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Magneto-x-ray effects in transition-metal alloys

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We present a theory that combines the relativistic spin-polarized version of the Koringa-Kohn-Rostoker coherent-potential approximation theory and the macroscopic theory of magneto-optical effects enabling us to calculate magneto-x-ray effects from first principles. The theory is illustrated by calculation of Faraday and Kerr rotations and ellipticities for transition-metal alloys. [S0163-1829(97)03820-4]

I. INTRODUCTION

A recent series of experiments by Siddons *et al.*,[1] Hart *et al.*,[2] McWhan *et al.*,[3] and Alp *et al.*[4] has demonstrated the existence of the analogue of some magneto-optical effects at x-ray frequencies. However, development of these into a probe of the magnetic properties of matter has been hampered because a satisfactory theory of magneto-x-ray effects has not been developed. Recently, a first-principles theory of x-ray Faraday effects was developed by Gotsis and Strange.[5] Using a relativistic quantum-mechanical description of the electronic structure of magnetic materials, they found that the theory of magneto-optical phenomena can be generalized to x-ray frequencies. The theory was illustrated by a calculation of the Faraday rotation and induced ellipticity in linearly polarized light incident at the K edge of pure iron.

Here we want to show that the same theory can be applied in the calculation of magneto-x-ray effects of random substitutional alloys. The alloys $Fe_{75}Pt_{25}$ (Ref. 4) and $Co_{90}Fe_{10}$ (Ref. 1) were investigated. In the first of these alloys Faraday rotation results at the iron K edge are available, and in the second they are available at the cobalt K edge. Furthermore, the only measurement of induced ellipticity of which we are aware is also available in the latter alloy.

II. CALCULATIONS FOR RANDOM SUBSTITUTIONAL ALLOYS

To describe random substitutional alloys we have used the generalization of the Koringa-Kohn-Rostoker coherent-potential approximation (KKR CPA) methods proposed by Ebert, Drittler and Akai[6] and more recently by Gotsis, Strange, and Staunton.[7] This involves combining the usual KKR CPA methods with the scattering theory of Strange, Staunton, and Gyorffy[8] to produce a method of determining the electronic structure of random alloys, which treats magnetism and relativity on an equal footing.

The CPA theory enables us to determine an effective medium in random alloys, in a self-consistent way, i.e., the fluctuations of the given quantity due to local fluctuations around the effective medium average out to zero. In the language of multiple scattering theory this means that the site diagonal part of the Green's function of an atom A or B embedded in the CPA medium, averaged over the possible occupations of a single site, should equal the Green's function of the medium itself. The previous statement forms the so-called CPA self-consistency condition.

The CPA condition can be expressed in terms of scattering-path operators as

$$c_A\tau^A + c_B\tau^B = \tau^{\mathrm{CPA}}. \tag{1}$$

The effective-medium-scattering-path operator $\tau^{\mathrm{CPA}}_{\mathrm{QQ'}}$ and the component projected scattering-path operators $\tau^{\alpha}_{\mathrm{QQ'}}$ ($\alpha = A,B$) can be calculated in terms of the usual KKR structure constants $g(\mathbf{q},E)$ and the single site t matrices:

$$\tau^{\mathrm{CPA}}_{QQ'} = \frac{1}{\Omega_{\mathrm{BZ}}}\int_{\mathrm{BZ}}[(t^{\mathrm{CPA}})^{-1} - g(\mathbf{q},E)]^{-1}_{QQ'}d\mathbf{q}, \tag{2}$$

$$\tau^{\alpha}_{QQ'} = [(t^{\alpha})^{-1} - (t^{\mathrm{CPA}})^{-1} + (\tau^{\mathrm{CPA}})^{-1}]^{-1}_{QQ'},$$

$$\alpha = A,B \tag{3}$$

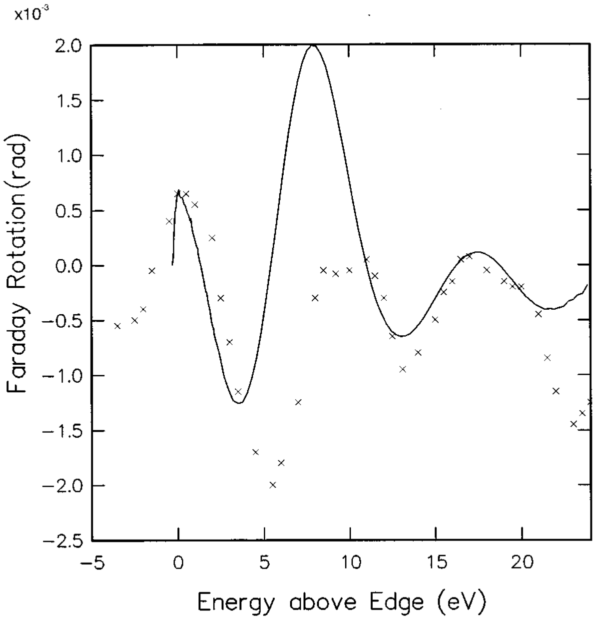

FIG. 1. The full line is the Faraday rotation at the iron K edge in $Fe_{75}Pt_{25}$. The crosses represent experimental data taken from Alp *et al.* (Ref. 4).

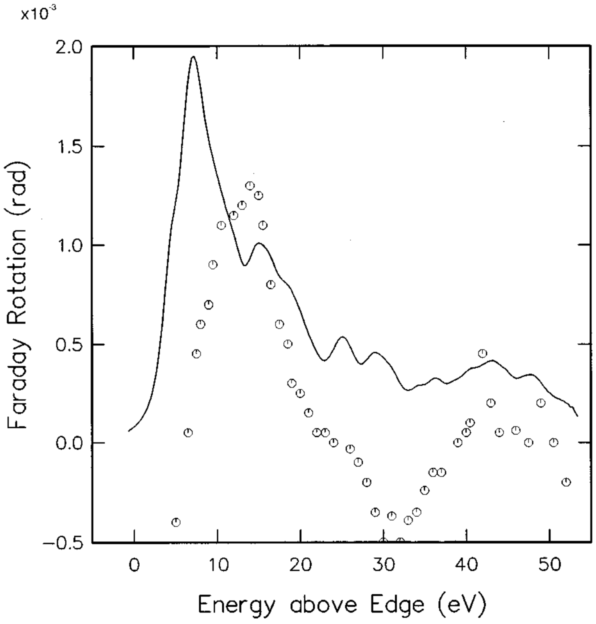

FIG. 2. The full line is the Faraday rotation at the cobalt *K* edge in $Co_{90}Fe_{10}$. The circles represent experimental data taken from Siddons *et al.* (Ref. 1).

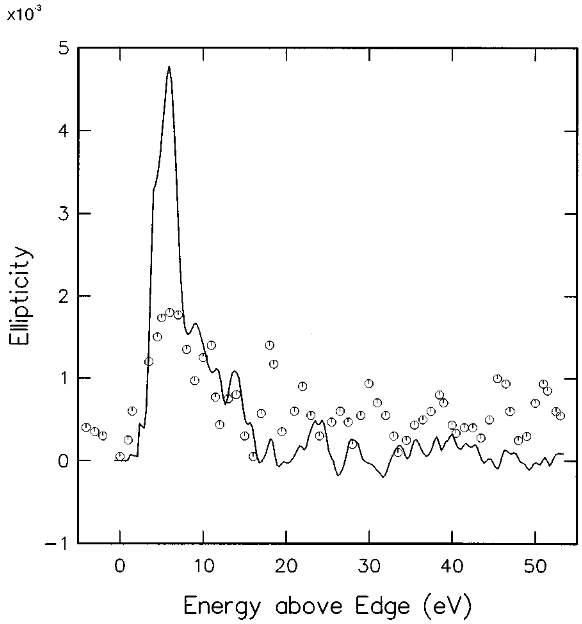

FIG. 3. The full line is the induced ellipticity at the cobalt *K* edge in $Co_{90}Fe_{10}$. The circles represent experimental data taken from Siddons *et al.* (Ref. 1).

Here Q and Q' are quantum numbers defining the representation. The component-projected scattering-path operators $\tau^{A}_{QQ'}$ and $\tau^{B}_{QQ'}$ are obtained from Eq. (3). Because $\tau^{\mathrm{CPA}}_{QQ'}$ is determined by Eq. (2), these coupled sets of equations for $\tau^{\mathrm{CPA}}_{QQ'}$ and $t^{\mathrm{CPA}}_{QQ'}$ have to be solved iteratively.

Obviously, the CPA equations (1)–(3) can be used without any modifications within the spin-polarized relativistic KKR formalism. The only difference from the paramagnetic case is that the single site t matrices $t^{A}_{QQ'}$ and $t^{B}_{QQ'}$, respectively, have to be determined by solving the Dirac equation for a spin-dependent potential.[7]

A general expression for the x-ray absorption rate of materials has been derived by Durham.[9] A relativistic spin-polarized version of this has been written down by Ebert, Strange, and Gyorffy.[10] The only modification to their theory due to the CPA is that the τ that enters the transition rate expression is replaced by τ^{A} or τ^{B} given by Eq. (1), whichever is appropriate, as the x ray is a site-specific probe.

In Fig. 1 we present our calculation of the Faraday rotation in $Fe_{75}Pt_{25}$. This has been broadened with a Lorentzian of width 1.8 eV in order to take into account lifetime and instrumental broadening effects. Also are shown the experimental points. Obviously, the agreement between theory and experiment is very satisfying. In Figs. 2 and 3 we see the Faraday rotation and induced ellipticity in $Co_{90}Fe_{10}$, respectively. The former has been broadened with a Lorentzian of width 1.8 eV. The latter has not been broadened because the experimental ellipticity is always positive, whereas our calculation gives positive and negative values. In experimenting with broadening we found that the shape of the curve was sensitively dependent on whether it was first made positive and then broadened, or the reverse. Therefore, in order for there to be no ambiguity, we have left the theoretical curve unbroadened. Again we have included the experimental results from Siddons *et al.*[1] The $Co_{90}Fe_{10}$ curves only agree qualitatively with the experimental points. There may be several reasons for this. The Faraday rotation looks rigidly shifted relative to the theory, suggesting a difference between theory and experiment in the energy calibration of the *K* edge. Of course the calculation of the absorption rates is underpinned by density-functional theory, which only describes the filled states, and which one might reasonably expect to get progressively more inaccurate as we get further above the Fermi energy.

In summary then, we have combined the spin-polarized relativistic KKR CPA electronic structure method with macroscopic optical constants to provide a theory that enables us to calculate magneto-x-ray effects from first principles. The theory has been illustrated with calculations of Faraday and Kerr rotations and ellipticities for transition-metal alloys. Comparison with recent experiments shows that the one-electron picture describes at least qualitatively the x-ray absorption process in transition-metal alloys.

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