Photoemission approach to spin motion in electron transmission through magnetic films

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Abstract

First-principles calculations demonstrate that the spin motion in electron transmission through ultrathin magnetic films can be investigated by means of spin- and angle-resolved core-level photoelectron spectroscopy. Spin motion can be viewed as precession around and relaxation towards the magnetization. For Fe films on Pd(0 0 1), its dependence on film thickness as well as on the Fe electronic structure is studied. Further, effects of the light polarization are discussed.
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1. Introduction

With decreasing size of magneto-electronic devices, scattering of electrons at ultrathin films and at interfaces becomes increasingly important with regard to spin-dependent transport. For example, the spin polarization (ESP) $\vec{P}$ of an electron transmitted through a ferromagnetic film precesses around and relaxes towards the magnetization $\vec{M}$. Whereas the precession is due to elastic scattering, the relaxation involves inelastic processes [1]. In order to investigate these fundamental spin-motion effects, one typically uses electron transmission through freestanding magnetic films or low-energy-electron diffraction (see, e.g., Refs. [2,3]).

We propose a new approach to spin motion in electron transmission through magnetic films [4].

Using spin- and angle-resolved core-level photoelectron spectroscopy, spin motion can be investigated in detail, with the advantages of easy orientation of the incoming ESP $\vec{P}^{\text{in}}$ and avoidance of freestanding films (Fig. 1, right). First, electrons from a core-level of the non-magnetic substrate (here: Pd $3d_{3/2}$) are excited to energies above the vacuum level E_{vac}. Depending on both polarization and incidence direction of the light, $\vec{P}^{\text{in}}$ can easily be oriented, an effect due to spin-orbit coupling [5]. Second, being subject to spin-dependent scattering, the electrons are transmitted through the covering magnetic film [here: fcc-Fe/Pd(0 0 1)] and display spin motion. The latter is eventually resolved by detecting the transmitted ESP $\vec{P}^{\text{tr}}$ of the photoelectrons. A similar method employing the spin-filter effect was used for spin-resolved band mapping in Fe/Cu(0 0 1) [6].

To demonstrate that the new approach can be used as a tool for detailed investigations of spin motion, we performed state-of-the-art

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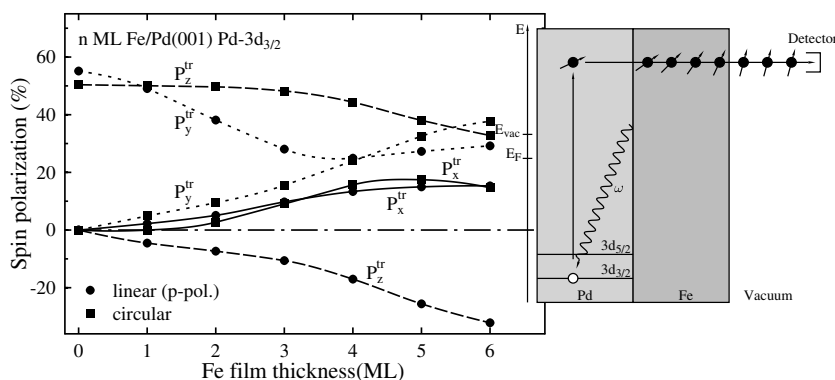
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Fig. 1. Light-polarization effects in spin motion. The transmitted ESP $\vec{P}^{\mathrm{tr}}$ for p- (circles) and circularly (squares) polarized light is shown vs. Fe film thickness (0–6 ML, normal emission, kinetic energy 17.5 eV). The inset on the right sketches the proposed photoemission approach to spin motion.

photoemission calculations. Model calculations corroborate our first-principles results.

2. Computational

Starting from first-principles calculations for 0–6 ML fcc-Fe/Pd(0 0 1) [7], spin- and angle-resolved photoemission spectra were calculated within the relativistic one-step model, as formulated in the layer-KKR (Korringa–Kohn–Rostoker) method (for details, see Ref. [8]). Inelastic processes were simulated by the imaginary part of the self-energy ('optical potential'), assuming a constant value of 1.8 eV. Considering several 'artificial' magnetic configurations proved that the spin motion is due to the Fe film. The results presented in the following were obtained for normal emission ($\vec{k}_{\parallel} = 0$). The magnetization $\vec{M}$ of the Fe films is in-plane, along the x axis.

3. Results and discussion

First, we address the spin-motion dependence on Fe-film thickness for two different light polarizations. For p-polarized light (e.g., incident with 45° polar angle), $\vec{P}^{\mathrm{in}}$ lies perpendicular to the scattering plane. By changing the azimuth of light incidence, it can be oriented within the surface plane (xy), e.g., perpendicular to $\vec{M}$. 'Optical ori-

entation' with normally incident circularly polarized light results in $\vec{P}^{\mathrm{in}}$ being along the surface normal (z axis). Hence, considering several directions of light incidence as well as light polarizations allows in principle to determine the orientation of the Fe magnetization since spin motion vanishes for $\vec{P}^{\mathrm{in}} \| \vec{M}$.

The spin motion for $\vec{P}^{\mathrm{in}} \perp \vec{M}$ vs. Fe-film thickness is displayed in Fig. 1, for p-polarized [$\vec{P}^{\mathrm{in}} \| \vec{y}$; cf. the value for uncovered Pd (0 ML)] and circularly polarized light ($\vec{P}^{\mathrm{in}} \| \vec{z}$). In both cases, the 'incoming' components (P_y^{tr} and P_z^{tr}, resp.) decrease, while the 'precessional' components P_z^{tr} and P_y^{tr} increase (in absolute value). In other words, one observes the onset of an anticlockwise spin precession around $\vec{M}$. Further, both P_x^{tr} increase in a similar manner, that is, the photoelectron spin relaxes towards $\vec{M}$ due to inelastic scattering.

The precession shows a wavelength of about 200 ML, meaning that a complete spin rotation cannot be observed in ultrathin films due to the small photoelectron escape depth of a few ML [9]. Further, multiple reflection at the boundaries of the Fe film (substrate/film and film/vacuum) induces a modulation of the spin motion with about 4 ML oscillation period, as being corroborated by model calculations for an asymmetric quantum well. This modulation shows up in $\vec{P}^{\mathrm{tr}}$ as deviation from the almost linear thickness dependence.

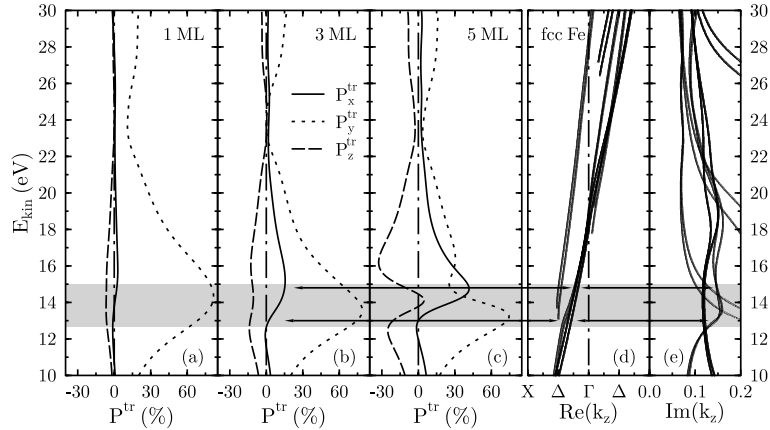Now we turn to effects of the electronic structures. The Pd substrate determines mainly the

Fig. 2. Band-structure effects in spin motion. (a)–(c) Transmitted ESP $\vec{P}^{tr}$ for Fe films 1, 3, and 5 ML thick vs. kinetic energy E_{kin}, for p-polarized light ($\vec{P}^{in} \| \vec{y}$). The components of $\vec{P}^{tr}$ are indicated by different line styles. (d) and (e) Complex band structure of fcc Fe. $Im(k_z)$ is given in units of $\Gamma-\Delta-X$. The horizontal arrows mark prominent features discussed in the text, whereas the grey areas roughly mark a band-gap range discussed in the text.

degree of $\vec{P}^{in}$. Further, Pd-band gaps result in intensity minima because the number of electrons incident on the Fe film is reduced. More important for the spin motion are details of the electronic structure in the Fe film, which will be discussed for p-polarized light ($\vec{P}^{in} \| \vec{y}$, as in Fig. 1). Whereas for 1 ML coverage the spin motion is very small (cf. P_x^{tr} and P_z^{tr} in Fig. 2a) and $\vec{P}^{tr}$ mainly samples the incoming P_y^{in}, the spin motion increases with film thickness (Fig. 2b and c) and shows up as considerably large P_x^{tr} and P_z^{tr}.

A feature between 12.5 and 15.0 eV kinetic energy (E_{kin}) attracts attention in particular (cf. the arrows in Fig. 2): P_x^{tr} and P_y^{tr} show significant min/max (i.e., a minimum followed by a maximum) and max/min structures (at about 13.0 and 14.8 eV), respectively, whereas P_z^{tr} displays a maximum in-between (at 14.1 eV). Since these structures get pronounced with increasing Fe-film thickness, their relation to the Fe electronic structure is obvious. Instead of discussing this effect in terms of layer-resolved spectral densities, we proceed by considering the complex band structure (BS) of fcc Fe (Fig. 2d and e). The latter was computed including the lifetime broadening that was used in the photoemission calculations [Considering only evanescent states decaying towards the bulk makes the band structure projected onto the $Re(k_z) - E_{kin}$ plane (Fig. 2d) non-symmetric with respect to Γ].

A significant feature in the BS in the particular energy range is an increase in $Im(k_z)$ of two exchange-split bands, which is typical for a band gap being smeared out by lifetime broadening (cf. the grey areas in Fig. 2). Since band gaps are hardly visible in $Re(k_z)$ (Fig. 2d), we checked the band-gap origin by computing BS's with reduced lifetime broadening (not shown here) in which the band gaps show up clearly. Note that the complex
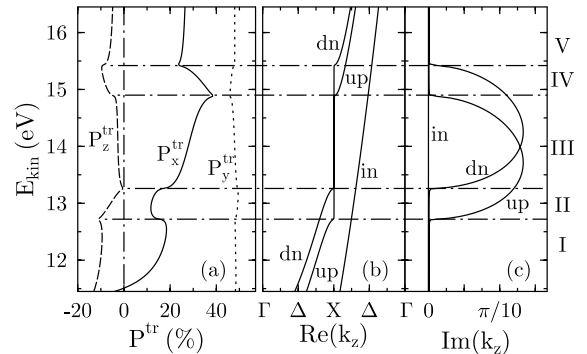

Fig. 3. Effect of band gaps on the spin motion in a nearly-free electron model. (a) Transmitted ESP $\vec{P}^{tr}$ for incident electrons with $P_y^{in} = 50\%$. (b) and (c) Complex band structure of the substrate (incident electrons, 'in') and in the magnetic film (spin up and down electrons, 'up' and 'dn'). The exchange split band gap in the film shows up at $Re(k_z) = X$. $Im(k_z)$ is given in units of $\Gamma-\Delta-X$. The energy ranges discussed in the text are indicated on the right ('I', . . ., 'V').

BS calculated with 1.8 eV lifetime broadening is strongly distorted with respect to the real BS. Especially band gaps become narrower and are shifted in both energy and $Re(k_z)$.

The above structures can be explained by the alternating (in E_{kin}) reduction of the transmission in one spin channel, as being confirmed by a model calculation for exchange-split nearly-free electrons (Fig. 3). To reveal the basic effect, lifetime broadening is not taken into account. In energy ranges I and V (Fig. 3, right), both spin channels are well transmitted through the film $[Im(k_z) = 0]$. In II and IV, one spin channel is suppressed $[Im(k_z) > 0$ for 'up' in II, for 'dn' in IV] while the other is transmitted, whereas in III both channels are suppressed. These energy-dependent transmissions affect the spin polarization of an electron that is polarized perpendicular to the spin-quantization axis (parallel to $\vec{M}$) because its spinor is a superposition of 'up' and 'dn' spinors. Consideration of the spin-density matrix of the transmitted electron yields the observed structures in $\vec{P}^{tr}$. For P_x^{tr}, the minimum in II and the maximum at the range boundary III/IV correspond to the min/max structure in Fig. 2c (note that the $\vec{P}^{tr}$ structures in Fig. 2a–c are smeared out due to lifetime broadening). Since the model calculation is based on rather crude approximations (e.g., number of bands, lifetime broadening), agreement with the ab initio results cannot be expected. For instance, P_y^{tr} shows much less structure in the model (Fig. 3a) than in the ab initio calculation (Fig. 2c).

4. Conclusions

The proposed photoemission approach to spin motion allows obtaining detailed information on the electronic and magnetic structure of ultrathin films. We hope that our calculations will stimulate corresponding experiments.

References

[1] M.D. Stiles, A. Zangwill, Phys. Rev. B 66 (2002) 014407.
[2] D. Oberli, S. Riesen, W. Weber, H.C. Siegmann, J. Magn. Magn. Mater. 198–199 (1999) 140.
[3] W. Weber, S. Riesen, C.H. Back, A. Shorikov, V. Anisimov, H.C. Siegmann, Phys. Rev. B 66 (2002) 100405(R).
[4] J. Henk, P. Bose, T. Michael, P. Bruno, Phys. Rev. B 54 (2003) 052403.
[5] J. Kessler, Polarized Electrons, Springer Series on Atoms and Plasmas, second ed., vol. 1, Springer, Berlin, 1985.
[6] W. Kuch, M.-T. Lin, K. Meinel, C.M. Schneider, J. Noffke, J. Kirschner, Phys. Rev. B 51 (1995) 12627.
[7] J. Henk, A. Ernst, J. Electron Spectrosc. Relat. Phenom. 125 (2002) 107.
[8] J. Henk, A.M.N. Niklasson, B. Johansson, Phys. Rev. B 59 (1999) 13986.
[9] M.P. Seah, W.A. Dench, Surf. Interf. Anal. 1 (1979) 2.