## Coulomb correlations and magnetic anisotropy in ordered $L1_0$ CoPt and FePt alloys

Alexander B. Shick

Institute of Physics ASCR, Na Slovance 2, 182 21 Prague 8, Czech Republic

Oleg N. Mryasov

Seagate Research, 1251 WaterFront Place, Pittsburgh, Pennsylvania 15222 (Received 7 January 2003; published 28 May 2003)

We present the results of the magnetocrystalline anisotropy energy (MAE) calculations for chemically ordered  $L1_0$  CoPt and FePt alloys taking into account the effects of strong electronic correlations and spinorbit coupling. The local spin density and the Hubbard U approximation (LSDA+U) are shown to provide a consistent picture of the magnetic ground-state properties when intraatomic Coulomb correlations are included for both 3d and 5d elements. Our results demonstrate a significant and complex contribution of correlation effects to large MAE of these materials.

DOI: 10.1103/PhysRevB.67.172407

PACS number(s): 75.30.Gw, 75.50.Ss, 71.15.Mb, 71.15.Rf

Recent progress in fabrication and characterization of the magnetic nanoparticles and thin films based on the ordered  $L1_0$  CoPt and FePt alloys, renewed interest in understanding the mechanisms contributing to the large magnetocrystalline anisotropy of these materials. While the earlier studies were primarily motivated by permanent magnet applications, current research efforts are focused on the use of CoPt and FePt alloys for the high-density magnetic recording. The large and controllable magnetic anisotropy energy (MAE) is then a crucial property to overcome a superparamagnetic limit.<sup>1</sup>

The chemically ordered  $L1_0$  phase of FePt has large uniaxial MAE ( $\approx 6.6 \times 10^7$  erg/cc), which is almost by two orders of magnitude higher than their disordered fcc phase (a dramatic MAE increase with chemical ordering is also typical for other alloys of this kind: CoPt and FePd). The cubic symmetry is broken in  $L1_0$  phase by (i) stacking direction; (ii) by tetragonal distortion due to 3*d* and 5*d* atomic size mismatch. For the tetragonal crystal with uniaxial symmetry, the MAE depends on polar  $\theta$  magnetization angle<sup>2</sup> as

$$E = K_1 \sin^2 \theta + K_2 \sin^4 \theta + \cdots, \tag{1}$$

where  $K_1$  and  $K_2$  are the anisotropy constants. The series, Eq. (1), is rapidly converging and  $K_1 \ge K_2$  for CoPt and FePt  $L1_0$  alloys.<sup>3,4</sup> The MAE is then computed as the total-energy difference when the magnetization is oriented along [110] and [001] crystal axes (MAE=E[110] - E[001]).

A significant amount of work has been done to calculate this energy difference from first principles, employing the local spin-density approximation (LSDA). For the case of CoPt alloy, the fully relativistic Korringa-Kohn-Rostoker method yields the MAE of 0.058 meV/f.u.,<sup>5</sup> which is very different from the results of linear muffin-tin orbitals method (LMTO) calculations in atomic-sphere approximation (ASA): 2.29 meV,<sup>6</sup> 1.5 meV,<sup>7</sup> 2 meV,<sup>8</sup> the augmentedspherical-wave (ASW) result of 0.97 meV,<sup>9</sup> and full-potential LMTO (FLMTO) calculation results<sup>10</sup> of 1.05 meV and 2.2 meV.<sup>11</sup> As can be seen, there is an apparent and significant scatter of the theoretical results, while the experimental measurements are known to be quite accurate and consistent yielding the MAE of 1 meV.<sup>3</sup> The situation is similar for the case of FePt alloy: the LMTO-ASA calculations yield 3.4 meV,<sup>6</sup> 2.8 meV,<sup>7</sup> 3.5 meV,<sup>8</sup> ASW yields (Ref. 9) 2.75 meV, and FLMTO yields 3.9 meV (Ref. 11) and 2.7 meV,<sup>10</sup> and none of these calculations reproduce the experimental MAE of 1.3-1.4 meV for the bulk,<sup>4</sup> and 1-1.2 meV for the films<sup>12</sup> (when extrapolated to T=0).<sup>13</sup>

The accurate ab initio calculation of the MAE in itinerant ferromagnet is a very difficult task due to its notorious sensitivity to numerical details.<sup>14</sup> More importantly, the LSDA [or generalized gradient approximation (GGA)], which is conventionally used in the first-principles theory, lacks proper orbital polarization due to the Coulomb correlation effects.<sup>15</sup> In this paper, we wish (i) to clarify the ability of the LSDA theory to reproduce the experimental MAE for CoPt and FePt alloys, when highly accurate full-potential relativistic linearized augmented plane-wave method (FP-LAPW) is used for the total-energy MAE calculations; (ii) to go beyond LSDA and to investigate the role of electron correlations. We account for the on-site Coulomb correlation effects by using the LSDA+U approach<sup>16</sup> and to show that correlations should be included for both "magnetic" (Fe and Co) and "nonmagnetic" (Pt) sites to describe consistently the magnetic ground-state properties, such as the MAE and spin and orbital magnetic moments. We quantitatively demonstrate a significant and complex character of the intra-atomic Coulomb repulsion contribution to the MAE of itinerant ferromagnet with strongly magnetic 3d and nonmagnetic 5delements.

We start with the conventional LSDA band theoretical method together with the relativistic FP-LAPW method<sup>17</sup> and apply them to perform total-energy electronic and magnetic structure calculations for the magnetization fixed along each of [110] and [001] axes, respectively, and the MAE. The special *k*-points method is used for the Brillouin-Zone integration with the Gaussian smearing of 1 mRy for *k*-points weighting.<sup>14</sup> For convergence of the total-energy differences within desired accuracy (better than a few  $\mu eV$ ), about 11 000 *k* points are used (the MAE as a function of *k*-points number is calculated to be very similar to the results of Ref. [10]). The experimental values for the lattice parameters (*a* = 7.19 a.u., *c* = 7.01 a.u. for CoPt and *a*=7.30 a.u., *c* 

	Ref. 9	Ref. 11	Ref. 10	Present		
CoPt	0.97	2.2	1.05	1.03		
Expt.	0.82 (T=293  K) (1)	0.82 (T=293  K) (Ref. 3);		1.00 (T=0  K) (Ref. 13)		
FePt	2.75	3.9	2.73	2.68		
Expt.	0.7 - 1.2 (T = 293  H)	0.7 - 1.2 (T = 293 K) (Refs. 4 and 12);		1 - 1.4 (T = 0  K) (Ref. 13)		

TABLE I. Magnetic anisotropy energy (meV/f.u.) calculated using the FP-LAPW method within the LSDA theory.

=7.15 a.u. for FePt) are used.<sup>10</sup> The calculated MAE is shown in Table I, in comparison with the recent total-energy calculations and experimental results. The present FP-LAPW results are in very good quantitative agreement with the ASW results of Oppeneer<sup>9</sup> and the FLMTO results of Ravindran<sup>10</sup> and disagree substantially with FLMTO results of Galanakis<sup>11</sup> for a reason which is unclear to us. For CoPt alloy, the MAE is calculated in a very good agreement with experimental data, while for FePt, our LSDA results (together with those of Refs. 9 and 10) overestimate the value of MAE by a factor of 2.

Very recently, the electron-electron interaction was shown to play an important role for the MAE in<sup>18</sup> itinerant d and f-electron<sup>19</sup> magnetic materials. Here, we use the LSDA + U method combined with relativistic FP-LAPW basis<sup>19,20</sup> to account for the intrasite Coulomb repulsion U. Minimization of the LSDA+U total-energy functional, with SOC treated self-consistently,<sup>17</sup> generates not only the groundstate energy but also one-electron energies and states providing the orbital contribution to the magnetic moment. The basic difference of LSDA + U calculations from the LSDA is its explicit dependence on on-site spin and orbitally resolved occupation matrices. The LSDA+U creates in addition to spin-only dependent LSDA potential, the spin and orbitally dependent on-site "+U" potential that produces the orbital polarization.<sup>21</sup> Since the LSDA+U method is rarely applied to metals, the appropriate values of intra-atomic repulsion Ufor Fe, Co, and Pt atoms in metals are not known precisely as they are strongly affected by the metallic screening. Here we choose  $U_{3d}$  from the range of 1-2 eV and  $U_{5d}$  from the range of 0-1 eV (according to the experimental values for pure metals),<sup>22</sup> in order to reproduce experimental values of the MAE. For the exchange J, we use the values of  $J_{Co}$ =0.911 eV,  $J_{Fe}$ =0.844 eV,  $J_{Pt}$ =0.544 eV, which are obtained as a result of the constrained LSDA calculations,<sup>23</sup> and are close to their atomic values.

First, we discuss the FePt alloy. The MAE as a function of  $U_{Fe}$  is shown in Fig. 1(a). When U is included on Fe site only and varied in the interval of 1–2 eV, MAE is decreasing from its LSDA value. The experimental value of the MAE cannot be reached without unreasonable increase of U. Further meaningful reduction of MAE can be achieved by including U on the Pt site [see, Fig. 1(a)] and for the value of  $U_{Pt}$  around 0.544 eV (= $J_{Pt}$ ), the MAE observed for the bulk FePt can be reproduced. We note that the correct value of the MAE can be obtained in the region of  $U_{Fe} \approx 1.5-1.6$  eV,  $U_{Pt} \approx 0.5-0.6$  eV.

We choose  $\{U_{Fe}=1.516 \text{ eV}, U_{Pt}=0.544 \text{ eV}\}$  as a representative material specific parameters set to analyze the spin

and orbital ground-state properties. The calculated spin  $M_s$ , orbital  $M_l$ , and total magnetic moments for the magnetization directed along [001] axis are shown in Table II. The LSDA+U agrees with the observed total magnetization/f.u.  $M^{tot}$ , yields a slight increase of  $M_s^{Fe}$  from its LSDA value of 2.88 $\mu_B$  and substantially increases  $M_l^{Fe}$  from 0.0657 $\mu_B$ . The change of  $M_s$  and  $M_l$  of Pt site is very small as compared with LSDA. The effect of U on the  $M_l$  is seen to be similar to the "orbital polarization correction" of Brooks *et al.* (LSDA+OP) (see, Table II).<sup>10</sup> This *ad hoc* LSDA+OP correction is known to improve  $M_l$  in a number of d- and f-electron compounds, but it does not reproduce the MAE for the FePt alloy.

We now describe the CoPt alloy. The MAE as a function of  $U_{Co}$  is shown in Fig. 1(b). When U is included on Co-site



FIG. 1. (Color online) The MAE vs intra-atomic Coulomb repulsion (U) on 3d site for (a) FePt alloy; (b) CoPt alloy for different values of U on Pt site. Note that we use the bulk experimental MAE values<sup>3,4</sup> extrapolated to T=0 K.

TABLE II. Spin  $(M_s)$ , orbital  $(M_l)$  magnetic moments for 3d and 5d atoms, and total magnetic moment  $(M^{tot})$  per formula unit  $(\mu_B)$ ; magnetic anisotropy energy (meV/f.u.) as results of LSDA + U calculations for FePt and CoPt alloys. The LSDA+U calculated  $M_s$  and  $M_l$  values for bcc-Fe and hcp-Co obtained with the same values for  $U_{3d}$  and  $J_{3d}$  as for Fe and Co atoms in FePt and CoPt alloys.

FePt[001]	MAE	M <sup>tot</sup>	Atom	$M_s$	$M_l$
LSDA+U	1.3	3.47	Fe	3.00	0.114
$\{U_{Fe} = 1.52 \text{ eV}, U_{Pt} = 0\}$	0.34	0.048			
LSDA+OP	2.9	3.36	Fe	2.89	0.110
			Pt	0.35	0.048
Expt.	1.3	3.4			
CoPt[001]	MAE	$M^{tot}$	Atom	$M_s$	$M_l$
LSDA + U	1.0	2.55	Co	1.93	0.253
$\{U_{Co} = 1.70 \text{ eV}, U_{Pt} = 0\}$	0.38	0.065			
LSDA+OP	1.64	2.37	Co	1.80	0.161
			Pt	0.39	0.062
Expt.	1.0	2.4	Co	1.9-2.1	0.284
			Pt	0.36	0.090
bcc-Fe[001]				$M_{s}$	$M_l$
LSDA + U	$U_{Fe} = 1.52 \text{ eV}$			2.234	0.085
LSDA+OP (Ref. 14)				2.193	0.078
Expt.				2.13	0.08
hcp-Co[0001]	$M_{s}$	$M_l$			
LSDA + U	$U_{Co}$	,=1.70	eV	1.631	0.153
LSDA+OP (Ref. 14)				1.591	0.123
Expt.				1.52	0.14

only and varied in the interval of 1-2 eV, the MAE increases from its LSDA value and deviates from the experiment. As in the case of FePt alloy, we need to include U on the Pt site. The increase of  $U_{Pt}$  yields the decrease of MAE and its correct value is found in the region of  $\{U_{Co} \approx 1.4 - 1.7 \text{ eV}, \}$  $U_{Pt} \approx 0.3 - 0.6 \text{ eV}$ . We choose the set  $\{U_{Co} = 1.698 \text{ eV}, \}$  $U_{Pt} = 0.544 \text{ eV}$  as a representative (note, that we use the same value of  $U_{Pt}$  as for the FePt alloy, indicating its transferability). The calculated ground state  $M_s$ ,  $M_l$ , and  $M^{tot}$ for the magnetization directed along [001] axis are shown in Table II. M<sup>tot</sup> is calculated in a good quantitative agreement with the results of LSDA+OP and experimental data.<sup>8</sup> There is only small increase in  $M_s^{Co}$  from the LSDA value of  $1.81\mu_B$ , while the  $M_l^{Co}$  is substantially enhanced from its LSDA value of  $0.093\mu_B$  (Table II). The change of  $M_s$  and  $M_l$  for Pt site is very small. The  $M_l^{Co}$  increase in the LSDA+U calculations is substantially more pronounced than obtained in the LSDA+OP approximation.<sup>17</sup>

Recently, the element-specific  $M_s$  and  $M_l$  for CoPt were measured by Grange *et al.* using the x-ray magnetic circular dichroism (XMCD).<sup>24</sup> The LSDA+U calculated values for  $M_s$  and  $M_l$  for the Co-site are in a good quantitative agreement with the XMCD results.<sup>25</sup> For the Pt site, the agreement is not so good. Probably, it is caused by the use of the atomiclike sum rules to extract  $M_s$  and  $M_l$  from the XMCD spectra. This procedure is not reliable for Pt due to the substantially itinerant character of Pt 5*d* electrons. The LSDA+*U*  calculations reproduce consistently the MAE, total, spin, and orbital ground-state magnetic moments for CoPt alloy (Table II). Both LSDA and LSDA+OP are only partially successful: LSDA yields the correct value of MAE but fails for  $M_l^{Co}$  and LSDA+OP improves somewhat  $M_l$  but does not reproduce the MAE.

To evaluate further the consistency of the LDSA+U results, we performed the LSDA+U calculations for the elemental 3*d*-ferromagnet bcc-Fe and hcp-Co with the same values of  $U_{3d}$  and  $J_{3d}$  as for Fe and Co atoms in FePt and CoPt alloys (see, Table II). It is seen that without any further adjustments of parameters, the LSDA+U provides very reasonable results for the orbital magnetization in elemental 3*d* ferromagnet. These results demonstrate that the on-site Coulomb interaction parameters  $U_{3d}$  are well transferable in the transitional *d*-metal systems.

As for the choice of the Coulomb U for Pt, the challenge lies in correcting the LSDA orbital polarization without harming the exchange splitting which is expected to be well accounted in LSDA. The choice of  $U_{Pt} = 0.5 - 0.6$  eV then looks quite reasonable. Indeed, for the Pt-5d states having almost equal on-site occupations, the choice of  $U_{Pt} \approx J_{Pt}$  corresponds to an effective Stoner exchange  $I_{LSDA+U} \approx I_{LSDA}$ preserving<sup>29</sup> the LSDA spin polarization. This allows to ensure that the LSDA + U correction contributes entirely to the orbital polarization. The LSDA+U method, while proposed to deal with the problems specific for the localized states, in fact, is not limited by this case. This method can be used as soon as the on-site Coulomb correlation in the form of the Hubbard model is physically meaningful. The above comparison with the available experimental data for the MAE and spin/orbital magnetic moments, and the physically reasonable choice of parameters justify the use of on-site LSDA+U correction<sup>16</sup> for the Pt-5d states as the way to correct the on-site orbital polarization.

We now discuss the relation between the MAE and the anisotropy of the orbital magnetic moment  $\Delta M_l$   $(=M_l \| [110] - M_l \| [001])$ . Bruno<sup>26</sup> showed that in the limit of strong exchange splitting  $\Delta_{ex} \ge$  spin-orbit coupling (SOC), the MAE is proportional to  $\Delta M_l$ . This model predicts the positive MAE of 0.2 meV for CoPt and negative MAE of -2.1 meV for FePt, in disagreement with the total-energy calculations and experiment (Table II).

A more general form for MAE was given in Ref. 27:

$$\text{MAE} \approx -\frac{\xi}{4} \Delta (M_l^{\downarrow} - M_l^{\uparrow}) + \Delta E_T [\uparrow \downarrow - \text{``spin flip''}], \quad (2)$$

where  $\xi$  is the SOC constant. The first term  $(\Delta E_L)$  is the  $\uparrow\uparrow;\downarrow\downarrow$ -spins contribution due to the orbital moment  $\vec{L}$  and the second term couples the  $\uparrow\downarrow$  spins and is related to the spin magnetic dipole moment  $\vec{T}$ . In the limit of SOC  $\ll \Delta_{ex}$ , the  $\Delta E_T \approx -3\xi^2/\Delta_{ex}[\Delta Q_{zz}]$  is proportional to the difference of quadrupole moments  $Q_{zz}$  for z=[110],[001]. Note, that this  $\Delta E_T$  form is valid for Fe and Co since their SOC (0.07–0.08 eV)  $\ll \Delta_{ex}$  (3–4 eV) and cannot be used for Pt which has the SOC (0.6 eV)  $> \Delta_{ex}$  (0.2 eV).<sup>28</sup>

Equation (2) gives for the CoPt alloy,  $\Delta E_L^{Co} = 1.4 \text{ meV}$ ,  $\Delta E_T^{Co} = -0.7 \text{ meV}$ , and  $\Delta E_L^{Pt} = 1.9 \text{ meV}$  and for FePt alloy,  $\Delta E_L^{Fe} = -0.1 \text{ meV}$ ,  $\Delta E_T^{Fe} = 1.0 \text{ meV}$ , and  $\Delta E_L^{Pt} = 1.2 \text{ meV}$ . Here, large  $\Delta E_T^{Fe,Co}$  contributions to the MAE naturally originate from the difference in the interplane  $\{xz, yz\}3d-5d$ and in-plane  $\{xy\}3d-3d$  hybridization. Without  $\Delta E_T^{Pt}$  contribution, the total MAE of 2.7 meV (CoPt) and 2.1 meV (FePt) can be estimated, exceeding substantially the experimental values (cf., Table II). We can only roughly estimate that  $\Delta E_T^{Pt} \sim -\Delta Q_{zz} (=0.12(\text{CoPt}), 0.09(\text{FePt}))$  provides additional negative MAE contributions that are expected to reduce a total MAE towards the experimental data. Thus, due to the strong Pt-SOC, neither of the commonly used MAE parametrizations<sup>26,27</sup> based on the SOC-perturbation theory expansions is valid on the quantitative and do not provide a substitute for the total-energy MAE calculations.

Still, it is of interest to apply Eq. (2) to analyze qualitatively the origin of MAE dependence on U, as shown in Fig. 1. This analysis shows that LSDA+U MAE vs U dependence is qualitatively consistent with Eq. (2), and the change in  $\Delta E_L^{Pt} \sim \Delta (M_l^{\perp} - M_l^{\uparrow})^{Pt}$  contributes substantially to the MAE variations with U. In particular, we find the "coupling" between  $U_{3d}$  and  $\Delta E_L^{Pt}$  which originates from the strong 3d-5d hybridization, so that tiny  $U_{3d}$ -induced changes in Pt- $\Delta(M_l^{\downarrow} - M_l^{\uparrow})$  produce substantial MAE change due to the strong Pt SOC. It also explains the surprisingly strong MAE dependence on  $U_{Pt}$  (cf., Fig. 1), as a variation of  $U_{Pt}$  causes a tiny Pt- $\Delta(M_l^{\downarrow} - M_l^{\downarrow})$  change ( $\sim 10^{-3}\mu_B$ ), which in turn changes the MAE substantially due to the strong Pt SOC.

To summarize, accounting for on-site Coulomb correlations beyond what is included in LSDA, and using the LSDA+U method in a very general implementation including SOC, we have provided a microscopic theory of the ground-state magnetic properties in  $L1_0$  FePt and CoPt alloys. It is shown by comparison with the experiment that the LSDA+U method is capable of describing quantitatively the MAE and the orbital magnetization in these alloys with physically reasonable choice of Coulomb-U parameters. Using the SOC-perturbation theory model, we provide interpretation of our numerical results. These results are believed to be important for quantitative microscopic understanding of the large MAE in these material, and will assist in the development of the next generation magnetic recording devices operating above  $Tbit/in^2$  recording densities.

We are grateful to D. Weller, V. Drchal, and P. Oppeneer for helpful comments and useful discussion.

- <sup>1</sup>D. Weller and A. Moser, Proc. IEEE Trans. Magn. 36, 10 (1999);
  S. Sun *et al.*, Science 287, 1989 (2000).
- <sup>2</sup>S. Chikazumi, *Physics of Magnetism* (Krieger, Malabar, FL, 1986).
- <sup>3</sup>A.Ye. Yermakov and V.V. Maykov, Phys. Met. Metallogr. **69**, 198 (1990), and references therein.
- <sup>4</sup>O.A. Ivanov et al., Phys. Met. Metallogr. 35, 92 (1973).
- <sup>5</sup>S. Razee *et al.*, Phys. Rev. Lett. **82**, 5369 (1999).
- <sup>6</sup>I.V. Solovyev et al., Phys. Rev. B 52, 13 419 (1995).
- <sup>7</sup>A. Sakuma, J. Phys. Soc. Jpn. **63**, 3053 (1994).
- <sup>8</sup>G.H.O. Daalderop *et al.*, Phys. Rev. B **44**, 12 054 (1991).
- <sup>9</sup>P. Oppeneer, J. Magn. Magn. Mater. **188**, 275 (1998).
- <sup>10</sup>P. Ravindran et al., Phys. Rev. B 63, 144409 (2000).
- <sup>11</sup>I. Galanakis, M. Alouani, and H. Dreysee, Phys. Rev. B **62**, 6475 (2000).
- <sup>12</sup>J.U. Thiele *et al.*, J. Appl. Phys. **84**, 5686 (1998); J.U. Thiele *et al.*, *ibid.* **91**, 6595 (2002); S. Okamoto *et al.*, Phys. Rev. B **66**, 024413 (2002).
- <sup>13</sup>We use E.R. Callen and H.B. Callen, J. Phys. Chem. Solids **27**, 1271 (1966), and experimental magnetization M(T) dependence (Refs. 3 and 4) to find MAE( $T \rightarrow 0$ ).
- <sup>14</sup>J. Trygg *et al.*, Phys. Rev. Lett. **75**, 2871 (1995). The numerical convergence of the calculated difference in the total energy was analyzed by following this work.
- <sup>15</sup>I.V. Solovyev, A.I. Liechtenstein, and K. Terakura, Phys. Rev. Lett. 80, 5758 (1998).
- <sup>16</sup>V.I. Anisimov, F. Aryasetiawan, and A.I. Lichtenstein, J. Phys.: Condens. Matter 9, 767 (1997).

- <sup>17</sup>A.B. Shick, D.L. Novikov, and A.J. Freeman, Phys. Rev. B 56, R14 259 (1997).
- <sup>18</sup>I. Yang, S. Savrasov, and G. Kotliar, Phys. Rev. Lett. 87, 216405 (2001).
- <sup>19</sup>A.B. Shick and W.E. Pickett, Phys. Rev. Lett. 86, 300 (2001).
- <sup>20</sup>A.B. Shick, A.I. Liechtenstein, and W.E. Pickett, Phys. Rev. B 60, 10763 (1999).
- <sup>21</sup>In these calculations, both  $V_{LSDA}$  and  $V_{+U}$  are determined selfconsistently. The charge/spin densities which are needed for the  $V_{LSDA}$  are converged better than  $5 \times 10^{-5}$  electron/(a.u.)<sup>3</sup> in order to achieve the total-energy convergence better than few  $\mu$ eV.
- <sup>22</sup>M.M. Steiner, R.C. Alberts, and L.J. Sham, Phys. Rev. B 45, 13 272 (1992).
- <sup>23</sup>I.V. Solovyev, P.H. Dederichs, and V.I. Anisimov, Phys. Rev. B 50, 16 861 (1994). Note that small variations of *J* are found not to affect the results of calculations.
- <sup>24</sup>W. Grange et al., Phys. Rev. B 62, 1157 (2000).
- <sup>25</sup> The XMCD measures the ratio of  $M_s$  and  $M_l$  to the number of holes  $n_d$  in d shell. To compare with the LSDA+U results, the calculated  $n_d^{Co} = 2.845$  and  $n_d^{Pt} = 2.370$  were used together with the experimental  $M_{s,l}/n_d$  ratios (Ref. 24).
- <sup>26</sup>P. Bruno, Phys. Rev. B **39**, 865 (1989).
- <sup>27</sup>G. van der Laan, J. Phys.: Condens. Matter **10**, 3239 (1998).
- <sup>28</sup>A.B. Shick *et al.*, Phys. Rev. B **54**, 1610 (1996).
- <sup>29</sup>A.G. Petukhov, I.I. Mazin, L. Chioncel, and A.I. Lichtenstein, Phys. Rev. B 67, 153106 (2003).