NOVEL IMAGING TECHNIQUE OF THE MAGNETIC BRILLOUIN ZONE OF THIN FILMS AND MAGNETIC SURFACES

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The energy and wave-vector resolved, spin-split electronic structure of thin magnetic films and surfaces can be mapped out under certain conditions by means of the polarized two-electron coincidence technique. This is demonstrated experimentally and theoretically for the case of a Fe (110) sample.

1 Introductory remarks

A number of important properties of materials, such as the magnetic, the optical and the transport properties, are determined mainly by the details of the underlining electronic structure. For probing the electronic structure a number of spectroscopic techniques have been established over the years, e.g. photoemission, optical and x-ray absorption spectroscopies and electron scattering techniques are widely used methods.

In this work we show theoretically and experimentally that the electronic structure of magnetic materials can be investigated by means of the spin polarized two-electron coincidence spectroscopy [1,2,3]. In addition, this technique allows to probe spin dependent excitations[1,2,3] which is the determining factor for a variety of dynamical properties of magnetic materials. In an inelastic electron scattering experiment, the sample is bombarded by electrons with a given primary energy E_0, and electrons which have suffered an energy loss are detected. In the simplest case, the energy lost by the primary electron has been transferred in a single collision to another electron in the solid, which thereby is excited from its initial state to a state with higher energy. Therefore, in principle, in the final state after the scattering event two hot electrons are present whose energies add up to the energy of the primary electron. If both final state electrons have sufficient energy, they may be emitted into the vacuum, where they can be detected. By employing two detectors in coincidence for detecting the escaping electrons, we can characterize the scattering process in more detail and under certain conditions map out the spin-split band structures [1,2,3].

2 Experimental details

The coincident two-electron emission experiments were performed in a time-of-flight apparatus which is shown schematically in Fig.1. For spin-dependent studies we developed a spin-polarized electron gun, which provides a monoenergetic beam of transversely polarized electrons pulsed 5 MHz to the sample [2,3].

The spin dependence of the two-electron spectrum is envisaged by recording the coincident electron-pair spectra when the spin polarization of the incoming electron beam (denoted by $\uparrow$ ($\downarrow$)) is parallel $W(\downarrow\Downarrow^{M})$ or antiparallel $W(\uparrow\Downarrow^{M})$ to the sample's magnetization direction (referred to as $\Downarrow^{M}$). The normalized difference (i.e. the asymmetry $\mathcal{A}$) between the spectra

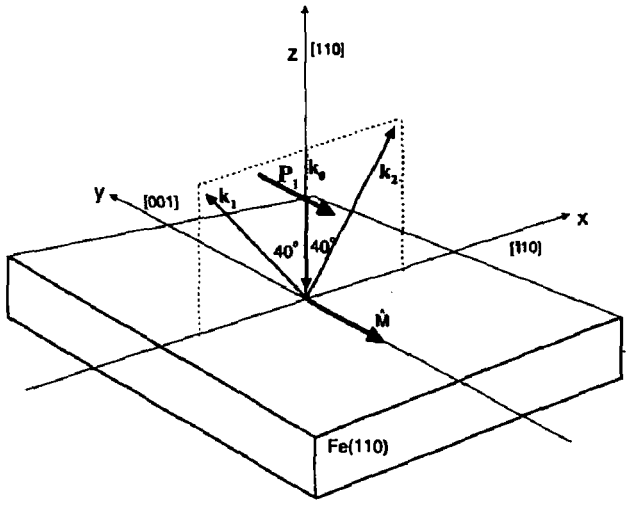

Figure 1. The experimental set-up as employed for the coincidence measurements shown in Fig. 3. The direction of the magnetization **M**, the spin polarization vector of the incoming beam $\mathbf{P}_1$ as well as the wave vectors of the incoming and the two emitted electrons $\mathbf{k}_0$ and $\mathbf{k}_1$ and $\mathbf{k}_2$ are indicated. The two emitted electrons are detected under an angle of 40° to the left and to the right of the z axis.

in these two cases quantifies the role of spin correlations, i.e. we define the quantity $\mathcal{A}$ as

$$\mathcal{A} = \frac{W(\uparrow\Downarrow^{\mathrm{M}}) - W(\downarrow\Downarrow^{\mathrm{M}})}{W(\uparrow\Downarrow^{\mathrm{M}}) + W(\downarrow\Downarrow^{\mathrm{M}})}. \tag{1}$$

The correlated electrons are detected by two channel plates, where energy and emission direction are determined from the flight time and from the detector hit position. The measurements have been performed for a series of materials. In this work we concentrate on the results for a magnetized Fe(110) single crystal. Before presenting the data, a careful theoretical analysis is due in order to understand the significance of the various facets of the spin dependent correlated electron pair spectra.

3 Theoretical considerations

A detailed account of the theory has been given in Refs.[1,2,3]. The conclusion of the theory are the following: a) The spin-dependence of the band-structure caused by the exchange interaction can be determined from the experiment. b) The detected coincidence signal originates from the top most layers which makes this technique predestinate for the analysis of surface magnetism and magnetic thin films. 3) The experiment is sensitive to the spin-resolved spectral density (rather then the density of states), as anticipated by theory [1]. This allows a detailed probe of certain regions of the magnetic Brillouin zone.

Briefly, the ingredients of the theoretical treatment are the following

1. A density matrix formalism to characterize the ensemble of the polarized electrons impinging onto the sample and to describe the magnetic state of the surface.

2. A realistic spin-split surface band-structure deduced on the ground of density functional theory within the local density approximation.

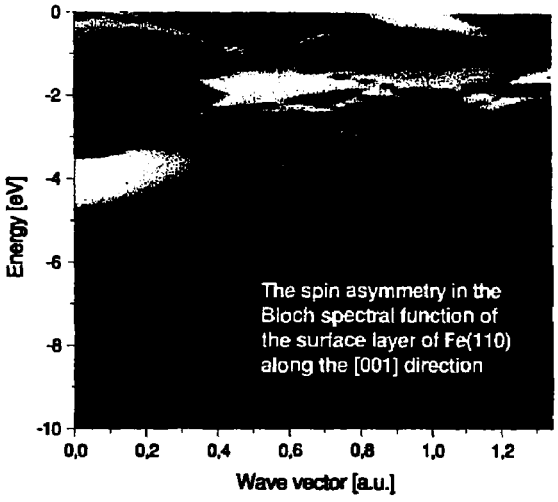

Figure 2. The spin asymmetry in the Bloch spectral function, as defined in Eq.(4), calculated for Fe(110) along the [001] direction (cf. Fig.1). The calculations have been done within the screened LKKR method for the first atomic surface layer. The zero energy point signifies the Fermi level. The weight color corresponds to positive asymmetry of 1 whereas the black color amounts to -1 spin asymmetry. The different grey shades correspond a linear scale in the interval $[-1, 1]$.

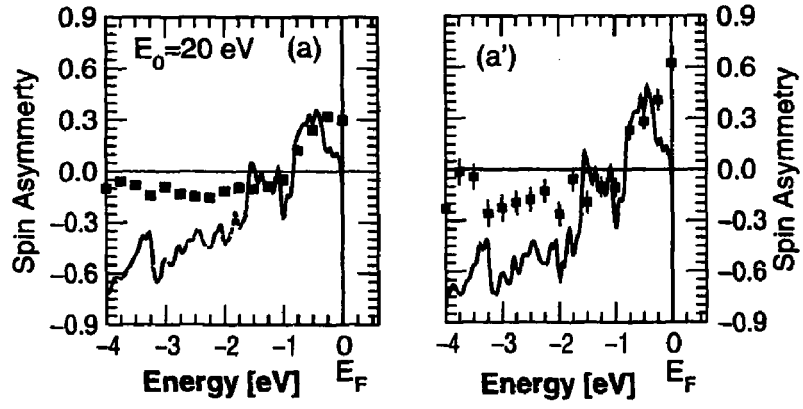

Figure 3. The spin asymmetry $\mathcal{A}$ measured in the set-up shown in Fig.1. The energies of the two emitted electrons are equal ($E_1 = E_2$). The asymmetry $\mathcal{A}$ is varied as function of the energy $\epsilon = E_1 + E_2 - E_0$. According to Eq.(2) ϵ corresponds to the binding energy of the ground state electrons and hence the Fermi energy is at $\epsilon = 0$. The incident energy is $E_0 = 20\,eV$. In the set (a) the angular integration for each of the detectors is $\theta_{1/2} = (40 \pm 15)°$. whereas in (a') the resolution is improved to be $\theta_{1/2} = (40 \pm 7.5)°$. Full squares with error bars are experimental data whereas the solid lines are the theoretical results.

3. A many-body Green function technique to propagate the two hot electrons in the presence of the multi-center potential of the surface.

4 Results and conclusions

From Fig. 1 it is obvious that for perfectly clean, ordered surfaces the energy and wave vector conservation are valid

$$E_0 + \epsilon = E_1 + E_2 \tag{2}$$

$$\mathbf{k}_{0\|} + \mathbf{q}_{\|} + \mathbf{g}_{\|} = \mathbf{k}_{1\|} + \mathbf{k}_{2\|}, \tag{3}$$

where ϵ is the energy of the initially bound valence band electron and $\mathbf{q}_{\|}$ is its (surface) Bloch wave vector. The surface reciprocal lattice vector is denoted by $\mathbf{g}_{\|}$. Experimentally we can tune the energies E_0, E_1, E_2 and the wave vectors $\mathbf{k}_0, \mathbf{k}_{1\|}, \mathbf{k}_{2\|}$. Thus, from Eqs.(2,3) the values of ϵ and $\mathbf{q}_{\|}$ can be deduced, i.e. one can zoom into certain states in the (magnetic) surface Brillouin zone (BZ).

For a comparison between theory and experiment we focus in this short report on one aspect, namely how the spin-dependence in the electronic band structure can be investigated: For bulk systems or for a free standing monolayer we showed [1] that due to symmetry the spin asymmetry $\mathcal{A}$ is directly related to the spin polarization P of the sample's electronic state, if the two electrons are emitted with the same energies and with equal emission angles as depicted in Fig. 1. This conclusion is valid for normal incident electron beam. Put in mathematical language this statement means

$$\mathcal{A} = P = \frac{w(\mathbf{q}_{\|}, l, \epsilon, \Uparrow) - w(\mathbf{q}_{\|}, l, \epsilon, \Downarrow)}{w(\mathbf{q}_{\|}, l, \epsilon, \Uparrow) + w(\mathbf{q}_{\|}, l, \epsilon, \Downarrow)} \quad \text{if} \quad \mathbf{k}_{0\|} = 0, \mathbf{k}_{1\|} = -\mathbf{k}_{2\|}, k_1 = k_2. \tag{4}$$

The quantities $w(\mathbf{q}_{\|}, l, \epsilon, \Uparrow)$ and $w(\mathbf{q}_{\|}, l, \epsilon, \Downarrow)$ are the Bloch spectral functions of respectively the majority and the minority band electrons. For the calculations of the spectral functions of the sample we utilized the self-consistent layer-resolved Korringa-Kohn-Rostoker method (LKKR) [4]. This method is based on the density functional theory within the local-density approximation which works well for the ground state of the material under study. As clear from Fig. 2 the spin polarization P has a rich structure that have been mapped out only partly with the present apparatus due the limited experimental angular resolution. An angular integration over the emission angles entails an integration in a regime in the BZ which is determined accroding the Eqs.(2,3). This is seen in Fig.3 where the finite angular resolution of the experiment imposes a sampling around the Γ point. Since P is not a smooth function of $\mathbf{q}$ and ϵ the outcome of the sampling depends sensitively on the integration region. This can be checked experimentally by improving on the resolution as shown in Fig.3. The oscillatory behaviour of $\mathcal{A}$ in Fig.3 can be related directly to a similar behaviour of $P(\epsilon)$ (Fig.2) at the Γ point. The diminishing experimental value of $\mathcal{A}$ for pair emission from deeper levels in the band is due to spin decoherence induced by inelastic spin-dependent electron-electron collisions. A detailed analysis of this issue and further results and discussions can be found in Ref.[3].

References

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