Magneto-Optic Materials I   Richard Gambino, Chairman

Magneto-optical properties of Co|Pt multilayer systems

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We are reporting, theoretical Kerr spectra of Co|Pt multilayer systems as obtained on a first principles basis including multiple reflections and interferences from all the boundaries in-between the layers. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1447501]

I. INTRODUCTION

Co|Pt multilayer systems are thought to be the next-generation magneto-optical recording media, because their performance is very similar to that of the rare-earth based materials, which are already in use.[1] Although, in the last decade a large amount of experimental investigations has been performed on these systems, realistic theoretical investigations, are still lacking up to now.

The propagation of electromagnetic waves in any multilayer system can exactly be described by using either a 2×2 matrix[2] or 4×4 matrix[3] formalism. However, up to date, these techniques have been only used to simulate magneto-optical properties of multilayers using exclusively bulk optical data from experiments. The present contribution completes these kind of theoretical investigations. Here the complex Kerr effect is calculated on a first principle basis by using the theoretical layer-resolved optical conductivity tensor of the investigated layered system as input for the 2×2 matrix formalism appropriate for polar geometry at normal incidence.

II. THEORETICAL FRAMEWORK

The complex optical conductivity tensor is calculated using Luttinger's formula[4] by means of a contour integration technique,[5] which permits the computation to be performed at nonzero temperatures and for finite lifetime broadening. In combination with the spin-polarized relativistic screened Korringa–Kohn–Rostoker band structure method,[6] this technique has been shown to provide the most adequate first principles computational scheme of the complex optical conductivity tensor for layered systems, without using Kramers–Konig relations, taking into account, however, both, the inter- and the intraband contributions on the same footing.[7]

The computational accuracy is permanently controlled applying the Gauss–Konrod quadrature and the recently developed cumulative special-points method.[8] In the present contribution, all the layer-resolved complex optical conductivity tensors have been obtained with an accuracy of 0.001 a.u. by taking 35 (2) Matsubara poles at 300 K in the upper (lower) complex semiplane and a lifetime broadening of 0.048 Ry. The Fermi level of -0.038 Ry corresponds to that of a paramagnetic fcc–Pt bulk substrate (lattice parameter of 7.4137 a.u.).

III. RESULTS AND DISCUSSIONS

The 2×2 matrix formalism has been adopted for polar geometry at normal incidence, for two reasons, namely (1) Kerr measurements are mainly recorded under these conditions,[9] and (2) in the case of polar geometry, the solutions of the characteristic equation are analytically known and, hence, within the iterative algorithm of Mansuripur,[2,10] the recursion relations are simple form. The form of 2×2 matrices can even be more simplified by neglecting the difference in the diagonal optical conductivity tensor elements.

Starting from the substrate, once the surface reflectivity matrix has been iteratively evaluated, the Kerr rotation angle θ_K and Kerr ellipticity ϵ_K, respectively, are obtained directly by using the following exact formulas:[11]

$$\theta_K = -\tfrac{1}{2}(\Delta_+ - \Delta_-), \tag{1}$$

and

$$\epsilon_K = -\frac{|r_+| - |r_-|}{|r_+| + |r_-|}, \tag{2}$$

where $r_\pm = |r_\pm| e^{i\Delta_\pm}$ is the complex reflectivity of the right- and left-handed circularly polarized light.
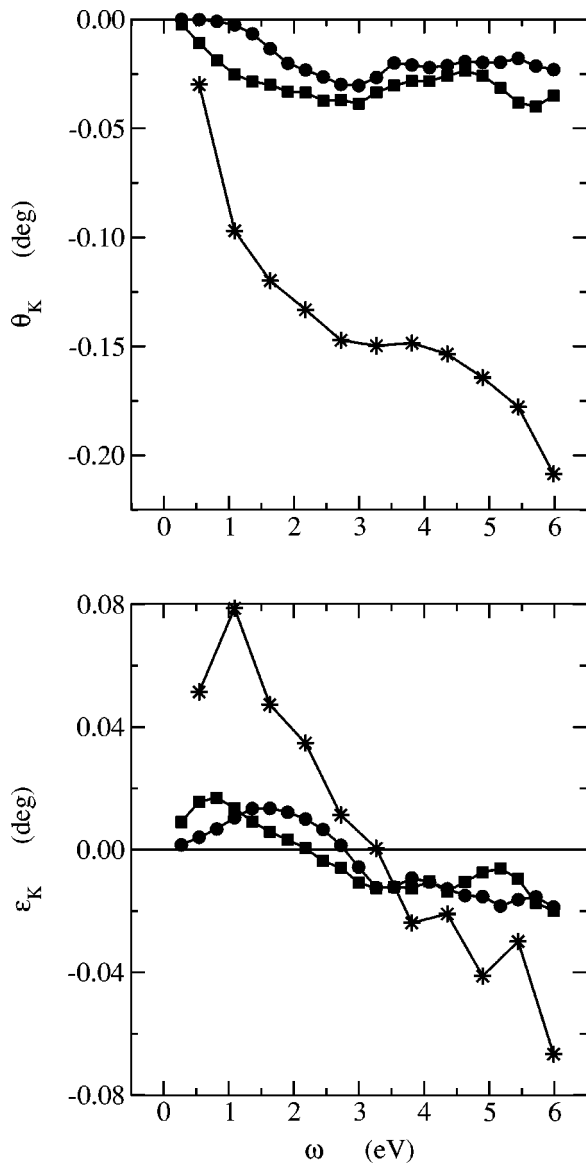
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FIG. 1. Kerr rotation angle and ellipticity as a function of the optical frequency for fcc(111) Co|Pt$_5$ (filled circles), Pt$_3$|Co|Pt$_5$(filled squares), and Pt$_3$|(Co|Pt$_3$)$_3$|Co|Pt$_5$ (stars), respectively, on top of a paramagnetic semi-infinite Pt bulk.

The theoretical Kerr spectra for fcc(111)–Co|Pt$_5$ layered system, with three Pt cap layers and in addition with three Co|Pt$_3$ bilayers in-between the cap layers and Co|Pt$_5$, respectively, are shown in Fig. 1. In the experiments the Pt cap layers on the top of Co layer are deposited to prevent the oxidation of the surface.[12] We have shown that in the absence of an applied field (magnetic ground state) strictly speaking the Co|Pt multilayer systems exhibit perpendicular magnetization only in presence of Pt cap layers. It is therefore not surprising that due to the Pt cap layers the Kerr effect is enhanced in comparison with uncapped Co|Pt$_5$. The three Co|Pt$_3$ bilayers on the top of Co|Pt$_5$ increase dramatically the Kerr effect, putting the theoretical Kerr rotation angle in shape and magnitude in a very good agreement with the experimental data.[9] However, because the systems considered here are much smaller than those used in experiments, a strict quantitative comparison of the Kerr spectra cannot directly be made.

In conclusion, by combining our technique, which permits to obtain the layer-resolved optical conductivity tensor on a first principle basis, with a proper description of the light propagation in multilayer systems, like the 2×2 matrix formalism, a very realistic description of the magneto-optical Kerr effect can be given.

ACKNOWLEDGMENTS

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