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Layer-resolved optical conductivity of Co | Pt multilayers

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Abstract

The complex optical conductivity tensor is calculated for the Co | Pt multilayer systems by applying a contour integration technique within the framework of the spin-polarized relativistic screened Korringa–Kohn–Rostoker method. It is shown that the optical conductivity of the Co | Pt multilayer systems is dominated by contributions arising from the Pt cap and/or substrate layers.

Keywords: Conductivity tensor; Ferromagnetic multilayers; Green's function; Magneto-optics

1. Introduction

Since Co | Pt multilayer systems can be used as magneto-optical recording media [1], in the last decade a large amount of experimental investigations has been performed in these systems; realistic theoretical investigations of these multilayer systems, however, are still lacking.

The contour integration technique [2] permits the evaluation of the complex optical conductivity tensor as given by the Kubo formula at nonzero temperatures and for finite life-time broadening. This technique used together with the spin-polarized relativistic screened Korringa–Kohn–Rostoker (SKKR) method [3] provides then the most proper description of magneto-optical properties in layered systems by accounting on the same footing for both the inter- and the intra-band contributions [4].

From a numerical standpoint of view, the computational accuracy is permanently controlled by using recently developed algorithms such as the cumulative special-points method [5]. All results given in the present contribution have been obtained with an accuracy of 0.001 a.u. by using 35 (2) Matsubara poles at 300 K in the upper (lower) semi-plane and a life-time broadening of 0.048 Ry. The Fermi level −0.038 Ry corresponds to that of FCC–Pt bulk (lattice parameter of 7.4137 a.u.).

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2. Results and discussion

Experimentally it has been shown that Pt as a substrate promotes an FCC(1 1 1) texture [6]. For this reason here only the results obtained for this particular surface orientation are presented.

As can be seen from Fig. 1, in the case of FCC(1 1 1)–Co | Pt_5—over the whole range of optical frequencies ω—the real part of the complex optical conductivity $\Sigma_{xx}(\omega)$ is mainly determinated by contributions arising from the Pt substrate layers. From 0 eV up to 3.5 eV the contribution of the first Pt-layer below the surface to the imaginary part of $\Sigma_{xy}(\omega)$ almost equals that of the Co-layer. Around 4 eV, the Co contribution to $\mathrm{Im}\,\Sigma_{xy}(\omega)$ has a local maximum and the first Pt-layer a minimum. The other Pt substrate layers contribute more or less in–between these two extrema. The other parts of the complex optical conductivity tensor, i.e., $\mathrm{Im}\,\Sigma_{xx}(\omega)$ and $\mathrm{Re}\,\Sigma_{xy}(\omega)$ show similarities with those given in Fig. 1. $\mathrm{Im}\,\Sigma_{xx}(\omega)$ is dominated by the contribution from the first Pt-layer and $\mathrm{Re}\,\Sigma_{xy}(\omega)$ is almost equally determined by the surface Co-layer and by the first Pt substrate layer. Furthermore, based on our calculations performed for FCC(1 0 0) and FCC(1 1 0) surface orientations, it can be said that the above listed features of layer-resolved optical conductivities are not surface dependent.

Pt cap layers on the top of the Co-layer deposited on FCC(1 1 1)–Pt are needed to prevent oxidation of the surface [7]. We found that only multilayer systems with

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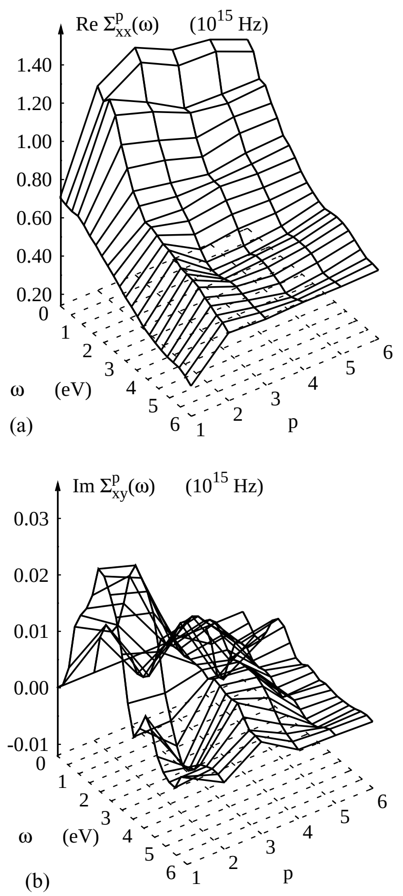

Fig. 1. Absorptive parts of the layer-resolved complex optical conductivity $\Sigma^{p}_{\mu\nu}(\omega)$ for FCC(1 1 1)–Co | Pt_5 as a function of the optical frequency ω and the layer index p. Heavy line marks the Co-layer resolved optical conductivity $\Sigma^{p=1}_{\mu\nu}(\omega)$.

Pt cap layers exhibit perpendicular magnetization to the surface. Furthermore, it has been found that the magnetic moments induced in the Pt-layers are symmetrically distributed above and below the Co-layer in such systems. Therefore, it is not surprising that a cap and the corresponding Pt substrate layer contribute in a similar manner to the layer-resolved optical conductivity tensor as is demonstrated in Fig. 2. Additional calculations performed for FCC(1 1 1)–Pt_m| Co |Pt_{8-m} for $m = 1, 2$ (not shown in Fig. 2), proved that this particular feature remains unchanged when increasing the number of Pt cap layers. A comparison of Fig. 1 with Fig. 2 shows that the Pt cap layers reduce the contributions from the Co and the Pt substrate layers, but do not change significantly their frequency dependence.

In conclusion, it can be said that over the whole range of frequencies besides the ferromagnetic Co-layer the optical conductivity tensor of Co | Pt multilayer systems is equally determined by Pt contributions arising from a Pt cap and/or substrate layers.

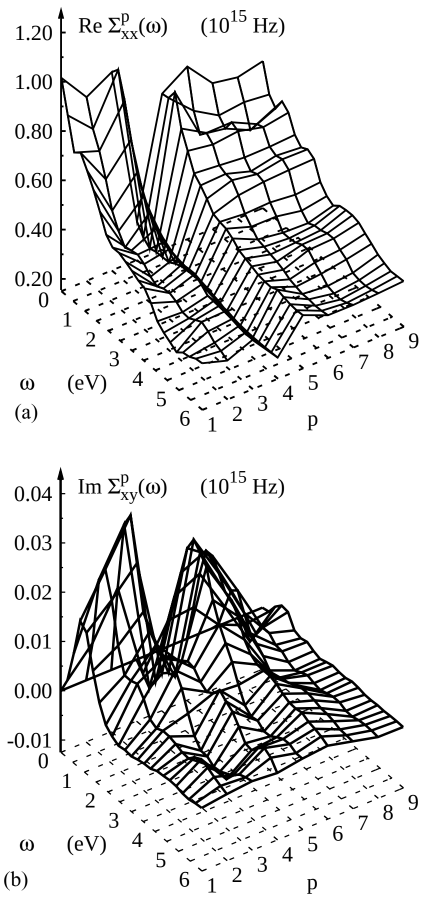

Fig. 2. Absorptive parts of the layer-resolved complex optical conductivity $\Sigma^{p}_{\mu\nu}(\omega)$ for FCC(1 1 1)–Pt_3 | Co | Pt_5 as a function of the optical frequency ω and the layer index p. Heavy line marks the Co-layer resolved optical conductivity $\Sigma^{p=1}_{\mu\nu}(\omega)$.

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