# Electron-yield saturation effects in *L*-edge x-ray magnetic circular dichroism spectra of Fe, Co, and Ni

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Saturation effects are determined in x-ray magnetic circular dichroism spectra, acquired by electron yield techniques. It is shown that sum-rule extraction of the number of *d* holes, orbital moment, and spin moment are affected for Fe, Co, and Ni. In particular, errors in the extracted orbital moment values due to saturation effects can be in excess of 100% and even yield the wrong sign for films as thin as 50 Å. They are significant even for film thicknesses of a few monolayers. Errors for the derived values for the number of *d* holes and the spin moment are considerably smaller but may be of the order 10-20 %. Correction factors are given for quantities obtained from sum rule analysis of electron yield data of Fe, Co, and Ni as a function of film thickness and x-ray incidence angle. [S0163-1829(99)01009-7]

#### I. INTRODUCTION

With the continued success in the utilization of x-ray magnetic circular dichroism (XMCD) spectroscopy to extract element-specific magnetic information from heteromagnetic systems, there is an increasing need to obtain reliable quantitative results from measured helicity dependent photoabsorption cross sections. As a variant of x-ray absorption spectroscopy, XMCD spectroscopy first introduced in 1987,<sup>1</sup> has been extensively used to determine element specific spin and orbital moments,<sup>2–12</sup> identify moment orientations in ultrathin films and monolayer magnetic materials,<sup>13,14</sup> and even characterize anisotropy in the orbital moment vector and spin density.<sup>15–17</sup>

As the analysis procedures become increasingly more powerful and sophisticated through sum rule analysis,<sup>18,19,15</sup> concerns over the presence of small systematic errors in the measured data have naturally risen. One area of repeated concern is the possible presence of saturation effects in the acquired data. Typically, saturation effects are discussed in conjunction with fluorescence or electron yield detection in x-ray absorption spectroscopy.<sup>20–23,9,10,24</sup> They are also called self-absorption effects<sup>22</sup> and in conjunction with x-ray transmission measurements they are commonly termed thickness effects.<sup>25–28</sup> Saturation effects result in a recorded signal which is not proportional to the photoabsorption cross-section as the photon energy is varied. In particular, the intensities of prominent absorption peaks are reduced or "saturated."

For the important 3*d* transition metals Fe, Co, and Ni soft x-ray absorption studies at the respective *L* edges are of particular interest and, for experimental convenience such measurements are typically carried out by means of electron yield detection.<sup>3–11</sup> Saturation effects arise if the electron yield sampling depth is larger than or comparable to the

absorption depth of the incident x rays. Owing to the small probing depth (of order 20 Å) in electron yield absorption measurements, which is a direct consequence of the short electron mean free path in solids,<sup>29</sup> it was originally thought that saturation effects would be insignificant. However, it is now known from careful transmission measurements<sup>30</sup> that in Fe, Co, and Ni the x-ray absorption lengths at the  $L_{2,3}$  edge thresholds ("white line" positions) are quite short (about 200 Å). The impact of saturation effects on extracted data from electron yield XMCD spectra must therefore be re-examined. The great sensitivity to saturation effects is a consequence of the requirement of accurate determination of the  $L_{2,3}$  resonance intensities for sum rule extraction of magnetic moments.<sup>18,19</sup>

In this paper we examine theoretically and experimentally the impact of saturation effects on electron yield XAS and XMCD measurements for extracting relevant material parameters such as the number of d holes  $N_{3d}$  (energy integral of the polarization-averaged absorption curve), and the orbital  $m_{\rm orb}$ , and spin  $m_{\rm spin}$ , moments (integrals of the XMCD difference curves). By using polarization dependent transmission spectra as absolute measures of the photoabsorption cross sections of Fe, Co, and Ni, and from measured values of the electron yield sampling depth we find that the saturation effect has a large impact on the orbital moment extraction and is significant even for films as thin as a few Å. Under unfavorable circumstances the derived orbital moment may even have the incorrect sign. The effect on the derived values for the number of d holes and the spin moment are considerably smaller but may be of the order 10-20 %.

# II. ELECTRON AND FLUORESCENCE YIELD IN MAGNETIC MATERIALS: SPIN DEPENDENT EFFECTS

The x-ray absorption cross section of an atom is directly proportional to the number of core holes created in the ab-

6421

sorption process.<sup>31</sup> Any process which is a true measure of the number of created core holes can therefore be used for quantitative x-ray absorption spectroscopy. For Fe, Co, and Ni core holes are created in the 2p core shell which is subsequently filled by Auger electron (99.2%) or fluorescence (0.8%) decay.<sup>32</sup> In magnetic materials the valence band is split into minority and majority spin subbands with unequal populations. In such cases the Auger and fluorescence decays become spin dependent <sup>33,34</sup> and one needs to consider the effects of spin dependent deexcitations and, for electron yield detection, spin-dependent transport. We shall discuss them, in turn, below.

We shall first consider spin-dependent decay effects of a valence electron into a core hole. The absorption of circularly polarized x rays creates spin polarized core holes.<sup>35</sup> The subsequent Auger (Coulomb operator) and fluorescence (dipole operator) decays then involve different matrix elements for transitions to final states with different spin configurations. For fluorescence decay spin flips are forbidden and the spin polarized core hole can only be filled by valence electrons of the same spin. In Auger electron decay the matrix element leading to a singlet final state (two valence holes with opposite spin) is larger than that leading to a triplet final state and the emitted Auger electrons exhibit a significant spin polarization.<sup>33</sup> Simple two-step models for core to valence excitation and valence to core  $(3d \rightarrow 2p)$ deexcitation<sup>33,34</sup> would then predict that neither  $L_{\alpha,\beta}$  fluorescence yield nor  $LM_{4.5}M_{4.5}$  Auger electron yield measurements are equivalent to XMCD absorption measurements. In particular, spin-resolved Auger electron yield measurements are predicted to yield enhanced XMCD effects and even spin-integrated measurements are expected to show deviations from the true absorption signal. However, a more realistic description of the fluorescence yield in terms of an inelastic scattering process, involving interference of intermediate states, shows quantitative agreement between the fluorescence yield signal and the x-ray absorption cross section in magnetic materials.<sup>36</sup> More sophisticated models for the spin-integrated Auger electron intensity are also expected to yield a direct proportionality to the x-ray absorption cross section. For total electron yield detection, the contributions of the various Auger decay channels (e.g., all  $LM_xM_y$  channels where x and y may be valence or core states) furthermore average out spin-dependent matrix element effects in the core hole decay.

The second effect caused by the spin-dependent band structure of magnetic materials is spin-dependent transport. Of particular interest in conjunction with total electron yield XMCD measurements, performed without spin analysis, is the electron yield sampling or escape depth. In our case, the electron escape depth  $\lambda_{\rho}$  is the average depth from which the measured spin-up and spin-down electrons originate. The further away the excited atom is from the surface, the less likely the primary and secondary Auger electrons will escape from the sample. The total electron yield signal from the sample is dominated by the inelastically scattered electron cascade (secondary electrons) originating from the primary spin polarized Auger electrons.<sup>37,31</sup> Measurements of the transmission of spin polarized electrons through a ferromagnetic metal reveal that high-energy (above about 50 eV) spin-up and spin-down Auger electrons produce an equal



FIG. 1. Qualitative description of (a) transmission and (b) electron yield methods for x-ray absorption measurements.

number of secondary electrons per primary electron.<sup>38</sup> There is no spin filter effect, unlike for low-energy elastic photoelectrons.<sup>39</sup> This fact is the reason for the difficulty of building a spin detector for electrons in the 100–1000 eV range. The total (spin-up plus spin-down) number of secondary electrons is therefore proportional to the number of elastic Auger electrons created in the core hole decay and it is a good measure of the x-ray absorption cross section.

In summary, the above discussion shows that in magnetic materials the spin-integrated total electron yield signal is a quantitative measure of x-ray absorption. In the following we can therefore ignore the electron spin in the discussion of electron yield saturation effects in XMCD spectra.

# **III. DESCRIPTION OF SATURATION EFFECTS**

Figure 1 depicts the mechanisms of transmission and electron yield measurements of x-ray absorption. Figure 1(a) shows the transmission method, where the transmitted photon intensity decays exponentially as a function of sample thickness t with a decay constant  $\mu$ , the linear absorption coefficient. The x-ray absorption coefficient  $\mu$  is directly obtained from transmission absorption measurements and is described by the familiar equation

$$I(\hbar\omega) = I_0 \ e^{-\mu t},\tag{1}$$

where I is the intensity of the transmitted photons,  $I_0$  is the incoming photon intensity,  $\mu$  is a function of photon energy  $\hbar \omega$ , and t is the sample thickness. We see here that transmission measurements give the x-ray absorption coefficient  $\mu$ from measuring  $I/I_0$  as a function of photon energy  $\hbar \omega$ , since  $\mu = -(1/t)\ln(I/I_0)$ . To maintain a measurable photon intensity after transmission, the sample must be of finite thickness (less than about  $2/\mu_{max}$ , where  $\mu_{max}$  is the maximum value of the energy-dependent absorption coefficient in the energy range of interest.<sup>40</sup>) With transmission measurements, saturation in the signal occurs when either the sample thickness t or the absorption coefficient  $\mu$  is too large. At these conditions, the transmitted intensity I "saturates" at zero, no matter what the variation in the energy-dependent  $\mu$ spectra might be. However, this is usually not a problem, since the sample thickness can typically be adjusted.

Figure 1(b) shows the electron yield method, where the number of electrons (and hence the rate of absorption) can be



FIG. 2. Illustration of saturation effect for Fe. Left: The difference in the x-ray intensity arriving at depth  $z = \lambda_e = 17$  Å is shown, compared to the incident x-ray intensity at z=0 ( $I_0=1$ ). Center: Probability of electron escape, plotted in a horizontal bar graph as a function of depth z. The probability of escape is unity at the sample surface (z=0) and drops to 1/e at  $z=\lambda_e$ . Right: Hypothetical electron yield spectra generated from the absorbed photons in layers at a depth z=0 and  $z=\lambda_e$ . The measured total electron yield spectrum outside the surface consists of contributions from the various layers weighted by the probability of escape from the surface (shown in center).

measured by counting the electrons which escape from the surface of the sample<sup>31</sup> (however, this signal may not accurately reflect the rate of absorption, as will be discussed below). In total electron yield measurement the intensity of the escaped electrons is recorded with a channeltron electron detector or, more simply by direct measurement of the electrical current from the sample to the ground by means of a picoammeter. In Fig. 1(b),  $\theta$  is the x-ray incidence angle from the surface normal,  $\lambda_x$  is the x-ray penetration *length* (also called the x-ray attenuation length) which is the inverse of the absorption coefficient ( $\lambda_x = 1/\mu$ ),  $\lambda_x \cos \theta$  is the x-ray penetration *depth*, and  $\lambda_e$  is the electron sampling or escape depth discussed in the previous section.

#### A. Illustration of saturation effects

The degree to which saturation of the signal occurs in the electron yield signal depends on the relative photon penetration depth and electron escape depth. The saturation mechanism in electron yield can be illustrated from an example in the extreme case where the x-ray penetration depth is much shorter than the electron escape depth. All incident photons will be converted into photoelectrons and therefore the electron signal is proportional only to the incident photon intensity  $I_0$  and not to the absorption coefficient  $\mu$ . Hence we see that the electron yield signal has completely saturated in the limit  $\lambda_e \gg \lambda_x \cos \theta$ .

Figure 2 illustrates the electron yield saturation effects in more detail. Our model calculations used parameters  $\lambda_e$  and  $\mu$  for Fe (see below) and assumed an x-ray incidence angle of  $\theta = 0^{\circ}$ . In this figure, the horizontal lengths of the gray bars in the center represent the "weight" of the electron yield signal for each layer—i.e., the length of the bar represents the number of electrons which actually reach the surface and escape if the rate of electron production were the same for every layer. The number of electrons that reach the surface  $dY_e(z)$  decays exponentially as a function of depth of the original x-ray absorption process<sup>41</sup>

$$dY_e(z) = dY_{e,0}(z) e^{-z/\lambda_e},$$
(2)

where z is the depth from the surface and  $dY_{e,0}(z)$  is the number of electrons produced in a layer of thickness dz at depth z. In the center panel of the figure, each bar represents a dz=2 Å thick layer of Fe, and the two darker bars represent the layers at the surface (z=0) and at one electron escape depth  $(z=\lambda_e=17 \text{ Å})$  below the surface.

In Fig. 2, it is assumed that the incident flux is constant over the photon energy region of the *L* edge (top left). At the surface layer, therefore, the electron yield will exactly resemble the shape of the true Fe absorption spectrum (top right). As the photons pass through the various layers, they are absorbed. In the bottom left figure, we see a 10% drop of the incident x-ray intensity at the  $L_3$  absorption edge at a depth  $z=\lambda_e$ , whereas there is hardly any drop in the preedge region. This reduced flux directly affects the electron yield from this layer as shown in the bottom right of Fig. 2. We see a 10% drop at the  $L_3$  edge in the hypothetical electron yield (unweighted for escape probability) from this layer. The total electron yield signal is simply the sum of the contributions from the various layers weighted by the electron escape probability shown in the center.

#### B. Quantitative description of saturation effects

The two important parameters which describe the energy dependence of the electron yield are the x-ray penetration depth  $\lambda_x \cos \theta$ , and the electron escape depth  $\lambda_e$ . The x-ray penetration length  $\lambda_x$  is the inverse of the x-ray absorption coefficient  $\mu$ , and its values for the  $L_{2,3}$  absorption edges for the elements Fe, Co, and Ni, obtained from reported transmission data,<sup>30</sup> are shown in Fig. 3. The electron escape depths for bulk Fe, Co, and Ni were experimentally determined by preparing a wedge sample for each element as shown in Fig. 4 and measuring the respective *L*-edge electron yield spectra at various sample thicknesses. From the measured spectra we determined the  $L_3$  and  $L_2$  and the con-



FIG. 3. X-ray penetration length at the  $L_{3,2}$  edges of Fe, Co, and Ni, obtained from transmission data (Ref. 30). The penetration depth is about 6000 Å in the pre-edge region (not shown), where the photon absorption rate is small.

tinuum (40 eV above  $L_3$  energy) edge jumps J,<sup>41</sup> defined as the differences in spectral intensity at the three energies relative to those below the  $L_3$  edge. For our wedge structures the Fe, Co, and Ni edge jumps increase with the thickness t of the magnetic layers according to

$$J = J_{\infty} [1 - \exp(-t/\lambda_e)]$$
(3)

assuming that the x-ray penetration depth is much longer than the electron yield sampling depth  $\lambda_x \cos \theta \gg \lambda_e$ . Here  $J_{\infty}$ is the edge jump value in the limit of large sample thickness  $t \ge \lambda_e$ . Within experimental error bars (~10%) we obtained the same values for  $\lambda_e$  from fits of the three edge jump curves, indicating that for the present analysis the approximation  $\lambda_r \cos \theta \gg \lambda_e$  is adequate. The results for the thickness dependent post-edge minus pre-edge jumps, normalized to  $J_{\infty} = 1$ , are shown in Fig. 4. From the fits we determine electron sampling depths of  $17\pm 2$  Å for Fe and  $25\pm 3$  Å for Co and Ni. We note that, in general, the electron sampling depth depends on the crystallographic and electronic structure. For the transition metals the most important parameter appears to be the number of d holes<sup>42,43</sup> which is approximately constant for different crystallographic phases of the metals Fe, Co, and Ni, respectively. We therefore believe the above values for  $\lambda_{e}$ , within the quoted error bars, to be representative for the three metals.

The electron yield signal is comprised of photoelectrons, Auger electrons, and secondary electrons generated from the



FIG. 4. Measured *L*-edge jump as a function of Fe, Co, and Ni layer thickness *t* using the wedge structure shown on top. The *L*-edge jump was defined as the difference in electron yield intensity in the pre-edge and post-edge regions of the measured spectra. The jumps are fit to an exponential function of the form  $1 - e^{-t/\lambda_e}$ , as discussed in the text, to determine the electron yield sampling depth  $\lambda_e$ .

inelastic cascade process of the high energy primary electrons (we ignore secondary processes such as the reabsorption of emitted fluorescence photons from core-hole relaxation). The high-energy Auger electrons created in the core hole decay are predominantly responsible for the secondary electron signal which dominates the total electron yield.<sup>37</sup> The number of Auger electrons created in the sample (including Coster-Kronig transitions) at depth *z* within thickness *dz* per unit time is  $dY_{e,0}(z)$ , and is given by<sup>41</sup>

$$dY_{e,0}(z) = I_0 e^{-\mu z/\cos\theta} \frac{\mu dz}{\cos\theta}.$$
 (4)

Here,  $I_0$  is the number of photons incident on the sample,  $I_0 e^{-\mu z/\cos \theta}$  is the same quantity at depth z of the sample,  $z/\cos \theta$  is the distance traversed by the photons through the sample before they reach depth z,  $\theta$  is the x-ray incidence angle from the surface normal, and  $\mu dz/\cos \theta$  is the fraction of photons absorbed within thickness dz. We assume negligible x-ray reflection at the sample surface which is a good assumption for x-ray incidence angles within the range  $10^{\circ}$   $<\theta \le 90^{\circ}$ , and that the probability for the emission of an Auger electron due to the filling of the vacancy is unity, which is true for the x-ray energy range in interest (500– 1000 eV) for Fe, Co, and Ni.<sup>41</sup>

The net total electron yield  $Y_e$  of a sample of semi-infinite thickness can be described by substituting Eq. (4) into Eq. (2) and integrating over the depth z from z=0 to  $z=\infty$  and accounting for the electron cascading process and escape into vacuum we obtain

$$Y_e = C\left(\frac{1}{1 + \lambda_e / \lambda_x \cos\theta}\right) \mu.$$
 (5)



FIG. 5. Correction factor  $f(\theta, \lambda_x, \lambda_e)$  as a function of (a) the electron escape depth to x-ray penetration depth ratio  $\lambda_e / \lambda_x$  and (b) the x-ray incidence angle  $\theta$  (for various values of  $\lambda_e / \lambda_x$ ). The plotted  $\lambda_e / \lambda_x$  values 0.003, 0.02, and 0.10 correspond to the preedge, post-edge, and  $L_3$  peak energies in Fe, respectively.

The proportionality constant is given by  $C = I_0 G \lambda_e / \cos \theta$ where the electron gain function *G*, which is proportional to the photon energy, describes the average number of electrons produced through a "cascade" process initiated by a single Auger electron.<sup>41</sup> *C* increases with the electron sampling depth  $\lambda_e$  and through the  $\cos \theta$  term it is enhanced at glancing x-ray incidence because the photons are absorbed closer to the surface and produce more photoelectrons.

The saturation effect in Eq. (5) is explicitly expressed by the correction factor

$$f(\theta, \lambda_x, \lambda_e) \equiv \frac{1}{1 + \lambda_e / \lambda_x \cos \theta}, \qquad (6)$$

which is a function of the ratio  $\lambda_e/(\lambda_x \cos \theta)$  as discussed earlier. When  $\lambda_x \cos \theta \gg \lambda_e$ , then f=1 and  $Y_e = C\mu$ , and there is no saturation effect, but when  $\lambda_e \gg \lambda_x \cos \theta$ , then  $f \approx \lambda_x \cos \theta / \lambda_e$  and  $Y_e = C/\lambda_e = \text{const}$ , and we have total saturation.

We can examine the dependency of this correction factor on the escape-to-penetration depth ratio and the x-ray incidence angle. Figure 5(a) shows *f* as a function of the ratio of the electron escape depth to x-ray penetration depth, for  $0 \le (\lambda_e / \lambda_x \cos \theta) \le 1$ . For the correction factor to approach unity within 1%,  $\lambda_e / \lambda_x \cos \theta$  must be less than 0.01. In the range  $0.01 \le \lambda_e / \lambda_x \cos \theta \le 1$ , the electron yield signal is neither directly proportional to  $\mu$  nor completely saturated, and this is the range where most of the resonance absorption data lies.

Figure 5(b) shows the correction factor as a function of the x-ray incidence angle  $\theta$  at selected  $\lambda_e / \lambda_x$  ratios. Here the values  $\lambda_e / \lambda_x = 0.003$ , 0.02, and 0.10 correspond to the preedge, post-edge, and  $L_3$  peak energies in the Fe XAS spec-



FIG. 6. Absorption spectra obtained by transmission measurements (Ref. 30), corresponding to 100% circular polarization and alignment of the photon spin and magnetization direction.

trum, respectively. As the x-ray incidence angle increases (approaches more grazing angles relative to the surface), the x-ray penetration *depth*  $\lambda_x \cos \theta$  is made artificially shallower, although the x-ray penetration *length*  $\lambda_x$ , remains unchanged. In such cases, the electron escape depth to x-ray penetration depth ratio increases dramatically, and we see that the saturation effect is larger at grazing angles than at normal x-ray incidence.

The above description for samples of semi-infinite thickness can readily be extended to samples of finite thickness t. Instead of Eq. (5) the electron yield is then given by

$$Y_e(t) = C \frac{1}{1 + \lambda_e / \lambda_x \cos \theta} \{ 1 - e^{-t(1/\lambda_e + 1/\lambda_x \cos \theta)} \} \mu.$$
(7)

We shall also consider this case below.

# IV. MODELING OF SATURATION EFFECTS IN Fe, Co, AND Ni

The quantitative form of the electron yield signal given by Eqs. (5) and (7) shows that, in general, the removal of the saturation effect is difficult, since this requires inverting the nonlinear energy dependent electron yield function. The problem is that the correction factor *f* is energy dependent. For example, one may fit the measured electron yield spectrum  $Y_e(\hbar \omega)$  to the true absorption coefficient  $\mu$  in the preand post-edge regions<sup>44</sup> where according to Fig. 5(b) the saturation effects are small, but then the white line intensities remain saturated. In contrast, the determination of the size of the saturation effect is an easy task if the electron mean free path  $\lambda_e$  and  $\mu = 1/\lambda_x \cos \theta$  are known, since the electron yield can be calculated and modeled. Below we shall use this procedure to determine the effect of signal saturation in electron yield XAS and XMCD spectra for Fe, Co, and Ni films.

In order to model the electron yield and hence its saturation, the absolute energy and polarization-dependent x-ray absorption coefficients for the relative alignment of photon



FIG. 7. Saturation effect modeling in electron yield mode for bulk Fe. We have plotted the fraction of the values for the number of holes  $(N_{3d})$ , the spin magnetic moment  $(m_{spin})$ , and the orbital magnetic moment  $(m_{orb})$  obtained by sum rule analysis of electron yield data relative to those obtained from ideal unsaturated data, as discussed in the text. Left: as a function of x-ray incidence angle, measured with respect to surface normal. Right: as a function of sample thickness, for normal  $(\theta=0^{\circ})$  and grazing  $(\theta=70^{\circ})$  x-ray incidence.

spin (helicity) and magnetic moment directions must be known near the  $L_{3,2}$  resonances. Data from transmission mode XMCD measurements,<sup>30</sup> used to determine the cross sections, are shown in Fig. 6. The absorption spectra  $\mu_{\text{theo}}^+$ and  $\mu_{\text{theo}}^-$  for bulk Fe, Co, and Ni shown in this figure have been recalculated to correspond to 100% circular polarization and alignment of the saturation magnetization direction along the photon spin direction. The spectra were obtained as follows. The background signal was removed from the measured transmission data according to tabulated pre- and postedge continuous cross sections.<sup>44</sup> The dichroism difference spectra, obtained by substraction of the measured helicity



FIG. 8. Saturation effect modeling in electron yield mode for bulk Co, similar to Fig. 7.



FIG. 9. Saturation effect modeling in electron yield mode for bulk Ni, similar to Fig. 7.

dependent absorption spectra, were then corrected for the finite angle between the photon helicity-direction and the sample magnetization direction in the transmission geometry (cos 45°) and for incomplete circular polarization (76%).<sup>30</sup> The corrected helicity dependent x-ray absorption spectra,  $\mu_{\text{theo}}^+$  and  $\mu_{\text{theo}}^-$ , were then calculated by adding and subtracting the corrected dichroism difference spectra (100% polarization) to the average of the measured absorption spectra ( $\mu_{\text{exp}}^+ + \mu_{\text{exp}}^-$ )/2.

The saturation effect was modeled (i) as a function of x-ray incidence angle for samples with semi-infinite thickness and (ii) as a function of sample thickness, for x-ray incidence angles of  $\theta = 0^{\circ}$  and  $70^{\circ}$ , for bulk Fe, Co, and Ni. For each point in the absorption spectra, Eq. (5) for semi-infinite thickness samples and Eq. (7) for finite thickness sample were applied (setting C=1), and a new theoretical electron yield spectrum was calculated, using the  $\lambda_e$  values obtained from the wedge sample measurements.

Once the calculated electron yield spectra  $Y_e^+$  and  $Y_e^$ were obtained, sum rule analyzes<sup>18,19,15</sup> were applied to obtain the orbital  $m_{\rm orb}$ , and spin  $m_{\rm spin}$  moments and the number of *d* holes  $N_{3d}$ . For the *d*-hole determination we used the white line intensity of the  $(Y_e^+ + Y_e^-)/2$  spectra. The determined values were then compared to those obtained from the corresponding  $\mu_{\rm theo}^+$  and  $\mu_{\rm theo}^-$  spectra, and their ratios are shown in Figs. 7–9, for Fe, Co, and Ni, respectively. In each case, the same procedures were used so that the calculated corrections are entirely due to saturation effects.

# V. RESULTS

In every case, we observe that the saturation effect results in a decrease in  $N_{3d}$  compared to the analysis of the true absorption spectra. The reduced values for  $N_{3d}$  determined from the electron yield signal originates from signal saturation at the resonance peaks. The orbital and spin magnetic moments behave similarly, since the dichroism signal (the difference of the  $\sigma = \pm 1$  photon absorption) also decreases in size due to the saturation effect: The signal from the higher resonance peak from one of the polarizations ( $\sigma =$ -1 absorption at  $L_3$ , for example) is saturated more than that of the other polarization ( $\sigma = +1$  at the same  $L_3$  peak),



FIG. 10. Saturation effect modeling in electron yield mode as a function of degree of circular polarization for bulk Fe. We have plotted the fraction of the values for the spin magnetic moment  $(m_{spin})$  and the orbital magnetic moment  $(m_{orb})$  obtained by sum rule analysis of electron yield data recorded at x-ray incidence angle  $\theta$ , relative to the values obtained with unsaturated 100% polarized data. The solid line is a linear fit to the calculated data points.

and hence the difference of the two, the XMCD effect, is smaller with electron yield detection compared to the true dichroism signal.

Of the three quantities  $m_{\rm orb}$ ,  $m_{\rm spin}$ , and  $N_{3d}$  the orbital magnetic moment is affected to a much larger degree compared to the spin moment or the number of d holes. Since the saturation effect is larger for the  $L_3$  than the  $L_2$  intensities the orbital moment is more effected since it corresponds to the difference between the absolute dichroism intensities at the two edges, as opposed to a sum of areas for the other two cases. For the case of Fe, we see that the orbital magnetic moment can actually appear to be negative due to electron vield saturation, for x-ray incidence angles larger than 70°. On the other hand, the hole count and the spin moment are affected less by saturation effects, up to 15 and 23 %, respectively. The degree of error for the hole count and the spin moment are related in going from Fe to Co to Ni. It is important to note that saturation effects can be significant for very thin samples. The extracted orbital moment for a 10 Å Fe film at 70° x-ray incidence angle is only 60% of the true value.

In practice, almost all measured electron yield spectra contain effects due to, both, saturation and incomplete circular polarization. The question arises whether the sequence of correction for saturation and polarization effects matters. This is addressed by the results shown in Fig. 10. Here we have plotted the dependence of the saturation effect for the spin and orbital moments on the degree of circular polarization for the case of Fe metal. The moments determined from

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the electron yield dichroism data, which contain saturation effects, are seen to depend linearly on the degree of circular polarization for all x-ray incidence angles. Therefore, according to Figs. 7-9, the order of correction of the measured electron yield data does not matter.

#### VI. CONCLUSION

We have modeled saturation effects in Fe, Co, and Ni  $L_{3,2}$ -edge photon absorption spectra recorded by electron yield detection for different sample thicknesses and x-ray incidence angles, and determined their effect on the derived values for  $N_{3d}$ ,  $m_{spin}$ , and  $m_{orb}$ . We have found that the values determined from electron yield data are always less than the actual values due to saturation, and that the orbital magnetic moment determination may be severely in error due to saturation effects. Smaller errors are found for the hole count and the spin magnetic moment. We have provided plots for Fe, Co, and Ni which allow the correction of experimental XAS and XMCD data obtained with electron yield detection. These should allow a more accurate determination of materials parameters from electron yield x-ray absorption spectra.

#### ACKNOWLEDGMENT

One of us (J.S.) would like to thank Boris Sinković for valuable discussions regarding spin-dependent Auger electron de-excitation and spin filtering effects.

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