X-ray resonant reflection from magnetic multilayers: Recursion matrix algorithm

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Recursion equations for 2×2 scattering matrices have been derived to calculate resonant x-ray reflection from magnetic multilayers. The solution has been basically reduced to that found in Stepanov *et al*, Phys. Rev. B **57**, 4829 (1998) for grazing incidence x-ray diffraction from crystalline multilayers.

I. INTRODUCTION

For a number of years the majority of magnetic materials studies were carried out with neutrons, while x rays were solely used as an auxiliary tool to obtain the crystal structure data of the materials.[1–5] The magnetic scattering of x rays was not of practical interest because of its weakness as compared to the usual x-ray charge scattering. The situation changed after the discovery of a huge resonant enhancement for the x-ray magnetic scattering near some absorption edges.[6,7] Since then the resonant x-ray magnetic scattering has become a new experimental tool for the investigation of magnetic materials.

At the beginning, the resonant magnetic x-ray scattering was mostly measured around high-angle Bragg peaks from bulk magnetic materials[6,8–12] or thick magnetic films.[13] Nowadays, the increasing interest in thin magnetic films and multilayers has stimulated the application of grazing incidence x-ray techniques that are specifically sensitive to the structure of thin surface layers. Grazing incidence resonant x-ray reflection has been utilized for the investigation of an iron film[14] and magnetically coupled Ag/Ni multilayer.[15] Resonant grazing incidence x-ray diffraction[16] has been applied to the studies of magnetic effects at UO_2 and Co_3Pt surfaces.[17,18] Resonant x-ray diffuse scattering at grazing incidence has been used to measure the magnetic roughness of Co/Cu multilayers,[19] a 50-Å-thick $Co_{0.95}Fe_{0.05}$ film[20] and a Fe/Gd multilayer.[21]

In the conditions of magnetic resonance, the amplitude of x-ray scattering becomes anisotropic[7,22] and the conventional Parratt[23] and Abeles[24] techniques to calculate the x-ray reflection are generally not applicable. Thus a theory is required to calculate the resonant x-ray reflectivity from magnetic multilayers. This would also provide the x-ray wave fields inside the layers which are required for the calculation of grazing incidence diffraction[25,26] and diffuse x-ray scattering[27] with the distorted wave Born approximation technique.

To our knowledge, the problem of calculating x-ray resonant reflection from magnetic multilayers has not been fully addressed. Perhaps, the closest analogs to this task are the theories for the reflection of visible light from a multilayer consisting of anisotropic layers.[28,29] In these theories the Maxwell equations for the electromagnetic waves are reduced to four linear equations containing the product of 4×4 transfer matrices of individual layers. The results of Ref. 29 have been applied to calculate the x-ray resonant reflectivity of a five-layer system with one resonant layer.[30] However, the details and the restrictions of the calculations were not discussed.

Another similar analysis has been carried out for the x-ray reflection from multilayers under the conditions of Mössbauer resonance.[31–33] In Ref. 31 a special case was considered where the two x-ray eigenpolarizations in each layer are orthogonal and directed in the same way for all of the layers. Then, the reflectivity of Mössbauer multilayer could be reduced to the Parratt scalar recursive equations. In Ref. 32 the set of four linear equations for 4×4 transfer matrices was obtained as in the optics of anisotropic multilayers.[28] Finally, in a thesis by Baron[33] the solution was obtained in the form of recursive equations for 2×2 reflection and transmission matrices. That approach is the closest to what is suggested in our paper. However, Ref. 33 did not contain the analysis of special cases such as possible matrix singularities or the simplifications for hard x rays, etc. Also, of course, the specifics of magnetic scattering were not discussed since the work was devoted to the Mössbauer resonance. Some other theoretical attempts to build the theory of x-ray resonant reflection from magnetic multilayers are underway[34,35] but we believe that they do not overlap with this presentation.

In our study we analyze the x-ray reflection from an arbitrary stack of resonant magnetic and nonmagnetic layers. The problem is basically reduced to that of dynamical grazing incidence x-ray diffraction from a crystalline multilayer,[36] i.e., to the (2×2) recursive matrix algorithm for scattering matrices of individual layers. The formulas derived are valid for the whole x-ray wavelength range, and the simplifications are demonstrated for the medium-energy and hard x rays with small grazing incidence angles and weak interaction with matter.

In Sec. II the conventional reflection from nonresonant media with scalar susceptibility is derived. The idea is to introduce a common approach to both magnetic and nonmagnetic reflection, noting, moreover, that magnetic multilayers are often sandwiches of resonant and nonresonant (or nonmagnetic) layers.

In Sec. III the reflectivity of a layer with an aligned orientation of resonant scatterers is analyzed. At the end of that

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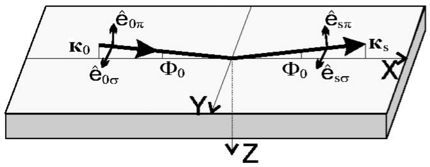

FIG. 1. X-ray reflection and our choice of coordinate system. Vectors $\boldsymbol{\kappa}_0$ and $\boldsymbol{\kappa}_s$ denote incident and specularly reflected waves, respectively; Φ_0 is the angle of these waves to the surface, $\hat{\mathbf{e}}_{\mathbf{m}n}$ are the unit vectors in the directions of σ and π polarization.

section the problem of resonant reflection from a magnetic layer is reduced to that of grazing incidence diffraction.

In Sec. IV a short survey of Ref. 36 is provided for the reader's convenience. Also some minor differences between our case and Ref. 36 are pointed out.

In Sec. V we present some model calculations using our technique and compare them with the data available in the literature.[30] Section V also contains the discussion of possible applications and further developments.

II. NONRESONANT X-RAY REFLECTION (SCALAR MEDIA SUSCEPTIBILITY)

Consider first the usual specular reflection of x rays from a slab with flat interface. The wave field in vacuum consists of the incident and specular waves with the amplitudes $\mathbf{E}_0$ and $\mathbf{E}_s$, respectively:

$$\mathbf{E}_\mathbf{v}(\mathbf{r})=(\mathbf{E}_0 e^{i\kappa\gamma_0 z}+\mathbf{E}_\mathbf{s} e^{-i\kappa\gamma_0 z})e^{i\boldsymbol{\kappa}_\parallel\cdot\mathbf{r}}. \qquad (1)$$

Here $\gamma_0=\sin\Phi_0$; Φ_0 is the incidence angle. Since electromagnetic waves in vacuum are transverse $(\mathbf{E}\cdot\boldsymbol{\kappa}=0)$, each of the waves $\mathbf{E}_0$ and $\mathbf{E}_\mathbf{s}$ can be split into σ- and π-polarization components chosen perpendicularly to the incidence plane, and in this plane respectively (see Fig. 1).

The electric field of the waves inside the isotropic slab must satisfy Maxwell's wave equation:[37]

$$\sum_{j=1}^{3}\{[\nabla^2+\kappa^2(1+\chi_0)]\delta_{ij}\}E_j(\mathbf{r})=0, \qquad (2)$$

where index $i=1,2,3$ lists the x,y,z components and χ_0 is the mean dielectric susceptibility of the media (see below).

Due to the lateral homogeneity of the problem, the lateral component of $\boldsymbol{\kappa}$ does not change at refraction and therefore the wave field $\mathbf{E}(\mathbf{r})$ inside the media can be represented as

$$\mathbf{E}(\mathbf{r})=\mathbf{E}e^{i\kappa u z+i\boldsymbol{\kappa}_\parallel\cdot\mathbf{r}}. \qquad (3)$$

The parameter u has the same physical meaning for the waves inside the slab as γ_0 for the vacuum waves, but unlike γ_0 it can be a complex number due to absorption or total reflection.

Substituting Eq. (3) into Eq. (2) we get

$$[(\gamma_0^2-u^2)+\chi_0]\mathbf{E}=0. \qquad (4)$$

The condition for a nonzero solution to Eq. (4)—the dispersion equation—is

$$(\gamma_0^2-u^2)+\chi_0=0, \qquad (5)$$

which brings

$$u^{(1,2)}=\pm(\gamma_0^2+\chi_0)^{1/2}. \qquad (6)$$

Thus in the general case of x-ray reflection from isotropic media there are two internal waves $\mathbf{E}^{(1)}$ and $\mathbf{E}^{(2)}$ corresponding to the $u^{(1)}$ and $u^{(2)}$, respectively. Since the waves in homogeneous media are transverse $(\mathbf{E}^{(j)}\cdot\mathbf{k}^{(j)}=0)$, each of the vectors $\mathbf{E}^{(j)}$ has only two independent components, $\mathbf{E}^{(j)}=(E_\sigma^{(j)},E_\pi^{(j)})$, where as in vacuum, π and σ polarizations are chosen in the plane of reflection and perpendicular to it, respectively.

On the other hand, the π and σ components can be viewed as separate waves because they are not linked through the wave equation [Eq. (4)]. Then, we can conclude that the reflection from homogeneous media produces four waves inside the slab—two σ and two π ones—and the polarizations are not exchanged.

The boundary conditions for the waves must be satisfied for the lateral components $\mathbf{E}_\parallel$ and $\mathbf{H}_\parallel$ of electric fields and magnetic fields, respectively. Since $\mathbf{H}\propto[\mathbf{k}\times\mathbf{E}]$, this gives

$$\gamma_0 E_{0\pi}-\gamma_0 E_{s\pi}=\sum_{j=1,2}E_x^{(j)}, \qquad (7)$$

$$E_{0\sigma}+E_{s\sigma}=\sum_{j=1,2}E_y^{(j)}, \qquad (8)$$

$$\gamma_0 E_{0\sigma}-\gamma_0 E_{s\sigma}=\sum_{j=1,2}u^{(j)}E_y^{(j)}, \qquad (9)$$

$$E_{0\pi}+E_{s\pi}=\sum_{j=1,2}[u^{(j)}E_x^{(j)}-n_x E_z^{(j)}], \qquad (10)$$

where Eqs. (9) and (10) are for $H_x\propto -k_z E_y$, $H_y\propto(k_z E_x-k_x E_z)$, respectively, and $n_x=\kappa_x/\kappa=(1-\gamma_0^2)^{1/2}$.

With the condition that the waves inside the media are transverse, Eqs. (7)–(10) can be transformed to

$$\gamma_0 E_{0\pi}-\gamma_0 E_{s\pi}=\sum_{j=1,2}u^{(j)}E_\pi^{(j)}/\epsilon^{1/2}, \qquad (11)$$

$$E_{0\sigma}+E_{s\sigma}=\sum_{j=1,2}E_\sigma^{(j)}, \qquad (12)$$

$$\gamma_0 E_{0\sigma}-\gamma_0 E_{s\sigma}=\sum_{j=1,2}u^{(j)}E_\sigma^{(j)}, \qquad (13)$$

$$E_{0\pi}+E_{s\pi}=\sum_{j=1,2}\epsilon^{1/2}E_\pi^{(j)}, \qquad (14)$$

where the parameter $\epsilon=1+\chi_0$ is the dielectric permittivity of the media.

Finally, Eqs. (11)–(14) can be presented in the 4×4 matrix form

$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ \gamma_0 & 0 & -\gamma_0 & 0 \\ 0 & \gamma_0 & 0 & -\gamma_0 \end{pmatrix} \begin{pmatrix} E_{0\sigma} \\ E_{0\pi} \\ E_{s\sigma} \\ E_{s\pi} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & \epsilon^{1/2} & 0 & \epsilon^{1/2} \\ u^{(1)} & 0 & u^{(2)} & 0 \\ 0 & u^{(1)}/\epsilon^{1/2} & 0 & u^{(2)}/\epsilon^{1/2} \end{pmatrix} \begin{pmatrix} E_\sigma^{(1)} \\ E_\pi^{(1)} \\ E_\sigma^{(2)} \\ E_\pi^{(2)} \end{pmatrix}. \quad (15)$$

For hard- and medium-energy x rays one can take $\epsilon \approx 1$ and the equations for σ and π polarizations become equivalent.

As follows from Eq. (6), the imaginary parts of roots $u^{(1)}$ and $u^{(2)}$ must have opposite signs. Let us choose $\mathrm{Im}[u^{(1)}] > 0$ and $\mathrm{Im}[u^{(2)}] < 0$. Then, the amplitudes of the waves corresponding to $u^{(1)}$ decrease and those for $u^{(2)}$ increase with z (i.e., towards the slab interior). The former and the latter waves can be interpreted as the refracted incident (or transmitted) waves and the ones specularly reflected from the lower interface of the slab, respectively. For a thick slab (no lower interface) one can take $E_\sigma^{(2)} = E_\pi^{(2)} = 0$. Then the four linear Eqs. (15) are sufficient to find the remaining four unknown amplitudes $E_{s\sigma}$, $E_{s\pi}$, $E_\sigma^{(1)}$, and $E_\pi^{(1)}$. If the slab is a multilayer, the boundary conditions like Eq. (15) can be applied at each interface, so that each layer adds four more unknown amplitudes and four more equations. Thus the problem remains soluble.

Of course, in the case of *nonresonant* x-ray reflection the boundary conditions for σ and π polarizations can be split into independent 2×2 matrix equations for each of the polarizations.[36] We make use of the 4×4 formalism in order to develop a common approach to both the usual case and the *resonant* x-ray reflection from magnetic layers where the polarizations interfere with each other.

III. RESONANT X-RAY REFLECTION (TENSOR MEDIA SUSCEPTIBILITY)

A. Susceptibility tensor

In the case of magnetic resonance the total amplitude for coherent elastic scattering of x rays from a magnetic atom is given by[6]

$$f = \left\{ f_0 + \frac{3\lambda}{8\pi}[F_{11} + F_{1-1}] \right\} (\hat{\mathbf{e}}_f^\star \cdot \hat{\mathbf{e}}_i) - \frac{3\lambda}{8\pi} i [F_{11} - F_{1-1}] (\hat{\mathbf{e}}_f^\star \times \hat{\mathbf{e}}_i) \cdot \hat{\mathbf{M}} + \frac{3\lambda}{8\pi}[2F_{10} - F_{11} - F_{1-1}](\hat{\mathbf{e}}_f^\star \cdot \hat{\mathbf{M}})(\hat{\mathbf{e}}_i \cdot \hat{\mathbf{M}}), \quad (16)$$

where f_0 is the usual nonmagnetic (charge scattering) part known as the Thompson scattering amplitude $[f_0 = r_0(-Z + f' + if'')$, r_0 is the classical electron radius, Z is the number of electrons in the atom, f' and f'' are the nonresonant dispersion corrections]; $\lambda = 2\pi/\kappa$ is the x-ray wavelength; $\hat{\mathbf{e}}_i$, $\hat{\mathbf{e}}_f$, and $\hat{\mathbf{M}}$ are the unit vectors representing the polarizations of incident and scattered waves and the direction of the magnetic moment of atom, respectively; F_{LM} are the resonant magnetic scattering amplitudes (see Ref. 6 for more details).

Since the directions of vectors $\hat{\mathbf{e}}_i$ and $\hat{\mathbf{e}}_f$ can be chosen arbitrarily, the dielectric susceptibility of a resonant magnetic medium is a tensor:

$$\chi_{ij} = (\chi_0 + A)\delta_{ij} - iB\epsilon_{ijk}M_k + CM_iM_j, \quad (17)$$

where by the usual constitutive relationship relating refractive index to scattering length,

$$\chi_0 = -\frac{\lambda^2 r_0}{\pi} \sum_a n_a(-Z_a + f'_a + if''_a), \quad (18)$$

$$A = \frac{\lambda^2 r_0}{\pi} n_M[\tilde{F}_{11} + \tilde{F}_{1-1}], \quad (19)$$

$$B = \frac{\lambda^2 r_0}{\pi} n_M[\tilde{F}_{11} - \tilde{F}_{1-1}], \quad (20)$$

$$C = \frac{\lambda^2 r_0}{\pi} n_M[2\tilde{F}_{10} - \tilde{F}_{11} - \tilde{F}_{1-1}]. \quad (21)$$

The sum in Eq. (18) is over all the types of atoms in the material, n_a is the density of the atoms of type ''a'' and in particular n_M is the density of magnetic atoms; ϵ_{ijk} is the antisymmetric Levi-Civita symbol ($\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1$, $\epsilon_{132} = \epsilon_{213} = \epsilon_{321} = -1$, all other $\epsilon_{ijk} = 0$). The renormalized amplitudes $\tilde{F}_{kl} = 3\lambda F_{kl}/(8\pi r_0)$ are substituted instead of the original F_{kl} because they are commonly discussed in the literature[6] and more convenient for comparing with Z_a. They are, in general, complex, the imaginary part being related to absorption.

Equations (19)–(21) correspond to the case where all the magnetic moments are aligned in one direction. In the case of a partial alignment, n_M must be corrected for some demagnetization factor.

B. Wave equation: General case

With the tensor media susceptibility given by Eq. (17) the wave Eq. (2) now becomes[37]

$$\sum_{j=1}^{3} [\delta_{ij}\nabla^2 - \nabla_i\nabla_j + \kappa^2(\delta_{ij} + \chi_{ij})]E_j(\mathbf{r}) = 0. \quad (22)$$

The substitution of $E_j(\mathbf{r})$ in the form of Eq. (3) brings

$$\sum_{j=1}^{3} [(\gamma_0^2 - u^2)\delta_{ij} + n_in_j + \chi_{ij}]E_j = 0, \quad (23)$$

where $n_i = k_i/\kappa$, i.e., $n_x = (1-\gamma_0^2)^{1/2}$, $n_y = 0$, $n_z = u$. A nontrivial solution for Eq. (23) requires the following dispersion equation:

$$\left\| \begin{matrix} 1 + \chi_{xx} - u^2 & \chi_{xy} & \chi_{xz} + un_x \\ \chi_{yx} & \gamma_0^2 + \chi_{yy} - u^2 & \chi_{yz} \\ \chi_{zx} + un_x & \chi_{zy} & \gamma_0^2 + \chi_{zz} \end{matrix} \right\| = 0, \quad (24)$$

which provides the fourth order polynomial equation for u:

$$u^4Q_1+u^3Q_2+u^2Q_3+uQ_4+Q_5=0. \tag{25}$$

Here

$$Q_1=1+\chi_{zz}, \tag{26}$$

$$Q_2=n_x(\chi_{xz}+\chi_{zx}), \tag{27}$$

$$Q_3=\chi_{xz}\chi_{zx}+\chi_{yz}\chi_{zy}-(1+\chi_{zz})(\gamma_0^2+\chi_{yy}) \\ -(1+\chi_{xx})(\gamma_0^2+\chi_{zz}), \tag{28}$$

$$Q_4=n_x[\chi_{xy}\chi_{yz}+\chi_{yx}\chi_{zy}-(\chi_{xz}+\chi_{zx})(\gamma_0^2+\chi_{yy})], \tag{29}$$

$$Q_5=(1+\chi_{xx})[(\gamma_0^2+\chi_{yy})(\gamma_0^2+\chi_{zz})-\chi_{yz}\chi_{zy}] \\ -\chi_{xy}\chi_{yx}(\gamma_0^2+\chi_{zz})-\chi_{xz}\chi_{zx}(\gamma_0^2+\chi_{yy}) \\ +\chi_{xy}\chi_{zx}\chi_{yz}+\chi_{yx}\chi_{xz}\chi_{zy}. \tag{30}$$

Let us prove that Eq. (25) always has two roots $u^{(j)}$ with $\mathrm{Im}[u^{(1,2)}]>0$ and the other two roots with $\mathrm{Im}[u^{(3,4)}]<0$ corresponding to transmitted and reflected waves in the medium, respectively. That can be done with the help of the following imaginary experiment. First we ''switch off'' the anisotropy by setting $\chi_{ij}=\chi_0\delta_{ij}$. Then, Eq. (25) reduces to the form

$$[u^2-(\gamma_0^2+\chi_0)]^2=0, \tag{31}$$

which clearly has the two roots with $\mathrm{Im}[u^{(1,2)}]>0$ and the other two with $\mathrm{Im}[u^{(3,4)}]<0$. Now let us continuously proceed from Eq. (31) to Eq. (25) by virtue of continuous variation in χ_{ij}. At such a transition the number of positive and negative imaginary parts cannot change at any point because that would imply the possibility of anisotropic media with zero absorption ($\mathrm{Im}[u^{(j)}]=0$) which is physically impossible. So, the number of roots with $\mathrm{Im}[u^{(j)}]<0$ and $\mathrm{Im}[u^{(j)}]>0$ must be always 2 and 2, respectively.

Thus, as distinct from a nonresonant x-ray reflection, the magnetic resonance produces four waves inside the media (the two transmitted and two reflected ones) with different critical angles for total external reflection (the latter are given by the condition $u^{(j)}=0$ at zero absorption).

For each of the waves Eqs. (23) give ($j=1,\ldots 4$):

$$E_x^{(j)}=P_x^{(j)}E_y^{(j)}, \\ E_z^{(j)}=P_z^{(j)}E_y^{(j)}, \tag{32}$$

where

$$P_x^{(j)}=[\chi_{xy}(\gamma_0^2+\chi_{zz})-\chi_{zy}(\chi_{xz}+u^{(j)}n_x)]/\mathcal{D}^{(j)}, \tag{33}$$

$$P_z^{(j)}=[\chi_{zy}(1-u^{(j)2}+\chi_{xx})-\chi_{xy}(\chi_{zx}+u^{(j)}n_x)]/\mathcal{D}^{(j)}, \tag{34}$$

$$\mathcal{D}^{(j)}=(\chi_{xz}+u^{(j)}n_x)(\chi_{zx}+u^{(j)}n_x) \\ -(1-u^{(j)2}+\chi_{xx})(\gamma_0^2+\chi_{zz}). \tag{35}$$

The boundary conditions are still given by Eqs. (7)–(10) with the only difference that now there are four wave modes instead of two on the right-hand side. Substituting Eq. (32) into the boundary conditions one arrives at

$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ \gamma_0 & 0 & -\gamma_0 & 0 \\ 0 & \gamma_0 & 0 & -\gamma_0 \end{pmatrix}\begin{pmatrix} E_{0\sigma} \\ E_{0\pi} \\ E_{s\sigma} \\ E_{s\pi} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ v^{(1)} & v^{(2)} & v^{(3)} & v^{(4)} \\ u^{(1)} & u^{(2)} & u^{(3)} & u^{(4)} \\ w^{(1)} & w^{(2)} & w^{(3)} & w^{(4)} \end{pmatrix}\begin{pmatrix} E_y^{(1)} \\ E_y^{(2)} \\ E_y^{(3)} \\ E_y^{(4)} \end{pmatrix}, \tag{36}$$

where

$$v^{(j)}=u^{(j)}P_x^{(j)}-n_xP_z^{(j)}, \tag{37}$$

$$w^{(j)}\equiv P_x^{(j)}. \tag{38}$$

For a thick slab with one interface only the reflected waves inside the slab vanish, $\mathbf{E}^{(3)}=\mathbf{E}^{(4)}=0$, and Eqs. (36) provide the remaining four unknown amplitudes $E_{s\sigma}$, $E_{s\pi}$, $E_y^{(1)}$, and $E_y^{(2)}$.

C. Wave equation: Special case of magnetization perpendicular to the reflection plane

Equations (36) can only be solved if the scattering matrix on the right-hand side is not singular. The singularity may occur when either some roots $u^{(j)}$ coincide or all the $v^{(j)}$ or $w^{(j)}$ become zero.

As we have seen in the previous section, the former situation occurs in the absence of magnetic resonance when all the off-diagonal terms of χ_{ij} become zero. Then one has to use Eq. (15) instead of Eq. (36). Note that there is no continuous transition between these two types of equations because they are for different sets of wave fields.

The matrix singularity of the latter type [$v^{(j)}=0$ or $w^{(j)}=0$] can only occur when $\chi_{xy}=\chi_{zy}=0$. Otherwise, the terms on the right-hand side of Eqs. (33), (34), and (37) have different orders of magnitude and cannot yield zero sum. The condition $\chi_{xy}=\chi_{zy}=0$ provides $P_x^{(j)}=P_z^{(j)}=0$ and thus implies decoupling of E_x and E_z from E_y.

Proceeding to Eq. (17), we find that the case of $\chi_{xy}=\chi_{zy}=0$ in the resonant magnetic media requires $M_x=M_z=0$, i.e., the magnetization vector must be parallel to the Y axis. For $\mathbf{M}\|\mathbf{Y}$ the dispersion equation [Eq. (24)] reduces to

$$\begin{Vmatrix} 1+\chi_{xx}-u^2 & 0 & \chi_{xz}+un_x \\ 0 & \gamma_0^2+\chi_{yy}-u^2 & 0 \\ -\chi_{xz}+un_x & 0 & \gamma_0^2+\chi_{zz} \end{Vmatrix}=0, \tag{39}$$

and gives ($\chi_{xx}=\chi_{zz}$)

$$(u^2-\gamma_0^2-\chi_{yy})(u^2-\gamma_0^2-\chi_{zz}-\delta)=0, \tag{40}$$

$$\delta=\chi_{xz}^2(1+\chi_{xx})=-B^2/(1+\chi_{xx}). \tag{41}$$

The two roots of this equation $u^{(1,3)}=\pm(\gamma_0^2+\chi_{yy})^{1/2}$ provide $E_x^{(1,3)}=E_z^{(1,3)}=0$ and an arbitrary $E_y^{(1,3)}$. The other two

$u^{(2,4)}=\pm(\gamma_0^2+\chi_{zz}+\delta)^{1/2}$ provide $E_y^{(2,4)}=0$ and $E_x^{(2,4)}=R_xE_z^{(2,4)}$, where $R_x^{(j)}$ are given by Eq. (39). Substituting these solutions into the boundary conditions (7)–(10), one obtains

$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ \gamma_0 & 0 & -\gamma_0 & 0 \\ 0 & \gamma_0 & 0 & -\gamma_0 \end{pmatrix} \begin{pmatrix} E_{0\sigma} \\ E_{0\pi} \\ E_{s\sigma} \\ E_{s\pi} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & v^{(2)} & 0 & v^{(4)} \\ u^{(1)} & 0 & u^{(3)} & 0 \\ 0 & w^{(2)} & 0 & w^{(4)} \end{pmatrix} \begin{pmatrix} E_y^{(1)} \\ E_z^{(2)} \\ E_y^{(3)} \\ E_z^{(4)} \end{pmatrix} \tag{42}$$

with

$$v^{(j)}=u^{(j)}R_x^{(j)}-n_x = -[u^{(j)}\chi_{xz}+n_x(1+\chi_{xx})]/(n_x^2-\delta), \tag{43}$$

$$w^{(j)}=R_x^{(j)} = -(u^{(j)}n_x+\chi_{xz})/(n_x^2-\delta). \tag{44}$$

Equation (42) looks similar to Eq. (15), but unlike the scalar case here one has an interaction between E_x and E_z and the x-ray waves in the magnetic media are not transverse.

D. Wave equation: Simplifications for hard x rays

With the assumptions that even at the resonance χ_{ij} remain small ($|\chi_{ij}|\ll 1$), and the angles of x rays to the surface are also small $[\gamma_0^2\sim O(\chi_{ij})]$, which are reasonable for hard- and medium-energy x rays, we can simplify the expressions for Q_j to

$$Q_1=1, \tag{45}$$

$$Q_2=\chi_{xz}+\chi_{zx}, \tag{46}$$

$$Q_3=-(\gamma_0^2+\chi_{yy})-(\gamma_0^2+\chi_{zz}), \tag{47}$$

$$Q_4=\chi_{xy}\chi_{yz}+\chi_{yx}\chi_{zy}-(\chi_{xz}+\chi_{zx})(\gamma_0^2+\chi_{yy}), \tag{48}$$

$$Q_5=(\gamma_0^2+\chi_{yy})(\gamma_0^2+\chi_{zz})-\chi_{yz}\chi_{zy}. \tag{49}$$

Further simplification is possible if the amplitude of resonance scattering does not essentially exceed the usual Thompson contribution $|\chi_{ij}|\lesssim|\chi_0|$. Then, estimating $u^2\sim\gamma_0^2\sim|\chi_{ij}|$ we find that the order of the terms at Q_2 and Q_4 in the dispersion Eq. (25) is small as compared to the others. Neglecting these terms, the roots $u^{(j)}$ can be found analytically:

$$u^2=\frac{u_\sigma^2+u_\pi^2}{2}\pm\left[\left(\frac{u_\sigma^2-u_\pi^2}{2}\right)^2+\chi_{\sigma\pi}\chi_{\pi\sigma}\right]^{1/2}, \tag{50}$$

where $u_s^2=\gamma_0^2+\chi_{ss}$, and σ and π axes for grazing x rays coincide with Y and $-Z$ respectively.

Equations (33)–(35) are considerably simplified as well and one obtains

$$v^{(j)}=-\chi_{\pi\sigma}/[u^{(j)2}-\gamma_0^2-\chi_{xx}], \qquad w^{(j)}=u^{(j)}v^{(j)}. \tag{51}$$

It is worth noting that the above simplifications are equivalent to neglecting E_x and using the transverse waves approximation for hard x rays inside magnetic slab. In this case, the main effect of magnetic resonance on x-ray reflection is the interaction between σ and π polarizations.

Consider now the cases where the magnetization vector **M** is directed along one of the coordinate axes.

1. M∥X

The dispersion Eq. (24) is reduced to

$$\begin{Vmatrix} 1 & 0 & u \\ 0 & \gamma_0^2+\chi_0+A-u^2 & -iB \\ u & iB & \gamma_0^2+\chi_0+A \end{Vmatrix}=0, \tag{52}$$

and provides the roots $u^{1,2,3,4}=\pm(\gamma_0^2+\chi_0+A\pm B)^{1/2}$, as also follows from Eq. (50). Thus, when the incident x rays are parallel to the magnetization direction, the magnetic resonance affects the reflection of any polarization. Also, the polarizations are interacting. There are two critical angles for total reflection $\Phi_c=(\chi_0+A\pm B)^{1/2}$, but they are close since B is in general small.

2. M∥Y

In this case the dispersion equation is given by Eq. (39) and the simplified form of it may be written as

$$\begin{Vmatrix} 1 & 0 & u \\ 0 & \gamma_0^2+\chi_0+A+C-u^2 & 0 \\ u & 0 & \gamma_0^2+\chi_0+A \end{Vmatrix}=0. \tag{53}$$

Note that Eq. (50) is also valid. The roots given either by Eq. (50) or Eq. (53) are $u^{(1,3)}=\pm(\gamma_0^2+\chi_0+A+C)^{1/2}$ and $u^{(2,4)}=\pm(\gamma_0^2+\chi_0+A)^{1/2}$. As we have discussed, the polarizations are not interacting in this case. If $F_{10}=0$, the contributions of A and C to $u^{(1,3)}$ cancel each other and then only the reflection of π polarization is affected by the resonance.

3. M∥Z

The dispersion Eq. (24) may be approximated as

$$\begin{Vmatrix} 1 & 0 & u \\ 0 & \gamma_0^2+\chi_0+A-u^2 & 0 \\ u & 0 & \gamma_0^2+\chi_0+A+C \end{Vmatrix}=0, \tag{54}$$

and the respective roots are $u^{(1,3)}=\pm(\gamma_0^2+\chi_0+A)^{1/2}$ and $u^{(2,4)}=\pm(\gamma_0^2+\chi_0+A+C)^{1/2}$. We find that in the approximation for hard x rays the polarizations are not interacting again. At $F_{10}=0$ the only affected polarization is σ.

Thus, in the case of hard x rays and the magnetization vector directed along the Y or Z axis (along σ or π polarization, respectively), Eqs. (36) and (42) become formally equivalent[38] to Eq. (15). This corresponds to ''viewing'' by hard x rays the resonant magnetic media as a nonmagnetic one. The only exception is that the critical angles $\Phi_c^s = (\chi_{ss})^{1/2}$ for the total x-ray reflection differ for the $s=\sigma$ and $s=\pi$ incident polarizations, respectively.

E. Reflectivity of magnetic multilayer

For a multilayer, the 4×4 matrix boundary conditions of the above type can be imposed at each interface:

$$\mathcal{S}_{\mathrm{v}}\mathcal{E}_{\mathrm{v}} = \mathcal{S}_1\mathcal{E}_1,$$

$$\mathcal{S}_1\mathcal{F}_1^{(L)}\mathcal{E}_1 = \mathcal{S}_2\mathcal{F}_2^{(U)}\mathcal{E}_2,$$

$$\ldots\ldots \qquad \ldots\ldots,$$

$$\mathcal{S}_{N-1}\mathcal{F}_{N-1}^{(L)}\mathcal{E}_{N-1} = \mathcal{S}_N\mathcal{F}_N^{(U)}\mathcal{E}_N. \tag{55}$$

Here $\mathcal{E}_{\mathbf{v}} = (E_{0\sigma}\ E_{0\pi},\ E_{s\sigma},\ E_{s\pi})$ and $\mathcal{E}_n = (E_{\sigma n}^{(1)},\ E_{\sigma n}^{(2)},\ E_{\sigma n}^{(3)},\ E_{\sigma n}^{(4)})$ are the four-component vectors. $\mathcal{S}_{\mathbf{v}}$ and $\mathcal{S}_n$ are the characteristic 4×4 matrices of the layers as introduced at the left and the right sides of Eq. (36), respectively. Finally, $F_n^{j(U,L)}$ are the diagonal 4×4 matrices

$$[F_n^{(j)U,L}]_{ij} = \delta_{ij}\exp[iu_n^{(j)}\kappa z_n^{U,L}], \tag{56}$$

$z_n^{U,L}$ denote the coordinates of the upper and the lower interfaces of layers, respectively.

At this point the problem of resonant x-ray reflection from magnetic media has been reduced to that of the grazing-incidence x-ray diffraction from a crystalline multilayer.[36] Thus the rest of this section as well as the next one presents a nearly complete repetition of Ref. 36. This review is provided for the reader's convenience. We also point out some minor differences.

A direct formal solution to Eqs. (55) is

$$\mathcal{E}_{\mathbf{v}} = \mathcal{S}_{\mathbf{v}}^{-1}\mathcal{S}_1F_1\mathcal{S}_1^{-1}\mathcal{S}_2F_2\cdots\mathcal{S}_{N-1}^{-1}\mathcal{S}_N\mathcal{F}_N^{(U)}\mathcal{E}_N, \tag{57}$$

where $(F_n)_{ij} = [\mathcal{F}_n^{(U)}(\mathcal{F}_n^{(L)})^{-1}]_{ij} = \delta_{ij}\exp(-iu_n^{(j)}\kappa t_n)$, and t_n is the thickness on the nth layer. Calculating the matrix product at the right-hand side of Eq. (57) and taking into account that the amplitudes of reflected waves in the substrate are zero ($E_{\sigma N}^{(3)} = E_{\sigma N}^{(4)} = 0$), one arrives at four linear equations for four unknown amplitudes: $E_{s\sigma}$, $E_{s\pi}$, $E_{\sigma N}^{(1)}$, and $E_{\sigma N}^{(2)}$. The other amplitudes are given by Eqs. (55) and (32). The above scheme provides a 4×4 transfer-matrix solution to the problem of resonant and nonresonant x-ray reflection from a multilayer.

As has been mentioned in the introduction, a similar 4×4 matrix formalism is used in the optics of visible light to calculate the reflectivity of anisotropic layered media.[28,29] It has also been applied to calculate the x-ray reflectivity from multilayers under the conditions of magnetic[30] and Mössbauer[32] resonances. Although formally the 4×4 matrix method is absolutely correct, its numerical implementation is often problematic because of possible numerical overflow while calculating the matrix product on the right side of Eq. (57).

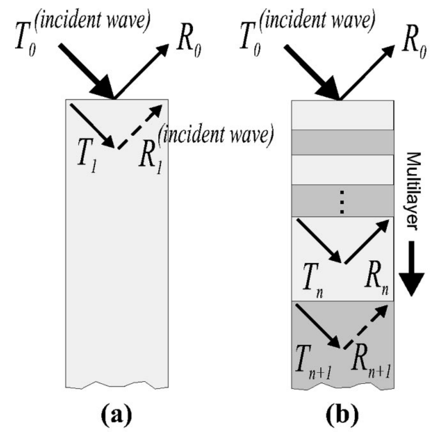

FIG. 2. Schematic illustrating the derivation of matrix recursion equations for x-ray resonant reflection in the cases of (a) a single layer and (b) a multilayer. T_k and R_k denote the two-component vectors containing the amplitudes of transmitted and reflected waves, respectively.

IV. RECURSION 2×2 MATRIX FORMULAS FOR RESONANT X-RAY REFLECTION FROM A MULTILAYER

In the following consideration we make use of the approach developed by Kohn[39] for nongrazing x-ray diffraction from multilayer with multiple Bragg- and Laue-case reflections. The Bragg- and Laue-case x-ray waves in that problem can be viewed as being analogous to the transmitted and reflected waves in our problem. The basic idea of Kohn is that Eq. (57) diverges because the vacuum amplitudes $\mathcal{E}_{\mathbf{v}}$ are sought together with the substrate amplitudes $\mathcal{E}_N$. The former amplitudes are of the order of 1, while the latter ones can be evanescent in a thick multilayer. A better way is to express the reflectivity of a multilayer containing $n+1$ interfaces via that of a multilayer with n interfaces. Then the recursion must converge because the effect of additional lower interfaces on the reflectivity decreases with the distance of the interfaces from the surface.

We start with the following renormalizing of x-ray amplitudes:[40]

$$\mathcal{E}_n' = \mathcal{F}_n^{(L)}\mathcal{E}_n, \tag{58}$$

and denoting $X_{n+1} = \mathcal{S}_n^{-1}\mathcal{S}_{n+1}$. Then, all Eqs. (55) assume the universal form (here and below the primes in $\mathcal{E}_n$ are left out)

$$\mathcal{E}_n = X_{n+1}F_{n+1}\mathcal{E}_{n+1}, \quad n=0,\ldots,N-1. \tag{59}$$

The amplitudes $\mathcal{E}_n$ are constant within the layers and change at the interfaces. Therefore the interfaces can be treated as "scatterers" for amplitudes. First, let us consider the scattering at a single interface. For clarity we discuss the reflection from the surface [Fig. 2(a)], but our consideration is applicable to any internal interface as well. The waves at the left-hand side of Eq. (59) can be classified as two incident and two scattered waves. We group them in the vectors $T_0 = (E_{0\sigma}, E_{0\pi})$ and $R_0 = (E_{s\sigma}, E_{s\pi})$, respectively. In their turn, the waves at the right-hand side of Eq. (59) can be viewed as the two transmitted (or scattered) waves and two ones "incident" onto the interface from the slab interior. The former and the latter waves are characterized by $\mathrm{Im}[u^{(1,2)}]>0$ and $\mathrm{Im}[u^{(3,4)}]<0$, respectively. Although the amplitudes of the latter waves are zero in a thick slab, we keep them for the general case where slabs have internal interfaces. Thus we group the waves below the surface as the vectors $T_1=(E_\sigma^{(1)},E_\sigma^{(2)})$ and $R_1=(E_\sigma^{(3)},E_\sigma^{(4)})$, respectively. Splitting matrices X and F into four 2×2 blocks we obtain

$$\begin{pmatrix} T_0 \\ R_0 \end{pmatrix}=\begin{pmatrix} X^{tt} & X^{tr} \\ X^{rt} & X^{rr} \end{pmatrix}\begin{pmatrix} F^{+} & 0 \\ 0 & F^{-} \end{pmatrix}\begin{pmatrix} T_1 \\ R_1 \end{pmatrix}, \tag{60}$$

where F^+ and F^- are the diagonal matrices containing the increasing and decreasing exponential functions, respectively.

Equation (60) enables the ''scattered'' waves R_0 and T_1 to be expressed via the ''incident'' waves T_0 and R_1:

$$\begin{pmatrix} T_1 \\ R_0 \end{pmatrix}=\begin{pmatrix} M^{tt} & M^{tr} \\ M^{rt} & M^{rr} \end{pmatrix}\begin{pmatrix} T_0 \\ R_1 \end{pmatrix}, \tag{61}$$

where

$$\begin{aligned} M^{tt}&=(F^{+})^{-1}(X^{tt})^{-1},\\ M^{tr}&=-M^{tt}X^{tr}F^{-},\\ M^{rt}&=X^{rt}(X^{tt})^{-1},\\ M^{rr}&=(X^{rr}-M^{rt}X^{tr})F^{-}. \end{aligned} \tag{62}$$

Equations (62) have a clear physical interpretation. For example, the block M^{rr} is responsible for the scattering of R_1 into R_0 and the last line in Eq. (62) implies that the scattering may be a direct transmission $R_1\rightarrow R_0$ and may be a multiple scattering process $R_1\rightarrow T_0\rightarrow T_1\rightarrow R_0$. We note that Eqs. (61) and (62) do not cause any divergences because the increasing exponentials F^+ are inverted. In the case of a thick substrate vector R_1 approaches zero, and then $R_0=M^{rt}T_0$.

Proceeding to multilayers [Fig. 2(b)], the solutions of the scattering problem for multilayers incorporating n interfaces and $n+1$ interfaces according to Eq. (57) can be presented as

$$\begin{pmatrix} T_n \\ R_0 \end{pmatrix}=\begin{pmatrix} W_n^{tt} & W_n^{tr} \\ W_n^{rt} & W_n^{rr} \end{pmatrix}\begin{pmatrix} T_0 \\ R_n \end{pmatrix}, \tag{63}$$

and

$$\begin{pmatrix} T_{n+1} \\ R_0 \end{pmatrix}=\begin{pmatrix} W_{n+1}^{tt} & W_{n+1}^{tr} \\ W_{n+1}^{rt} & W_{n+1}^{rr} \end{pmatrix}\begin{pmatrix} T_0 \\ R_{n+1} \end{pmatrix}, \tag{64}$$

respectively. Here W_n and W_{n+1} are 2×2 matrices. At the same time, according to Eq. (61) the scattering equations for interface $(n+1)$ are

$$\begin{pmatrix} T_{n+1} \\ R_n \end{pmatrix}=\begin{pmatrix} M_{n+1}^{tt} & M_{n+1}^{tr} \\ M_{n+1}^{rt} & M_{n+1}^{rr} \end{pmatrix}\begin{pmatrix} T_n \\ R_{n+1} \end{pmatrix}. \tag{65}$$

The combination of Eqs. (63)–(65) results in the following recursion formulas for W_n:

$$\begin{aligned} W_{n+1}^{tt}&=A_nW_n^{tt},\\ W_{n+1}^{tr}&=M_{n+1}^{tr}+A_nW_n^{tr}M_{n+1}^{rr},\\ W_{n+1}^{rt}&=W_n^{rt}\ \ +B_nM_{n+1}^{rt}W_n^{tt},\\ W_{n+1}^{rr}&=B_nM_{n+1}^{rr}, \end{aligned} \tag{66}$$

where we define

$$\begin{aligned} A_n&=M_{n+1}^{tt}(1-W_n^{tr}M_{n+1}^{rt})^{-1},\\ B_n&=W_n^{rr}(1-M_{n+1}^{rt}W_n^{tr})^{-1}. \end{aligned} \tag{67}$$

Starting with the surface and progressively applying Eqs. (66) to lower interfaces, one arrives at the matrices W_N^{xy} determining the reflectivity of the whole multilayer. The recursion matrix (RM) solution does not cause any divergences in the numerical calculations. As follows from Eq. (62), the order of M^{rt} is about one, while the other three blocks are small due to the factors F^- and $(F^+)^{-1}$. According to Eq. (66), the same ratio of orders is preserved for the blocks W^{xy}. Thus the block W_N^{rt} is the only one significant for a thick multilayer and the solution to the reflection problem is

$$R_0=W_N^{rt}T_0. \tag{68}$$

The other matrix blocks converge to zero at the recursions (66). The reflectivity is calculated as $I=|E_{s\sigma}|^2+|E_{s\pi}|^2\equiv|R_0^{(1)}|^2+|R_0^{(2)}|^2$.

Equation (68) can also be used to calculate the difference in the reflectivity for ''+'' and ''−'' circularly polarized incident x rays. Substituting $E_{0\pi}^{\pm}=\pm iE_{0\sigma}$ we obtain

$$\frac{I^+-I^-}{I^++I^-}=\frac{2\ \mathrm{Im}[W_{N11}^{rt}W_{N12}^{rt*}+W_{N21}^{rt}W_{N22}^{rt*}]}{|W_{N11}^{rt}|^2+|W_{N12}^{rt}|^2+|W_{N21}^{rt}|^2+|W_{N22}^{rt}|^2}. \tag{69}$$

Finally, let us find the x-ray wave field amplitudes R_n and T_n inside the layers. These are required for the interpretation of x-ray standing waves and diffuse scattering in reflection from multilayers. Equation (63) gives $R_0=W_n^{rt}T_0+W_n^{rr}R_n$. However, the direct solution $R_n=(W_n^{rr})^{-1}(R_0-W_n^{rt}T_0)$ leads to uncertainties like 0/0 for thick multilayers and one has to make use of recursions. A combination of Eqs. (63) and (65) yields

$$\begin{aligned} R_n&=(1-M_{n+1}^{rt}W_n^{tr})^{-1}(M_{n+1}^{rr}R_{n+1}+M_{n+1}^{rt}W_n^{tt}T_0),\\ T_n&=W_n^{tt}T_0+W_n^{tr}R_n. \end{aligned} \tag{70}$$

Equations (70) must be progressively applied to all the layers starting at the multilayer substrate where $R_N=0$.

V. NUMERICAL EXAMPLES AND DISCUSSION

The theory presented above has been put into the computer code for calculating the reflectivity and the x-ray wave fields at the x-ray resonant reflection from magnetic multilayers. Since the general recursion matrix formalism is used, the core part of the code is directly borrowed from the grazing incidence diffraction, specular reflectivity, and diffuse scattering programs presented at [http://sergey.bio.aps.anl.gov] and numerously verified through the World Wide Web (WWW) interface.

Here we discuss several numerical examples which are

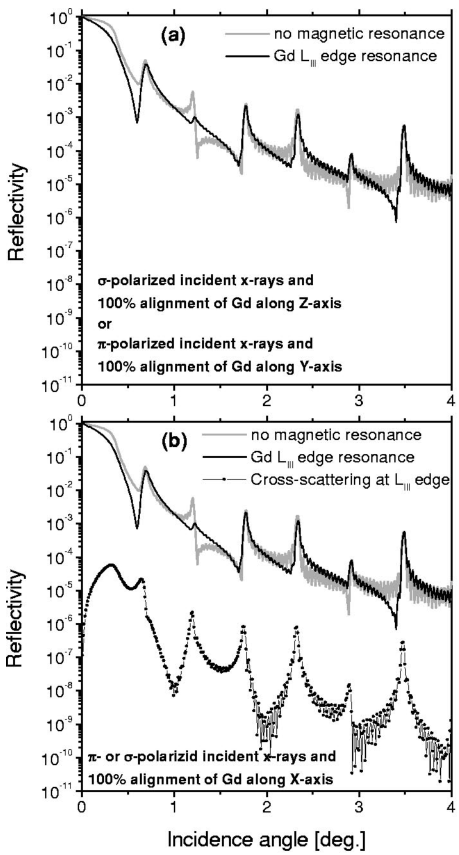

FIG. 3. Calculated resonant reflection of linearly polarized x rays from Gd/Fe multilayer at the Gd L_{III} edge (7.243 keV) for different directions of the magnetization and incident polarization.

aimed at better understanding the effects of magnetic resonance on x-ray reflection. Figure 3 presents the calculated effect of magnetic resonance for the case of a Gd/Fe multilayer consisting of 15 periods of 50-Å Gd and 35-Å Fe. The calculations are for the resonance in Gd at the Gd L_{III} edge (7.243 keV). The incident x rays are chosen either σ- or π-linearly polarized, while the reflected intensity is calculated as a sum of σ and π polarizations (i.e., with the assumption of no analyzer at the detector side),

$$R=|E_{s\sigma}|^2+|E_{s\pi}|^2. \tag{71}$$

The resonant scattering amplitudes $\tilde{F}_{10}\approx 0$, $\tilde{F}_{11}=-0.22+9.35i$, and $\tilde{F}_{1-1}=0.37+9.65i$ are taken from Ref. 41. These values correspond to the x-ray energy at the exact center of the resonance peak.[22]

Figure 3(a) compares the reflectivity without resonance (gray line) with the resonant reflectivity for the cases where either the incident x rays are σ polarized and the magnetization vector is along the Z axis, or the incident x rays are π polarized and the magnetization vector is along the Y axis. The latter two cases ($\sigma\Leftrightarrow Z$ and $\pi\Leftrightarrow Y$) give the same reflectivity curve shown by the black line.

For the other combinations ($\sigma\Leftrightarrow Y$, and $\pi\Leftrightarrow Z$), the calculated effect is zero, i.e., the calculated curves completely coincide with the nonresonant one. This happens due to the choice $F_{10}=0$ in our parameters of calculations. Then, $A=-C$ and the critical angle for the total reflection $\Phi_c^{\sigma}=|\chi_{\sigma\sigma}|^{1/2}=|\chi_0+A+C|^{1/2}=|\chi_0|^{1/2}$ becomes the same as for the nonresonant media. When, however, $F_{10}\neq 0$, these two combinations are also affected by the resonance but the effects for $\sigma\Leftrightarrow Y$, and $\pi\Leftrightarrow Z$ are equivalent. In any of the above cases there is no polarization exchange ($\sigma\rightarrow\pi$ or $\pi\rightarrow\sigma$) because the effects are due to the A and C terms in Eq. (17) which contribute to the diagonal terms of χ_{ij} only.

Figure 3(b) shows the calculated reflectivity for X orientation of the magnetization vector, i.e., when the magnetization is along the projections of the incident and reflected x-ray wave vectors onto the surface. Here also the reflections of both σ- and π-polarized x rays are equally affected. However, in addition, a $\sigma\rightarrow\pi$ and $\pi\rightarrow\sigma$ cross scattering appears due to the interaction between the polarizations, as shown by the lower curve. This curve plots the intensity of reflected π-polarized x rays when the incident wave is 100% σ polarized or vice versa. To measure this effect one needs an x-ray polarization analyzer at the detector side.

To measure the polarization exchange without the analyzer, one can use circularly polarized incident x rays. Figure 4(a) plots the calculated reflectivity curves I^+ and I^- for the clockwise and counterclockwise circularly polarized x rays, respectively. In these two cases the spin of the photons is, respectively, parallel and antiparallel to the magnetization vector directed along X. Though it is difficult to see the difference between these two reflectivity curves in the absolute scale, the relative difference presented on Fig. 4(b) clearly demonstrates systematic oscillations with the rms value about 10%. To calculate this curve we have used Eq. (69).

The oscillations of the relative difference imply a small angular shift of polarization exchange from the multilayer reflectivity peaks. This is a typical standing-wave effect. Thus the measurements of $(I^+-I^-)/(I^++I^-)$ can clearly display the magnetic resonance in the sample.

In order to provide a test of our theory, we have attempted to reproduce the results by Kao *et al.*[30] Figure 5 presents the calculated reflectivity of circularly polarized x rays for a multilayer consisting of 36-Å Al_2O_3, 39-Å Co, 5-Å Fe, and 560-Å ZnSe on GaAs substrate. The calculations are for the magnetic resonance in Co at the Co L_{III} edge (0.7865 keV) and the magnetization vector directed along X. The resonance scattering amplitudes used in the calculations are $\tilde{F}_{10}=0$, $\tilde{F}_{11}=12+6i$, and $\tilde{F}_{1-1}=20-14i$. The qualitative agreement of our plot with Fig. 5 of Ref. 30 is quite satisfactory. We could not achieve a better fit because many parameters of the calculations presented in Ref. 30 were missing.

Concluding the discussion of numerical examples, we have found that the effect of magnetic resonance on x-ray specular reflection is manifested as both a change of refraction and a polarization exchange. The former effect is at least three to four orders of magnitude stronger and thus easier to observe than the latter one. Perhaps it is one of the major distinctions between grazing incidence resonant reflection and resonant Bragg diffraction where the refraction effects are small.

Although the polarization exchange is relatively weak, it can be measured with circularly polarized x rays. For the reflection from a periodic multilayer one may find the

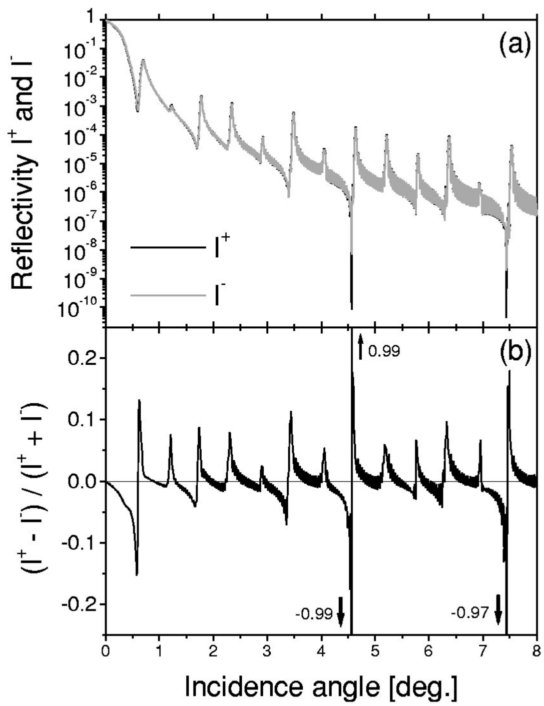

FIG. 4. Calculated resonant reflection of circularly polarized x rays from Gd/Fe multilayer at the Gd L_{III} edge (7.243 keV). (a): the reflectivity curves I^+ and I^- for the clockwise and counterclockwise incident polarizations respectively; (b): their normalized difference. In (a) the difference between the two cases is not appreciable, but in (b) the normalized difference is well seen to vary at the level of about $\pm 10\%$.

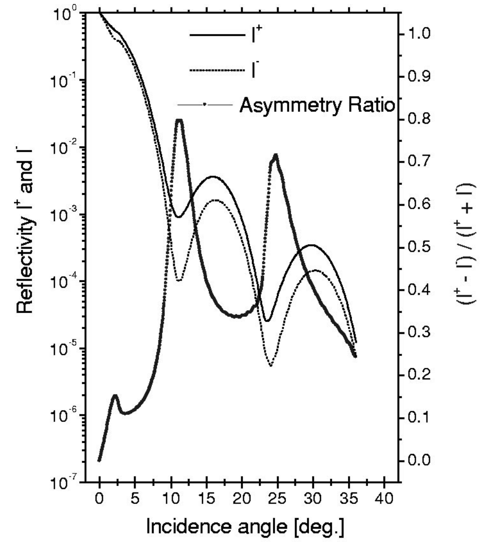

FIG. 5. The calculations of I^+ and I^- for the case presented in Ref. 30. The sample consists of 36-Å Al_2O_3, 39-Å Co, 5-Å Fe, and 560-Å ZnSe on GaAs substrate; the x-ray energy corresponds to the Co L_{III} edge (0.7865 keV).

standing-wave effects in the difference between the reflectivity for clockwise and counterclockwise circular polarizations.

VI. CONCLUSIONS

We have developed a formalism and a numerical procedure to calculate the x-ray resonant reflection from magnetic multilayers. Using this theory we have predicted the major peculiarities of the effect of magnetic resonance on the x-ray reflectivity and provided some tips for their measurement.

Further developments will need to include the real structure effects such as magnetic inhomogeneities and interface roughness. However, the treatment for some imperfections can be implemented with the present model too. For example graded magnetization profiles can be taken into account by slicing the real layers into sublayers. Also, a simple account for the roughness can be added following the procedure developed in Ref. 42 which gives the usual Debye-Waller-like factors in the dependence of x-ray reflectivity on the incidence angle.[27] Using the latter technique we have calculated the effect of 5-Å interface roughness on the curves presented in Fig. 3. The calculations predict that the roughness should cause a faster decrease of the reflectivity with the incidence angle, but the ratio $(I^+ - I^-)/(I^+ + I^-)$ would not be affected.

Finally, the x-ray wave fields provided by our theory can be used to calculate the x-ray diffuse scattering from chemical and magnetic roughness in magnetic multilayers. The common approach to such calculations is to apply the distorted wave Born approximation which requires the wave fields for the target without roughness.[27,20,21]

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