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# Analysis of results from x-ray magnetic reflectometry for magnetic multilayer systems

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To determine the magnetization profiles for magnetic multilayer systems by x-ray magnetic reflectometry, it is generally assumed that the local magnetic contributions $\Delta\delta(\omega)$ and $\Delta\beta(\omega)$ to the optical constants are proportional to the local atomic magnetic moment. In the present paper, the validity of this basic assumption is explored by general theoretical arguments as well as by *ab initio* calculations for a Co-Pt multilayer system. It turns out that the assumption may be at least approximately valid under two circumstances: (i) the width of the x-ray line should not be much smaller than the width of the dichroic spectra, and (ii) the spin-orbit coupling should not be too strong.

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## I. INTRODUCTION

Multilayer systems consisting of magnetic and nonmagnetic components are of overwhelming importance for technological applications such as systems with giant magnetoresistance (GMR), with tunnel magnetoresistance (TMR), with perpendicular magnetic anisotropy for magneto-optical recording, etc. To obtain guidelines for a successful design of devices, a layer-resolved characterization of the magnetic properties is indispensable. These properties are influenced by growth preparation conditions, subsequent heat treatment, hydrogen charging etc., which determine the morphology of the interface, in particular, the interface roughness and the interdiffusion. One method for the element- and layer-selective magnetic characterizations is the resonant magnetic x-ray scattering[1] in the variant of x-ray reflectometry.[2]

In multilayer systems, the magnetic moments of the various layers may differ in magnitude and/or in orientation. In the present paper, we comment on the use of the resonant magnetic reflectometry for the investigation of the variations of the magnitudes of the magnetic moments. There are other papers (e.g., Ref. 3) which focus on the determination of the orientations of the magnetic moments in the various layers and to which the problems discussed in the present paper do not apply.

In the magnetic x-ray reflectometry, the reflectivities $R_+$ and $R_-$ for right and left circularly polarized x rays are measured for an energy close to an absorption edge, and the asymmetry ratio $A(\theta)=[R_+(\theta)-R_-(\theta)]/[R_+(\theta)+R_-(\theta)]$ is determined as a function of incident angle $\theta$.[4] Then the reflectometry for a given polarization (+ or −) is modeled. To do this, it is assumed that a complex index of refraction $n_\pm=1+(\delta\pm\Delta\delta)+(\beta\pm\Delta\beta)i$ can be assigned to each layer, where $\Delta\delta$ and $\Delta\beta$ describe the magnetic contributions to the optical constants $\delta$ and $\beta$. A precondition for this assignment of a layer-resolved index of reflection is[5] that the electric field of the x ray varies only slowly compared to the range of variation of the nonlocal conductivity tensor $\underline{\underline{\sigma}}(\mathbf{r},\mathbf{r}')$ across the inequivalent layers, which in general requires a grazing incidence of the x rays. Then, the reflectometries $R_+$ and $R_-$ are determined from a multiple-scattering approach for the incident x ray (magnetically modified Parratt algorithm[2,6]) which takes into account the interference effects between all the layers. The layer-resolved quantities $\Delta\delta$ and $\Delta\beta$ are determined by fitting the theoretical result for $A(\theta)$ to the experimental data. Finally, the basic assumption is made[2,7] that the quantities $\Delta\delta$ and $\Delta\beta$ are proportional to the magnetic spin moment of the respective layer, thus yielding the magnetization profile.

By the method discussed above the Pt magnetization profile in a Pt/Co bilayer was determined and compared with results from the *ab initio* electron theory for an ideal Pt-Co interface (see Fig. 7 of Ref. 8). The reflectometry yielded a constant magnetization of Pt for a range of 0.3±0.1 nm at the Co interface, followed by an exponential decay, whereas the theoretical profile did not exhibit such an initial plateau, but it decreased continuously and rapidly, starting from a value that is considerably larger than the experimental plateau value. The differences between the theoretical and the experimental profiles probably may arise because the interface in the real sample was not ideal due to interdiffusion, roughness, etc. An alternative explanation would be that the basic assumption of a proportionality between $\Delta\delta$, $\Delta\beta$, and the magnetic moment is not correct. Indeed, this proportionality has been questioned by calculations within the density-functional electron theory for two special systems.[9] In the present paper, we will figure out under which general circumstances this basic assumption is valid.

## II. THEORETICAL CONSIDERATIONS

We consider the propagation of a plane x ray in matter, i.e., a plane wave for the electric field vector of the form

$$\mathbf{E}=\mathbf{E}_0\exp\left(i\frac{\omega}{c}\mathbf{n}\cdot\mathbf{r}-i\omega t\right), \tag{1}$$

where $\omega/(2\pi)$ is the frequency and $c$ is the speed of light. The complex index of refraction $\mathbf{n}=(n_x,n_y,n_z)$ is represented in the usual way,

$$n_j=1+(\delta_j+\Delta\delta_j)+(\beta_j+\Delta\beta_j)i, \tag{2}$$

where $\delta_j$ $(\Delta\delta_j)$ and $\beta_j$ $(\Delta\beta_j)$ are the nonmagnetic (magnetic) contributions to the optical constants. Accordingly, we can define a nonmagnetic contribution $\mu$ and a magnetic contribution $\Delta\mu$ of the absorption coefficient via

$$I \sim |\mathbf{E}|^2 \sim \exp[-(\boldsymbol{\mu}+\Delta\boldsymbol{\mu})\cdot\mathbf{r}]. \tag{3}$$

Comparison of Eq. (3) with Eqs. (1) and (2) yields

$$\mu_j = 2\frac{\omega}{c}\beta_j, \tag{4}$$

$$\Delta\mu_j = 2\frac{\omega}{c}\Delta\beta_j. \tag{5}$$

We consider the above described reflectometry experiment where we have a circularly polarized x ray. The objective is to determine $\Delta\delta_j$ and $\Delta\beta_j$ for the two circular polarizations (left and right) as a function of the angle of incidence for a material with a given orientation of the magnetization relative to the crystal axes and relative to the surface normal of the reflecting surface, and to figure out whether $\Delta\delta_j$ and $\Delta\beta_j$ are proportional to the magnetic moment. In general, the quantities $\mathbf{E}_0$ and $\mathbf{n}$ for the reflected and for the diffracted waves, respectively, are determined by the electromagnetic boundary conditions at the surface of reflection, and the diffracted wave will attain a form different from a circularly polarized wave. A circularly polarized x ray propagating in the material is obtained only for the following situation. We consider a system in which the magnetization is parallel to an axis (which we denote as $z$ axis) of at least threefold rotational symmetry. The optical conductivity tensor then has the form (see, e.g., Ref. 10)

$$\underline{\underline{\sigma}} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}. \tag{6}$$

Furthermore, we consider a propagation of the x ray parallel to the magnetization, i.e., $\mathbf{n}=(0,0,n)$. The Fresnel equation,

$$(n^2\underline{\underline{1}} - \mathbf{n}{:}\mathbf{n} - \underline{\underline{\varepsilon}})\mathbf{E}_0 = 0, \tag{7}$$

with the dielectric tensor $\underline{\underline{\varepsilon}}=\underline{\underline{1}}+\frac{4\pi i}{\omega}\underline{\underline{\sigma}}$ then yields two normal modes, $\mathbf{E}_0^{\pm}=\frac{E_0}{\sqrt{2}}(\hat{\mathbf{e}}_x \pm i\hat{\mathbf{e}}_y)$, where $\hat{\mathbf{e}}_x$ and $\hat{\mathbf{e}}_y$ are unit vectors in the $x$ and $y$ directions, and these two modes correspond to right (+ sign) and left (− sign) circularly polarized x rays, with

$$n_\pm = \sqrt{\varepsilon_{xx} \pm i\varepsilon_{xy}} = \sqrt{1+\frac{4\pi i}{\omega}(\sigma_{xx} \pm i\sigma_{xy})}. \tag{8}$$

Because for x rays $n_\pm$ is close to 1, we can linearize the relation between $n_\pm$ and $\sigma_{xx}$, $\sigma_{xy}=\sigma_{xy}^{(1)}+i\sigma_{xy}^{(2)}$. From a comparison with Eq. (2), we then obtain

$$\Delta\delta(\omega) = \frac{2\pi}{\omega}\sigma_{xy}^{(1)}(\omega), \tag{9}$$

$$\Delta\beta(\omega) = \frac{2\pi}{\omega}\sigma_{xy}^{(2)}(\omega). \tag{10}$$

Furthermore, Eq. (5) yields

$$\mu_c(\omega) = \frac{1}{2}[\mu_+(\omega) - \mu_-(\omega)] = \frac{4\pi}{c}\sigma_{xy}^{(2)}(\omega), \tag{11}$$

and hence

$$\Delta\beta(\omega) = \frac{c}{2\omega}\mu_c(\omega). \tag{12}$$

The quantity $\Delta\delta(\omega)$ may be obtained from $\Delta\beta(\omega)$ with the help of a Kramers-Kronig relation,

$$\Delta\delta(\omega) = \frac{2}{\pi}\mathcal{P}\int_0^\infty d\omega' \frac{\omega'\Delta\beta(\omega')}{\omega'^2 - \omega^2}. \tag{13}$$

We thus have managed to relate $\Delta\beta(\omega)$ to the dichroic absorption signal $\mu_c(\omega)$ for circularly polarized x rays in the material. For all other geometries $\Delta\beta(\omega)$ is not directly related to $\mu_c(\omega)$ because there are no circularly polarized waves in the material. At least for systems with only moderate spin-orbit coupling, however, the difference between the real $\Delta\beta(\omega)$ and the quantity given by Eq. (12) will be small. In this context, it should be noted that many multilayers are anyway polycrystalline rather than monocrystalline, and then it is rather unlikely that there are grains for which the above discussed geometry holds strictly. However, as just mentioned, Eq. (12) should still hold in good approximation for systems with only moderate spin-orbit coupling.

The advantage of Eq. (12) is that we can now use the theoretical results for $\mu_c(\omega)$ to try to relate $\Delta\beta(\omega)$ to the magnetic moment. It has been shown[11] that in dipole approximation the x-ray absorption spectrum is determined by eight ground-state operators, e.g., the spin operator, the orbital angular momentum operator and the spin magnetic dipole operator $\hat{T}_z$. For systems with small or moderate spin-orbit coupling, the influence of the spin operator is strongly dominating, and then we have (see, for instance, the two-step model[12])

$$\frac{\mu_c(\omega)}{\mu(\omega)} \sim \frac{D_\uparrow(\omega) - D_\downarrow(\omega)}{D_\uparrow(\omega) + D_\downarrow(\omega)}, \tag{14}$$

where $D_\uparrow(\omega)$ and $D_\downarrow(\omega)$ denote the density of electronic $d$ states for majority and minority electrons and where $\mu(\omega) = [\mu_+(\omega)+\mu_-(\omega)]/2$.

At the moment, we assume for simplicity that the linewidth of the resonant magnetic reflectometry is arbitrarily small. Then, the excited core electrons are deposited into empty valence states of a well-defined energy $E$ close to the Fermi energy $E_F$ (measured with respect to the energy of the core electron), and we have

$$\Delta\beta(\omega) \sim \mu_c \sim D_\uparrow(E) - D_\downarrow(E). \tag{15}$$

The atomic spin magnetic moment, however, is given by an integral over the spin polarization $D_\uparrow(E)-D_\downarrow(E)$,

$$m = -\mu_B\int_{E_F}^\infty [D_\uparrow(E) - D_\downarrow(E)]dE. \tag{16}$$

In general, the value of the integrand at some fixed energy has nothing to do with the value of the integral, and therefore it is—for arbitrarily small linewidth—very unlikely that $\Delta\beta$ is proportional to $m$. In an extreme situation, it might even be that $D_\uparrow(E\approx E_F)-D_\downarrow(E\approx E_F)$ has another sign than the integral [Eq. (16)]. Then, the assumption $\Delta\beta\sim m$ would yield even a magnetic moment with wrong orientation.

In the following, we want to discuss first a situation where $\Delta\beta(\omega)\sim m$ holds for a wide range of frequencies even for small linewidth, in spite of the doubts raised above. To do this, we consider a material which is described by the Stoner model of magnetism. In this model, the density of states $D(E)$ of the unpolarized system is rigidly split into a majority density of states, $D_\uparrow(E)=D(E+Um/2)$, and a minority density of states, $D_\downarrow(E)=D(E-Um/2)$, due to the action of the mean-field exchange splitting $Um$ with the Hubbard parameter $U$. For systems for which $D(E)$ varies only slowly on a range $Um$, this yields

$$\Delta\beta(E)\sim D\left(E+\frac{Um}{2}\right)-D\left(E-\frac{Um}{2}\right)\approx\frac{\partial D}{\partial E}Um, \quad (17)$$

i.e., $\Delta\beta(E)$ is proportional to $m$ for a range of energy $E$ much larger than $Um$. Such a situation probably appears for layers of simple $s$-$p$ metals (SM) in a multilayer structure $(\mathrm{SM})_n(\mathrm{TM})_m$ for which a small magnetization is induced by a nearby magnetic layer of a transition metal (TM). Then, the magnetic optical constant $\Delta\beta(E)$ in any one of the $m$ layers of simple metals will be proportional to the induced magnetic moment in that layer.

In transition metals with spontaneous or induced magnetization, however, there is not just a rigid shift between $D_\uparrow$ and $D_\downarrow$, and the spin-resolved density of state curves are strongly structured on a scale given by the exchange splitting; i.e., the above discussed preconditions for the validity of $\Delta\beta(\omega)\sim m$ at arbitrarily small width of the x-ray line are not fulfilled. However, in a real experiment there is a finite linewidth due to the finite lifetime of the excited core state (described by a Lorentzian broadening function) and due to the instrumental broadening (described by a Gaussian broadening function). We will see that under favorable circumstances, this broadening will allow us to assume that the contributions $\Delta\beta$ for transition-metal layers in a multilayer system measured at a fixed $\omega$ are approximately proportional to the magnetic moments of the layers. Describing the total broadening by a broadening function $g(E-E',\Gamma)$ with a broadening parameter $\Gamma$, the dichroic signal $\tilde{\mu}_c(E)$ measured in a real experiment is related to the "intrinsic" dichroic spectrum $\mu_c(E)$ via a convolution

$$\tilde{\mu}_c(E)=\int_{E_F}^{\infty}\mu_c(E')g(E-E',\Gamma)dE'. \quad (18)$$

Because of $g(E-E',\Gamma)\geqslant 0$, we may use the mean-value theorem of the integral calculus to obtain

$$\begin{aligned}\tilde{\mu}_c(E)&=\mu_c[E_0(E,\Gamma)]\int_{E_F}^{\infty}g(E-E',\Gamma)dE'\\&=\mu_c[E_0(E,\Gamma)]G(E,\Gamma)\end{aligned} \quad (19)$$

for some $E_0(E,\Gamma)\in[E_F,\infty]$. Accordingly, we have

$$\Delta\tilde{\beta}(E)\approx\frac{c\hbar}{4E_F}\tilde{\mu}_c(E)\sim\mu_c[E_0(E,\Gamma)]G(E,\Gamma), \quad (20)$$

with the same $E_0$. Instead of demanding that $\mu_c(E)$ be proportional to $m$ for all energies which was the precondition for the validity of $\Delta\beta(E)\sim m$ in the case of arbitrarily small linewidths, we arrive at the demand that $\mu_c[E_0(E,\Gamma)]\sim m$ for all energies $E$. This is a much less stringent demand because $\mu_c[E_0(E,\Gamma)]$ varies more slowly with $E$ than $\mu_c(E)$. In fact, if $\Gamma$ is very much larger than the range of extension of $\mu_c(E)$, then $\mu_c[E_0(E,\Gamma)]$ is just the mean value of $\mu_c(E)$ which, according to Eqs. (15) and (16), is proportional to $m$. In that case, we would have

$$\Delta\tilde{\beta}(E)\approx mG(E,\Gamma), \quad (21)$$

i.e., the value of $\Delta\tilde{\beta}(E)$ at some fixed energy $E$ would be proportional to $m$.

Please note that the energies are measured with respect to the energy of the excited core level of the considered atom. Due to a core-level shift, they may be different for crystallographically different layers of the same material in a multilayer system, and this would result in a corresponding small shift of the respective spectrum $\Delta\tilde{\beta}(E)$.

In many real experiments, the linewidth $\Gamma$ is not very much larger than the extension of $\mu_c(E)$ which is approximately given by the width of the considered valence band above $E_F$. For the absorption at the $L_2$ and $L_3$ edges of $3d$ transition metals, e.g., this is the $3d$ band. The full width of the $3d$ band is of the order of 5 eV, but the width of the unoccupied part of the $d$ band of course decreases when going from the early to the late transition metals. The lifetime broadening (full width at half maximum) is between 1 and 1.5 eV for the $L_2$ edge and below 1 eV for the $L_3$ edge of the typical $3d$ transition metals.[13] The instrumental broadening is often chosen in such a way that the intensity of the x ray is reasonably large (which rules out the use of extremely small instrumental linewidths), yet a bit smaller than the lifetime broadening. Altogether, it becomes clear from this reasoning that under these circumstances, the quantity $\mu_c[E_0(E,\Gamma)]$ and hence $\Delta\tilde{\beta}(E)$ will not be strictly proportional to $m$. As a consequence, the ratio $\Delta\tilde{\beta}_i(E)/\Delta\tilde{\beta}_j(E)$ for two crystallographically different layers $i\neq j$ of the same material in a multilayer system will depend to some degree on the broadening parameter $\Gamma$, and hence it is obvious that it need not be necessarily directly related to the ratio of the respective magnetic moments.

One example for which Eq. (21) fails is given in Ref. 9. There, the broadened quantities $\Delta\tilde{\beta}(E,x)$ and $\Delta\tilde{\delta}(E,x)$ per Pt atom in disordered bulk $\mathrm{Co}_x\mathrm{Pt}_{1-x}$ have been calculated by the *ab initio* density-functional electron theory. For fixed energy, $\Delta\tilde{\beta}(E,x)$ increases monotonically with $x$, whereas the directly calculated average Pt spin moment $m$ runs through a shallow maximum at $x\approx 0.5$ and then decreases slightly with increasing $x$. Obviously, in this system the assumption that $\Delta\tilde{\beta}(E,x)$ is proportional to $m(x)$ fails even qualitatively. There are two possible reasons for this failure. First, the linewidth due to the finite lifetime is considerably smaller than the extension of the spectrum $\Delta\tilde{\beta}(E)$. Second, the spin-orbit coupling for the Pt atoms is very large so that the absorption spectrum is not nearly exclusively determined by the spin moment but also by the an orbital moment, and then Eq. (15) is no longer valid.

## III. NUMERICAL RESULTS FOR A Co-Pt MULTILAYER SYSTEM

We consider a periodic fcc-like stacking $Co_2Pt_7$ of densely packed Co and Pt layers with magnetization perpendicular to these planes (parallel to the $z$ direction) and x-ray propagation parallel to the magnetization. The conductivity tensor then has the form given in Eq. (6). The x-ray absorption at the $L_2$ and the $L_3$ edge of Pt is considered, i.e., the excitation of an electron in the initial core state $|i\rangle=|2p_{j_i}^{m_{j_i}}\rangle$, with $j_i=1/2$ and $m_{j_i}=1/2$ and $-1/2$ for the $L_2$ edge and $j_i=3/2$ and $m_{j_i}=3/2$, $1/2$, $-1/2$, and $-3/2$ for the $L_3$ edge to an unoccupied final $5d$ valence state with wave vector $\mathbf{k}$ (the minor contribution of $2p$-$5s$ excitations is neglected). The absorptive part $\sigma_{xy}^{(2)}$ of the nondiagonal component (per volume $V$ of the elementary unit cell of the multilayer system) then is calculated from

$$\sigma_{xy}^{(2)}(\omega)=\frac{\pi e^2}{m^2\hbar V\omega}\sum_{i,\text{occ.}}\int d^3k\;\theta[E_{\mathbf{k}}-E_F]\,\delta(\hbar\omega-(E_{\mathbf{k}}-E_{c,i}))]\mathrm{Im}(\Pi^x_{i\mathbf{k}}\Pi^y_{\mathbf{k}i}). \tag{22}$$

Here, $e$, $m$, and $\hbar$ denote the electronic charge, mass, and Planck's quantum, and the sum runs over all occupied states $|i\rangle$ of the $2p_{1/2}$ or $2p_{3/2}$ core level $E_{c,i}$, respectively. The $\mathbf{k}$ integration runs over the Brillouin zone and $\theta(E_{\mathbf{k}}-E_F)$ is a step function that selects only unoccupied final states with $E_{\mathbf{k}}>E_F$. The matrix elements $\Pi^x_{i\mathbf{k}}$ are given by

$$\Pi^x_{i\mathbf{k}}=\langle i|\hat{p}_x|\mathbf{k}\rangle, \tag{23}$$

and an analogous relation holds for $\Pi^y_{\mathbf{k}i}$. They are calculated by the *ab initio* density-functional electron theory in local-spin-density approximation and by the linear-muffin-tin-orbital method in atomic-sphere approximation[14] in which the spin-orbit coupling has been implemented.[8] For the calculation of the spectrum $\sigma_{xy}^{(2)}(\omega)$, the range of considered photon energies $E=\hbar\omega$ is subdivided into equally sized regimes of width $\Delta=0.84$ mRy. Then, the Brillouin-zone integration is replaced by a summation over a discrete mesh of 21 600 $k$ points. The so-obtained nonbroadened histogram then is broadened with a Lorentzian

$$g(E-E',\Gamma)=\frac{1}{\pi}\frac{\Gamma}{(E-E')^2+\Gamma^2} \tag{24}$$

of half-width at half maximum $\Gamma$. By this, the finite lifetime of the excited core state is taken into account which is not included in our band-structure calculation which approximates the excited states by Kohn-Sham orbitals of infinite lifetime.

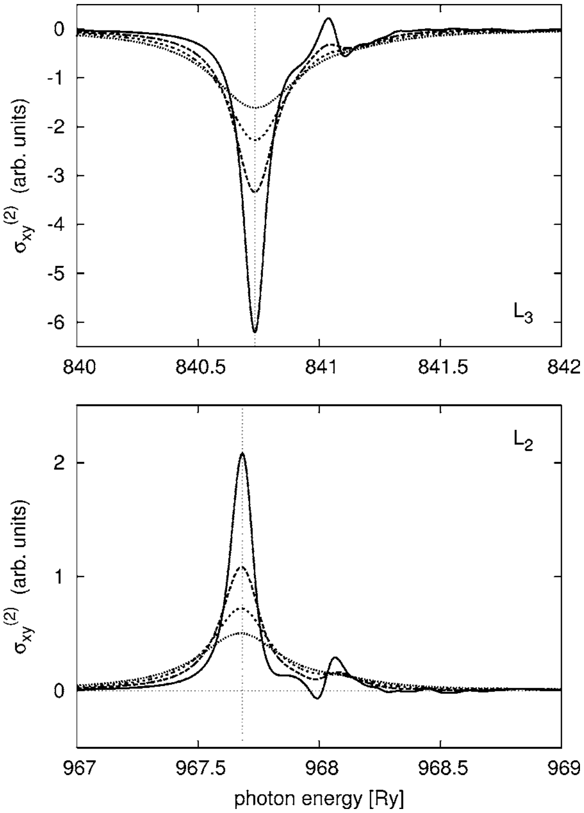

FIG. 1. Spectrum $\tilde{\sigma}_{xy}^{(2)}(E)$ for the $L_3$ and $L_2$ edge of Pt1. The spectra are broadened with a Lorentzian of widths $\Gamma=50$ mRy (solid), 100 mRy (long dashes), 150 mRy (short dashes), and 215 mRy (dotted).

Figure 1 exhibits the spectrum $\tilde{\sigma}_{xy}^{(2)}(E)$ of the Pt layer at the Co-Pt interface (Pt1) for the $L_3$ and the $L_2$ edge for various values of $\Gamma$. For the $L_2$ and the $L_3$ edge of Pt, the natural broadenings $\Gamma$ due to the finite lifetime of the $2p_{1/2}$ and $2p_{3/2}$ core holes are 2.93 eV (215 mRy) and 2.65 eV (195 mRy), respectively.[15] The spectra with small broadening ($\Gamma=50$ mRy) exhibit some structure in a range of about 1 Ry. This structure is completely smeared out for a broadening which corresponds to the natural linewidth, although $2\Gamma$ is always smaller than the range of extension of $\tilde{\sigma}_{xy}^{(2)}(E)$. Figure 2 exhibits the ratio $r=\tilde{\sigma}_{xy,\text{Pt}n}^{(2)}(E_{\text{edge}})/\tilde{\sigma}_{xy,\text{Pt1}}^{(2)}(E_{\text{edge}})=\Delta\tilde{\beta}_{\text{Pt}n}(E_{\text{edge}})/\Delta\tilde{\beta}_{\text{Pt1}}(E_{\text{edge}})$ for the various Pt layers Pt$n$, where Pt1 refers to the Pt layer at the Co-Pt interface and Pt4 to the innermost Pt layer between the Co layers. We thereby considered a photon energy corresponding to the maximum value of $\tilde{\sigma}_{xy,\text{Pt1}}^{(2)}$ (see Fig. 1) at the $L_3$ and the $L_2$ edge. Furthermore, the figures exhibit the ratio $m_{\text{Pt}n}/m_{\text{Pt1}}$ of the magnetic spin moments as obtained directly from the *ab initio* calculations. For the $L_3$ edge which has been used in the experimental study of Ref. 2, the magnetization profile obtained from the spectra with the assumption $\Delta\tilde{\beta}_{\text{Pt}n}\sim m_{\text{Pt}n}$ is similar to the directly calculated profile, albeit for the inner layers the values still differ considerably. For the $L_2$ edge, however, the agreement between the directly calculated ratios and the spectral ratios is much worse. The ratios of the magnetic moments obtained from the spectra broadened according to the natural linewidth differ by a factor of 2 from those of the directly calculated moments. Interestingly

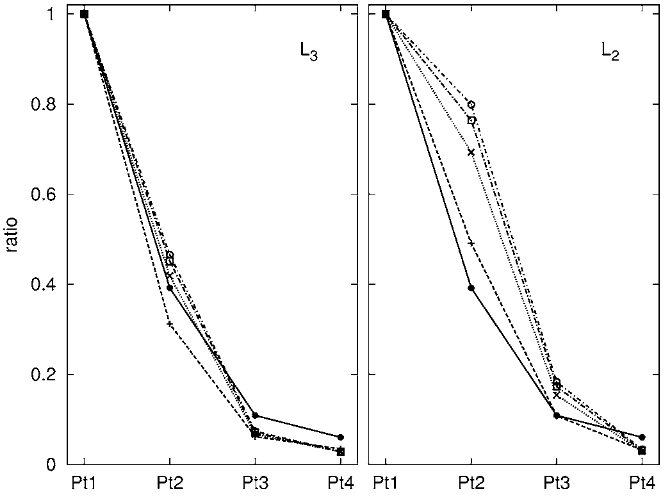

FIG. 2. Magnetization profile $m_{\mathrm{Pt}n}/m_{\mathrm{Pt}1}$ as obtained from the direct *ab initio* calculation (•) and from the ratio $\tilde{\sigma}^{(2)}_{xy,\mathrm{Pt}n}/\tilde{\sigma}^{(2)}_{xy,\mathrm{Pt}1}$ for energies corresponding to the $L_3$ and $L_2$ edges. The spectra $\tilde{\sigma}^{(2)}_{xy}(E)$ thereby have been broadened with a Lorentzian of widths $\Gamma = 50$ mRy (+), 100 mRy (×), 150 mRy (□), and 215 mRy (○). Lines are merely guides to the eye.

enough, the agreement between the two ratios deteriorates when going to larger broadening, both for the $L_2$ and the $L_3$ edge. The possible reasons for the deviations between the two ratios are the same as those discussed at the end of Sec. II. For instance, the orbital moments $m_\ell$ are not very much smaller than the spin moments $m$ (Table I). In addition, it has been shown in Ref. 8 that for the Pt layer at the Co-Pt interface, the $\hat{T}_z$ contribution to the dichroic signal cannot be neglected, and also because of this reason Eq. (15) does not hold exactly.

The result that a linear relation between the optical constants and the induced Pt spin moment appears to be a rather good approximation for the Pt $L_3$ edge but not for the $L_2$ edge may be rationalized in the following way. In a system such as Pt with strong spin-orbit coupling, our Eq. (14) should be replaced by Eqs. (21) and (22) of Ref. 16 where the ratios $\mu_c(\omega)/\mu(\omega)$ for the $L_2$ and $L_3$ edges are approximately related to the $\kappa$-projected spin polarizations of the $5d_{3/2}$ and $5d_{5/2}$ states, respectively, rather than to the total $5d$ spin polarization. However, the behavior of each of the $\kappa$-projected spin polarizations is not necessarily the same as the behavior of the total spin polarization which is composed of the $d_{3/2}$ and $d_{5/2}$ contributions as well as of cross terms between them. For the case of Pt impurities in Fe, e.g., it has been shown[17] that the $d_{3/2}$ part contributes only slightly to the total $5d$ spin polarization, whereas there is a substantial contribution of the $d_{5/2}$ part. It thus becomes plausible that a linear relation between the optical constants and the total $d$ spin moment is a much better approximation for the $L_3$ edge than for the $L_2$ edge.

TABLE I. Atomic magnetic spin ($m$) and orbital ($m_\ell$) moments of the crystallographically inequivalent Pt layers given in units of Bohr magneton.

| | Pt1 | Pt2 | Pt3 | Pt4 |
|---|---|---|---|---|
| $m$ | 0.22 | 0.085 | 0.024 | 0.013 |
| $m_\ell$ | 0.044 | 0.015 | 0.0015 | 0.0014 |

Altogether, our calculations show that for the Co-Pt multilayer system, the x-ray magnetic reflectometry may yield semiqualitative results for the magnetization profile when photon energies corresponding to the $L_3$ edge are used (as in Ref. 2). Deviations between the so-obtained magnetization profile from the profile calculated directly by the *ab initio* electron theory for an ideal Co-Pt layer therefore probably give a hint to the fact that the Co-Pt interface in the real sample was not ideal due to interdiffusion, roughness, etc.

## IV. CONCLUSIONS

At present the x-ray magnetic reflectometry is probably the best available method for the element- and layer-selective characterizations of the technologically important multilayer systems (possible alternatives are absorption experiments with polarized x rays by detecting the total electron yield for different angles of incidence and neutron reflectometry experiments). The basic assumption thereby is that the magnetic contributions to the optical constants of the various layers are proportional to the magnetic moments of these layers. Our theoretical considerations and our explicit *ab initio* calculations for the multilayer system $\mathrm{Co_2Pt_7}$ have shown that this assumption is not always quantitatively justified, and thus the validity of this assumption has to be justified for each individual system under consideration. To do this, we suggest combining the experiments on a specific multilayer system always with *ab initio* calculations for the corresponding (or a very similar) ideal multilayer system with ideal interfaces. If the results of the *ab initio* calculations confirm the approximate validity of the basic assumption, then the reflectometry can be used to study the magnetization profile in the real multilayer system for which the interface is most probably not ideal due to interdiffusion, roughness, etc. If there is no chance to perform simultaneous experimental and theoretical studies, we suggest performing the reflectometry experiment at least at two different energies, e.g., at energies corresponding to the $L_2$ and the $L_3$ edge. If the magnetization profiles for the two energies are rather different, then the system cannot be safely characterized by the magnetic x-ray reflectometry.

In general, we expect that the basic assumption is well justified if the following two preconditions are fulfilled.

(a) The spin-orbit coupling should not be too strong because then the magnetic x-ray absorption spectrum is not nearly exclusively determined by the spin moment but also by the orbital moment, and then Eq. (14) is not strictly valid. This, unfortunately, means that extreme care has to be taken when considering systems with potential application for magneto-optical recording because those usually involved atoms with large spin-orbit coupling.

(b) The width of the x-ray line should not be much smaller than the range of extension of the spectrum $\Delta\tilde{\beta}(\omega)$. The minimum width is the one determined by the natural linewidth due to the finite lifetime of the core hole. The total width of the line can be manipulated by the experimentalist by manipulating the instrumental linewidth. We suggest using large instrumental linewidth but of course still compatible with the other requirements of the experiment (e.g., good angular resolution).

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