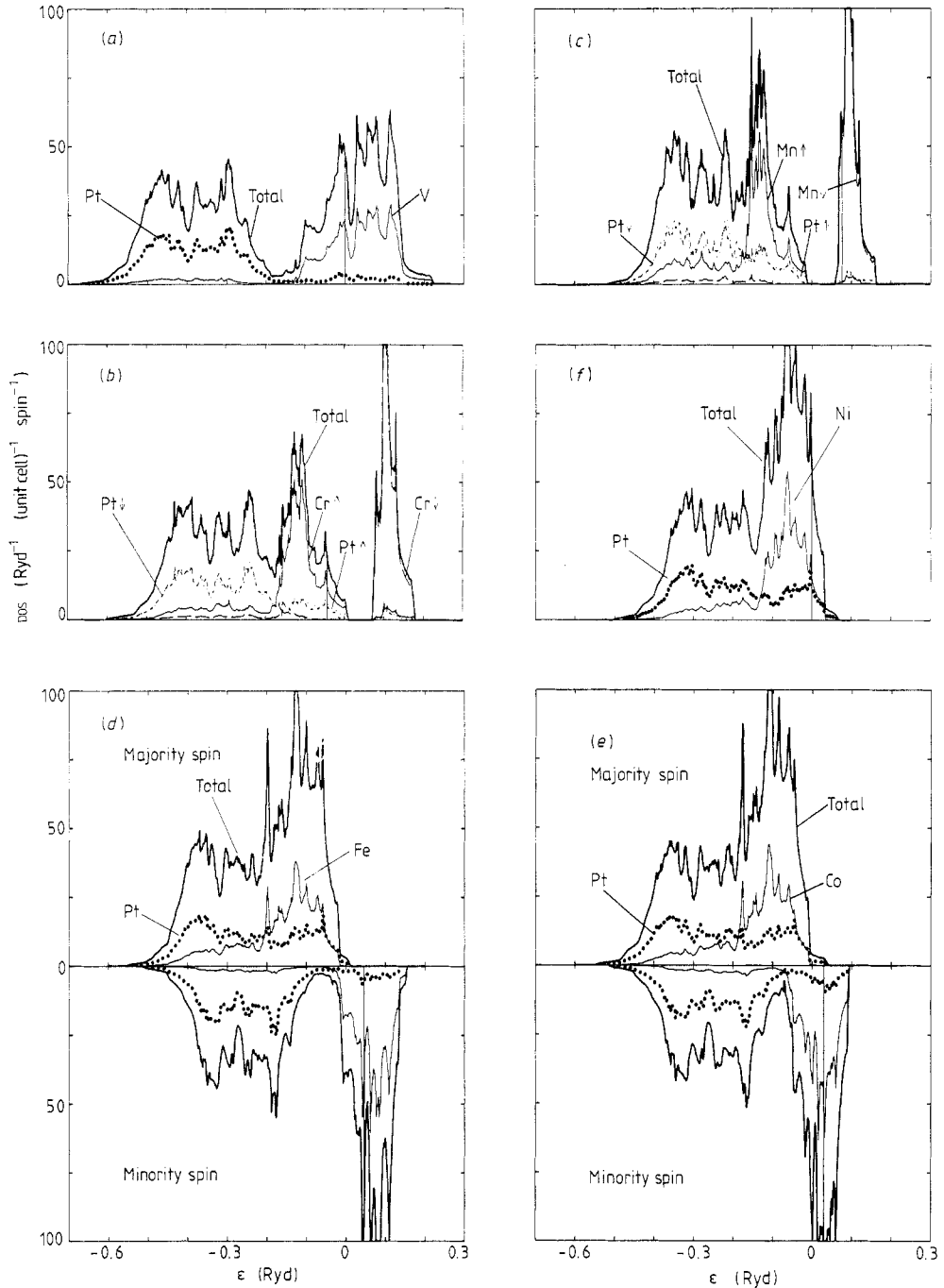


Figure 1. The total and local DOS curves calculated for the experimental magnetic orderings (the unit cell contains four atoms): —, total DOS; —, DOS on T site; ···, —, DOS on Pt site. The results for (a) VPt (paramagnetic), (b) CrPt (antiferromagnetic), (c) MnPt (antiferromagnetic), (d) FePt (ferromagnetic), (e) CoPt (ferromagnetic) and (f) NiPt (paramagnetic) are shown. The vertical lines indicate the Fermi levels.

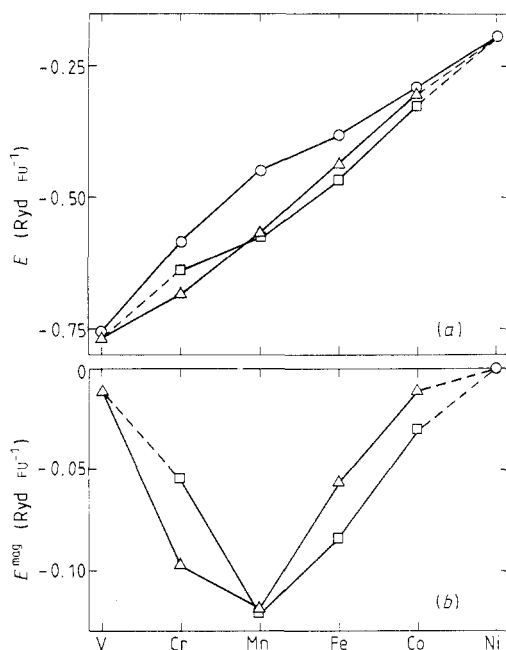


Figure 2. (a) The total electronic energy E and (b) the magnetic energy E^{mag} for the paramagnetic (\circ), ferromagnetic (\square) and antiferromagnetic (\triangle) states of TPt ($T \equiv V, \text{Cr}, \text{Mn}, \text{Fe}, \text{Co}$ and Ni) ordered alloys.

Table 2. The stable magnetic order, local magnetic moments m_T and m_{Pt} and total electronic energies E : P, paramagnetic; AF, antiferromagnetic; F, ferromagnetic.

Parameter (units)	VPt	CrPt	MnPt	FePt	CoPt	NiPt
Experiment	P ^a	AF ^b	AF ^c	F ^d	F ^e	P ^f
m_T (μ_B)	0	2.24	4.3	2.8	1.6	0
m_{Pt} (μ_B)	0	small	0	-0.25 ^g	0.25	0
Theory	AF	AF	F \approx AF	F	F	P
Paramagnetic						
E^{P} (Ryd FU^{-1})	-0.755	-0.585	-0.447	-0.381	-0.293	-0.196
Ferromagnetic						
E (Ryd FU^{-1})	—	-0.639	-0.569	-0.465	-0.324	—
m_T (μ_B)	—	4.21	4.17	3.09	1.93	0
m_{Pt} (μ_B)	—	0.20	0.32	0.30	0.34	0
Antiferromagnetic						
E (Ryd FU^{-1})	-0.765	-0.682	-0.566	-0.436	-0.303	—
m_T (μ_B)	2.13	3.96	4.00	2.87	1.64	0
m_{Pt} (μ_B)	0.03	0.04	0.04	0.06	0.07	0

^a Bieber *et al* (1980).

^b Pickart and Nathans (1963).

^c Kr n *et al* (1968) and P l *et al* (1968).

^d Kelarev *et al* (1973).

^e Franse and Gersdorf (1986).

^f Cadeville *et al* (1986).

^g Hypothetical value of Men'shikov *et al* (1974).

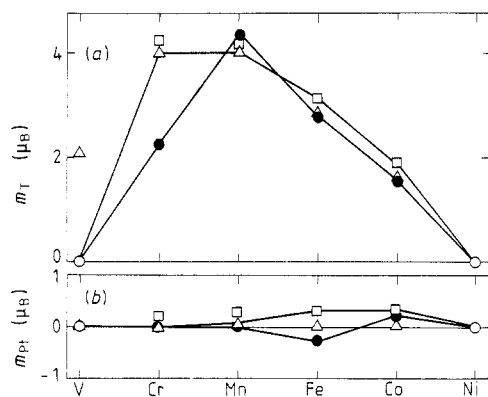


Figure 3. The local magnetic moments for ferro-magnetic (\square) and anti-ferromagnetic (\triangle) states of TPt ($T = V, Cr, Mn, Fe, Co$ and Ni) ordered alloys, which is compared with experiment (\bullet) (a) for T sites and (b) for Pt sites. The paramagnetic states (\circ) are also indicated for VPt and NiPt. The calculated points of the local moments corresponding to the experimental magnetic phases are connected together using bold lines.

almost the same energy as the anti-ferromagnetic state. The calculation for the alloys with a hypothetical cubic lattice ($c/a = 1$ with the volume preserved) produces no qualitative differences in the total energies.

The calculated local magnetic moments on each atom are shown in figure 3 and table 2. The global features, i.e. the large moments on T atoms which show a maximum in the middle of the series and the small moments on Pt atoms, are reproduced satisfactorily. The large local moments on the Mn atom in MnPt are the results of the large exchange splitting of the local bands. We note the largest discrepancy at CrPt in figure 3. It is known that the magnetic properties of the Cr–Pt systems are very sensitive to the state of atomic order (Goto 1977). For example, the m_{Cr} -value of $2.33\mu_B$ measured for CrPt₃ (Pickart and Nathans 1963) has been updated to the larger value of $3.37\mu_B$ by the new experiment of Burke *et al* (1980). Thus, the m_{Cr} -value of $2.24\mu_B$ for CrPt measured by Pickart and Nathans (1963) might possibly be unreliable. We cannot exclude, however, the possibility that our theory estimates too large an m_{Cr} -value because the method that we adopt may be justified only for obtaining a qualitative estimation of the magnetism. The anti-ferromagnetic structures of CrPt and MnPt on T-atom layers are in agreement with experiment (Pickart and Nathans 1963, Pál *et al* 1968) although the present calculation does not provide the directions of the moment vectors. The moments on Pt-atom layers, although they are very small, show anti-ferromagnetic ordering as well. For FePt, Men'shikov *et al* (1974) suggests hypothetically from experiment that the small moments on Pt atoms are antiparallel to the large Fe moments (ferrimagnetism), but our result indicates that they are parallel to each other although the moments on the Pt atom are very small. For disordered NiPt alloys, both experiment (Alberts *et al* 1974) and theory (Parra and Medina 1980) show the existence of local moments. For the ordered NiPt alloy, however, our calculation clearly indicates that only the paramagnetic solution is stable and this is consistent with the recent careful experiment of Cadeville *et al* (1986). We may thus conclude that the local moments in the NiPt system are induced by the effect of disorder. To determine the effect of the tetragonality on the magnetic properties, we examine the changes in the local magnetic moments by assuming a cubic lattice ($c/a = 1$ with the volumes preserved) for all the alloys. It is found that the changes are at most $0.05\mu_B$ on any atoms and thus unnoticeably small.

The electronic specific heat coefficient γ is calculated and compared with experiment (Kuentzler 1981) in figure 4. Although the orders of magnitude are reproduced satisfactorily, precise agreement is not obtained. To achieve better agreement with exper-

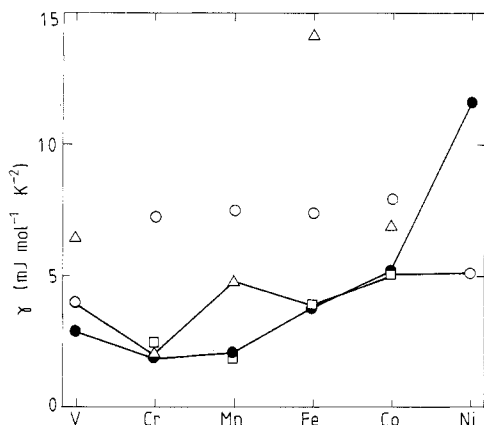


Figure 4. The electronic specific heat coefficients for paramagnetic (○), ferromagnetic (□) and antiferromagnetic (△) states of TPt ($T = \text{V, Cr, Mn, Fe, Co and Ni}$) ordered alloys compared with experiment (●). The calculated points of the coefficients corresponding to the experimental magnetic structures are connected together using bold lines.

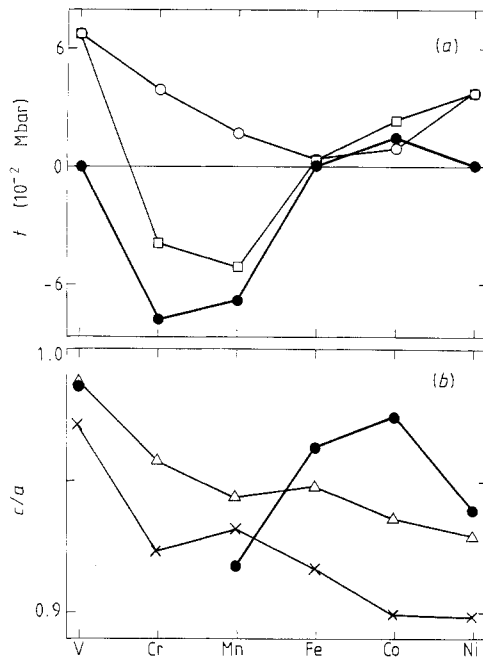


Figure 5. (a) The estimated electronic uniaxial pressure for non-magnetic (○) and spin-polarised (□) states of TPt ($T = \text{V, Cr, Mn, Fe, Co and Ni}$) ordered alloys. The magnetic contribution f^{mag} is also shown (●). The experimental magnetic orderings are assumed for each alloy. (b) The experimental c/a ratios (●) compared with the ratios obtained from the hard-sphere-packing model (×) and the pair-potential model (△).

iment, we need fine adjustments of the parameters n and U as well as the inclusion of the phonon (and other) enhancements, because non-integrated quantities such as γ reflect the sharp oscillations of the DOS curve directly.

The tetragonality c/a of the lattice has the characteristic alloy dependence that the ratio c/a is always smaller than unity and shows an oscillation as seen in figure 5. We now consider this tetragonality. The hard-sphere-packing model readily explains the reason for $c/a < 1$ from mismatch of the sizes of T and Pt atoms. The results may be seen in figure 5(b) where we assume that the atomic volumes of pure metals represents the sizes of the elements. The values of c/a thus obtained are, however, generally too small except for MnPt. The pair-potential model improves these values of c/a because the softness of the spheres is taken into account. We adopt here the form $\varphi(r) = \alpha r^{-10} - \beta r^{-5}$ with the inter-nuclear separation r . This particular power-law dependence is chosen on the basis of the theory of d-band cohesion (Pettifor 1983). The two positive coefficients α and β are determined to reproduce the atomic volumes and bulk moduli of the elemental metals. The coefficients between different kinds of atom are assumed to be the geometrical means of the coefficients for corresponding pure metals. The distortion of the lattice is calculated by minimising the total energy with respect to a and c . The results obtained are also shown in figure 5(b), with the characteristic oscillation observed

experimentally being left unexplained. To explain the oscillation, we consider the quantum mechanical behaviour of the electrons to be essential. Thus the electronic part of the uniaxial pressure for the hypothetical cubic state ($c/a = 1$ with the volume V preserved) is estimated from the computed difference between the total electronic energy E at $c/a = 0.95$ and at $c/a = 1.05$ as $t \approx -V^{-1} \Delta E / \Delta(c/a)$ where we assume the experimental magnetic orderings. We can thus expect a smaller c/a if t is small. The results obtained are shown in figure 5(a), where t^{mag} is obtained by subtracting t for the non-magnetic state from that for the spin-polarised state (see equation (4)). It is clear that t in the non-magnetic state shows no correlation with the experimental c/a but that the magnetic contribution t^{mag} exhibits a characteristic alloy dependence which correlates very well with experiment. The order of magnitude of t^{mag} , about 0.01 Mbar, is also sufficient to explain the few per cent distortion of the lattice provided that the relevant tetragonal elastic constant has the standard value, about 1 Mbar, of transition metals. We may therefore conclude that the spin polarisation is responsible for the characteristic tetragonality of the system. For quantitative arguments, we need to relax the lattice by taking into account both electronic and repulsive terms using, for example, the TB bond model (Ohta *et al* 1987).

4. Conclusions

In this paper, we have performed the TB-type self-consistent band calculation for the ordered TPt alloys with CuAuI structure and have investigated the magnetic properties of these alloys. The global features of their ground-state magnetic properties such as the magnetic phase stability and the local moments have been explained successfully. The characteristic tetragonality of the lattice has also been examined through the calculated uniaxial pressures and it has been concluded that the spin polarisation is responsible for its oscillatory variation along the series.

To make more quantitative calculations within the TB framework, we need to include the s-d hybridisation and spin-orbit coupling in the band calculation and to take into account the full-orbit exchange interactions in the Hamiltonian (Yamada and Shimizu 1987).

The TB parametrisation method employed in this paper will be used conveniently to assess the global trends of the electronic properties, to study very complex systems where the first-principles band calculation is too elaborate to perform, or to make an instant calculation as a preliminary work of the fully consolidated quantitative calculations.

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