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Magnetic dichroism in core-level photoemission from Gd(0001)

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This work reports on magnetic dichroism in photoemission from the Gd $4l(l=s,p,d,f)$ core level of in-plane magnetized Gd films excited with linearly, circularly, and unpolarized light. Thin Gd films of about 100 ML thickness were evaporated onto a W(110) substrate at room temperature, and subsequently annealed to 700 K to form an ordered layer exhibiting a (0001) surface. The dichroism measurements were performed by physically rotating the sample azimuth so as to change the direction of the magnetization axis relative to the incident light. The magnetic dichroism asymmetries were obtained by calculating the normalized difference between spectra obtained with the two mutually orthogonal orientations of the magnetization. Strong asymmetries were observed, even if exciting the spectra by means of unpolarized light. The experimental results are compared to three-step photoemission cluster calculations based on a relativistic full potential algorithm respecting magnetic exchange. © *2000 American Institute of Physics.* [S0021-8979(00)89808-4]

I. INTRODUCTION

Magnetic dichroism in core-level photoemission from solids represents a promising new element-specific probe to investigate the magnetic structure of surfaces and interfaces. One way of measuring such effects is to use photoelectrons excited by circular-polarized radiation, for which even the spin-integrated intensity depends on the relative orientation of the photon helicity (left or right circularly polarized) and the sample magnetization. In fact, if the magnetization lies in a surface mirror plane, then inverting its direction can provide a second way of measuring magnetic circular dichroism (MCD). Purely atomic models have been successfully applied to explain many aspects of such data.[1] By varying the direction of emission, one additionally probes the geometric structure of the sample. Such MCD in photoelectron angular distributions (MCDAD) then has to be interpreted in terms of photoelectron diffraction.[2] We studied such effects in core-level emission from Gd(0001).

II. EXPERIMENTAL DETAILS

The experiments have been performed at beamline 9.3.2 (Ref. 3) using the recently completed advanced photoelectron spectroscopy/diffraction endstation.[4] Photoelectron spectra were measured with a Scienta-ES200 electron analyzer. The overall (photon plus analyzer) energy resolution was about 1 eV. The spectra shown below have been taken utilizing both synchrotron and Al $K\alpha$ radiation. The helicity of the photons provided by the synchrotron was chosen by selecting light from above or below the storage ring plane by means of a movable aperture, resulting in about 85% circular polarization.[3] In the experiments presented here, we mostly used left circularly polarized light (LCP), but spot checks were also made to see if inverting magnetization in a mirror plane yielded the same effects as switching to right circularly polarized light (RCP).

The investigated samples were atomically smooth Gd films of about 100 ML (≅300 Å) evaporated at room temperature onto a clean W(110) substrate. The thickness of the films was monitored by a quartz crystal microbalance. A final annealing at 700 K ensures that the surface is flat on the atomic scale. The cleanness and crystalline order of the substrate and the final films were checked by x-ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED). The magnetic properties of the Gd films were studied with remanent in-plane magnetization, as induced by an *in situ* magnetic field of about 200 G lying along a high-symmetry direction. The sample temperature was kept at 240 K during the measurements, which is well below the Curie temperature for bulk Gd (293 K). The geometry chosen for the measurements is shown as an inset in Fig. 1; the photon propagation $\mathbf{q}$, the surface normal $\mathbf{n}$, and the photoelectron momentum $\mathbf{k}$ lie all in one plane with the light impinging on

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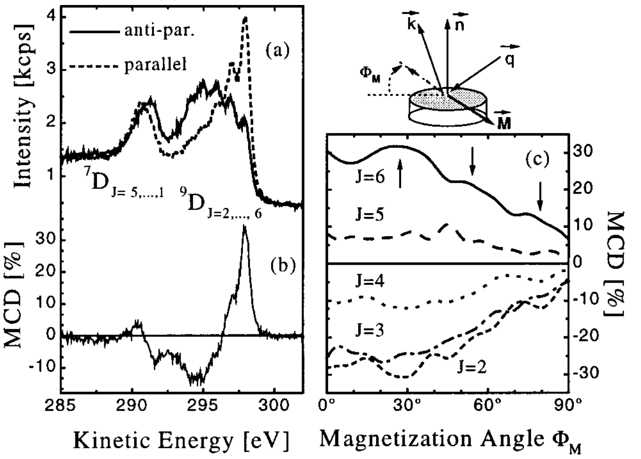

FIG. 1. (a) Gd 4*d* core-level photoemission spectra excited by circularly polarized light (450 eV) with in-plane magnetization (solid line $\Phi_M=0°$, dotted line $\Phi_M=180°$). (b) The MCD asymmetry. The inset shows the experimental geometry. (c) Angular dependence of the *state-specific* MCD for Gd 4*d* core-level emission. Vertical arrows indicate the positions of diffraction features.

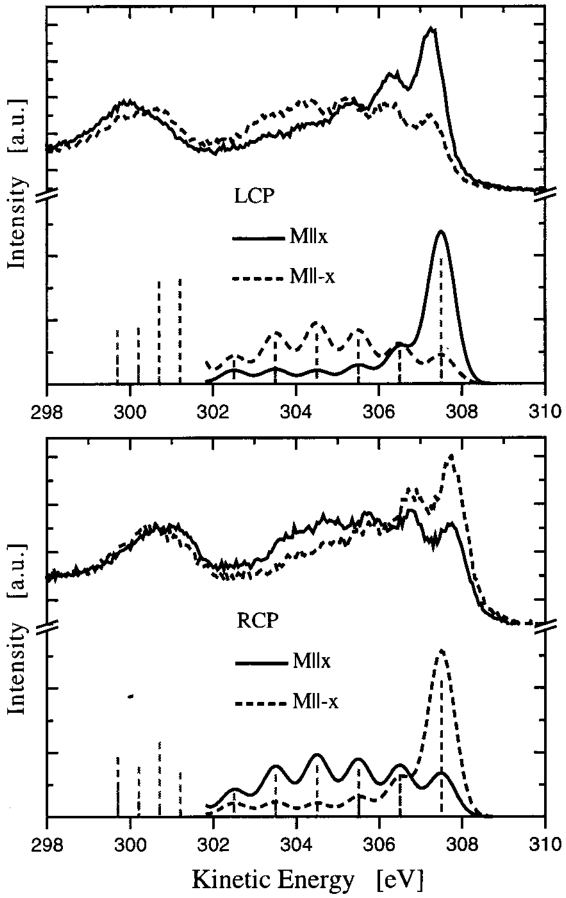

FIG. 2. Comparison between experiment and full-relativistic *jj* multiplet calculations with single photoelectron scattering for the MCD in Gd 4*d* photoemission.

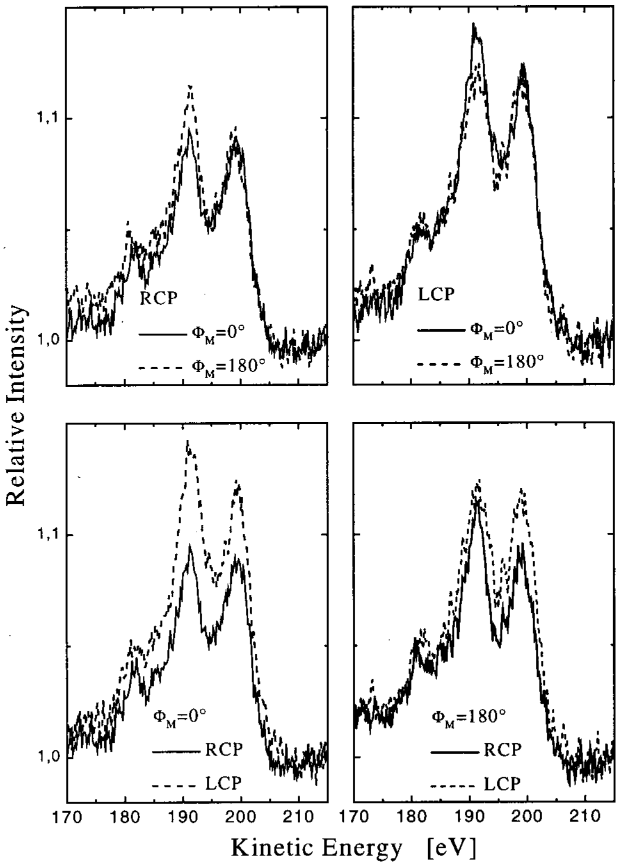

FIG. 3. Magnetic circular dichroism in photoemission from the Gd 4*s* state excited by circularly polarized light.

the sample at 70° angle of incidence. Photoelectrons were collected either in normal emission or at 20° with respect to the surface normal. The sample was rotated stepwise about the surface normal so as to vary the azimuthal emission angle. The MCD measurements were performed by inverting the magnetization direction that is rotating the sample azimuth by 180°. The angle Φ_M varied in the angle-dependent spectra is thus also the angle between the magnetization directions and the plane defined by **q**, **n**, and **k**.

III. RESULTS AND DISCUSSION

Figure 1(a) shows an example of Gd 4*d* core-level spectra taken with two different orientations of the magnetization axis [here denoted as parallel (I_p) and antiparallel (I_a)]. Also shown in Fig. 1(b) is a normalized MCD difference or asymmetry curve obtained from these two spectra. This asymmetry agrees very well with a free-atom theoretical description by van der Laan *et al.*[1] The present data resolve the individual final states of the Gd ion better than the previous experimental results and therefore they can be used as a state-specific measure of the MCD. Figure 1(c) shows the MCD as a function of Φ_M for emission at 20° off normal emission being taken for the first five *J* states of the ^9D multiplet. All states basically exhibit a cosine-like behavior, which would be expected from the free atom case, although it shows noticeable deviations from free-atom behavior (arrows). The additional MCD modulations riding on the overall cosine-like curve are due to photoelectron diffraction. Results of a simulations using single-scattering cluster calculations, including spin-orbit splitting and exchange splitting in the initial state were shown elsewhere.[5] In addition, we performed cluster calculations based on a relativistic full potential method with magnetic exchange to obtain the relative intensities of the $4d$ and $4s$ multiplets. In these calculations, each core-hole multiplet state was described fully, and the photoelectrons resulting from each state were then scattered singly by the surrounding Gd atoms. We have considered two types of angular momentum coupling, starting either from *LSJ* or *JJ*. Comparing these calculations with experiment, we found that starting with *jj* coupling and relativistic $|j,mj\rangle$ wave functions fits the measured results much better than treating the spin-orbit interaction as a perturbation, as usually used in *LSJ* schemes based on $|I,s\rangle$ type wave functions. Some results of such calculations for the 4d spectra are shown in Fig. 2 together with the experimental data. Deviations between experiment and theory seen in the ^7D part of the 4*d* multiplet are due to an incomplete usage of parentage terms.

MCD effects were also observed in the Gd $4f$ excitation utilizing both circular and unpolarized light (not shown here). The observed magnetic dichroism was about 15% for excitation by circularly polarized photons (450 eV) and 35% for excitation with unpolarized Al $K\alpha$ radiation. For the MCD, a zero crossing of the asymmetry was observed within the ^7F_J multiplet, even so its fine structure was not resolved. The asymmetry observed from the $4p$ excitation was about 6% for circular polarized photons (580 eV) and negligible for unpolarized light.

In Fig. 3, experimental results for the $\mathrm{Gd}^{3+}4s^2 4f^7(^8S_{7/2})+h\nu\rightarrow \mathrm{Gd}^{4+}4s^1 4f^7(^{9,7}S_J)+\epsilon(p)$ excitation are shown, in particular, the circular (switching helicity) and the magnetic (switching magnetization) dichroism at normal emission. This demonstrates clearly the existence of a magnetic dichroism in the angular distribution even in emission from initial states with zero orbital angular momentum. The presence of such dichroism for s subshells can only be explained by using full relativistic wave functions in the initial and final states. The atomic part of the dichroism in emission from s states is proportional to $R_{3/2}/R_{1/2}\sin(\delta_{3/2}-\delta_{1/2})$ (R and δ are the *relativistic* radial matrix elements and phases of the $j=1/2$ or 3/2 final state partial waves), which vanishes in the nonrelativistic description.

IV. CONCLUSIONS

The magnetic circular dichroism in the angular distributions (MCDAD) of the $4s$, $4p$, $4d$, and $4f$ core levels was measured for Gd(0001) grown on W(110). Asymmetries up to 35% have been found in all cases. Due to the high resolution, we were able to measure the state-specific MCD for the ^9D branch of the Gd $4d$ excitation. The asymmetry measured in the Gd $4s$ photoemission points clearly on the relativistic nature of the MCD process. The MCD spectra were compared to full relativistic calculations with magnetic exchange. We obtained good agreement with the calculations and more investigations of these issues, from both experimental and theoretical perspectives, are underway.

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