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Core-valence interactions in the linear dichroism of Cr 2p photoelectron spectra

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The linear dichroism in the $2p$ photoelectron spectra of free Cr atoms and Cr atoms bound to an Fe surface has been determined. The spectra of free laser-oriented atoms are compared to Hartree-Fock calculations and the corresponding spectra of magnetized surface layers. The importance of satellites and of the $2p$-$3d$ Coulomb interaction in the final ionic state is demonstrated in both cases.

I. INTRODUCTION

The linear magnetic dichroism in the $2p$ photoelectron spectra of $3d$ transition metal surfaces and thin films has attracted great interest because it promises element specific and surface-sensitive information on the magnetic properties.[1] For the interpretation of the results various models have been proposed ranging from single-particle band-structure approaches to ligand-field multiplet models.[2–9] One of the key issues is the treatment of the interaction of the $2p$ hole with the $3d$ valence electrons. This is intimately related to the local-delocal character of the $3d$ valence electrons in the core excited state. In order to address this problem we studied the linear magnetic dichroism in the $2p$ photoelectron spectra of laser-oriented free Cr atoms. The comparison of the free atom spectra with the corresponding spectra of a Cr surface layer allows for a direct assessment of the importance of the intra-atomic interactions. This approach has proved to be very successful for the photoelectron spectra of the subvalence $3p$ electrons where the intra-atomic $3p$-$3d$ interactions clearly dominate.[10] In the case of the $2p$ spectra the situation should be different due to the reduced overlap of the wave functions of the $2p$ core states and the $3d$ valence electrons and the considerable $2p$ spin-orbit coupling. Therefore a detailed comparison of the spectra of free and bound Cr atoms is of great interest. In addition Cr has very interesting magnetic properties ranging from the antiferromagnetism of the bulk metal to the ferromagnetic order observed for thin films[11] on ferromagnetic substrates which can be probed in great detail by the linear magnetic dichroism.

II. EXPERIMENT

Free Cr atoms in a collimated beam emanating from a resistively heated furnace were oriented by pumping the optical transition $4s \rightarrow 4p$ with circularly polarized laser radiation. Due to the selection rules for the excitation, the magnetic sublevels m_J of the Hund's rule ground state of the free atoms (Cr $3d^5\ 4s\ {}^7S_3,\ J=3$) were populated asymmetrically, corresponding to an orientation of the spin of the atoms. The laser radiation counterpropagated to the linearly polarized undulator radiation from beamline BW3 at HASYLAB which was used to $2p$ core ionize the Cr atoms. Photoelectrons emitted close to the magic angle of 54.7° relative to the polarization axis of the undulator radiation were registered with the aid of a high-resolution Scienta SES 200 electron energy analyzer. Pumping with right and left circularly polarized laser radiation resulted in antiparallel and parallel orientations of the atoms with respect to the propagation direction of the undulator beam. The $2p$ photoelectron spectra of the free Cr atoms were taken for the two opposite orientations of the atoms.

The $2p$ photoelectron spectra of a Cr surface layer deposited on Fe were taken for two opposite magnetizations of the sample. The 0.5 monolayer thick Cr film was deposited on an Fe film grown epitaxially on W(110). The magnetization was reversed by applying pulsed fields of 80 Oe along the easy axis for magnetization of iron. The photoelectron spectra were taken in remanence. The sample was magnetized in plane, the photon incidence angle was 45° with respect to the surface, and the electrons were collected under normal emission with a conventional hemispherical analyzer. The measurements have also been performed at the BW3 station at HASYLAB.

The linear magnetic dichroism in the angular distribution (LMDAD) is defined as the difference of two photoelectron intensities and for atomic orientations and for sample magnetizations of opposite sign.[12,1]

III. RESULTS AND DISCUSSION

Figure 1(a) shows the $2p$ photoelectron lines of atomic Cr. The spectra were taken at a photon energy of 706 eV and have been corrected for the electron analyzer transmission. The binding energies have been established using well-

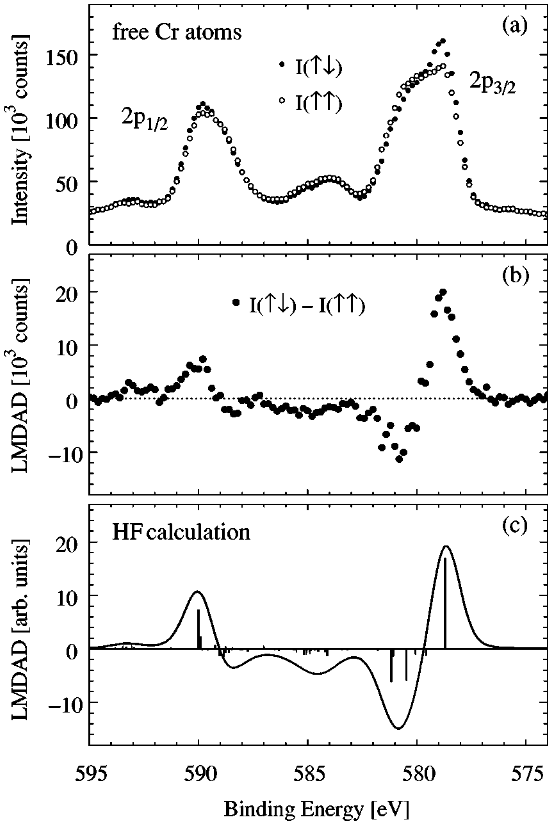

FIG. 1. The $2p$ photoelectron lines of free oriented Cr atoms excited with linearly polarized undulator radiation ($h\nu = 706$ eV) for two opposite orientations of the atoms are depicted in the upper part (a). The difference of the two curves [LMDAD$=I(\uparrow\downarrow)-I(\uparrow\uparrow)$] is displayed in the center (b) and the result of the HF calculation (see text) in the bottom (c).

known rare gas photoelectron lines. As expected from earlier studies of the $2p$ photoabsorption of atomic Cr,[13] the photoelectron spectra are dominated by the spin-orbit splitting of the $2p$ hole. The two main photoelectron lines can therefore in a first attempt be assigned to the $2p_{1/2}$ line at higher binding energy and to the $2p_{3/2}$ line at lower binding energy.

The two photoelectron spectra correspond to opposite orientations of the atoms. The photoelectron intensity considerably depends on the atomic orientation. The difference of the two spectra shown in Fig. 1(a), i.e., the LMDAD in the $2p$ photoionization of the free Cr atoms, is displayed in Fig. 1(b). Both main photoelectron lines clearly display the characteristic pattern of LMDAD:[1,11,14,15] one positive and one negative lobe. However, for the $2p_{1/2}$ line the pattern is inverted and the negative lobe is much less pronounced than the positive one.

The $2p$ LMDAD of the free Cr atoms is interpreted with the aid of the calculated spectrum shown in Fig. 1(c). Following the theory of the angular distribution of photoelectrons from polarized atoms the photoionization cross section can be presented in the form[16]

$$\frac{d\sigma}{d\Omega}=\frac{\pi\alpha\omega}{3\sqrt{2J_0+1}}\sum_{k_0kk_\gamma}\rho_{k_00}B_{k_0kk_\gamma}F_{k_0kk_\gamma}, \tag{1}$$

where ω and α are the frequency of the ionizing photon and the fine-structure constant, respectively. J_0 denotes the total angular momentum of the initial state of the atom. The statistical tensors (state multipoles) ρ_{k_00} with rank $k_0 = 0,1,\ldots,2J_0$ describe the atomic polarization of the initial state. The geometrical factors $F_{k_0kk_\gamma}$ contain the direction of the atomic polarization, the direction of the photoelectron emission, and the polarization state of the ionizing photon. The coefficients $B_{k_0kk_\gamma}$ contain the many-electron dipole matrix elements $\langle \gamma_f J_f,\varepsilon lj{:}J\|D\|\gamma_0 J_0\rangle$ and describe the dynamics of the photoionization process.[16] The total angular momentum J_f and other quantum numbers γ_f characterize the final ionic state. The photoelectron with kinetic enery ε has orbital and total angular momenta l and j, respectively. J denotes the total angular momentum of the final system (ion + photoelectron). The expressions for $F_{k_0kk_\gamma}$ and $B_{k_0kk_\gamma}$ in Eq. (1) are given in Ref. 16.

Only terms proportional to odd statistical tensors $\rho_{10},\rho_{30},\ldots$ in Eq. (1) contribute to the difference of cross sections for two opposite atomic orientations, i.e., to the LMDAD.[16] Simulating the pumping process of the free Cr atoms by solving the rate equations for the optical transition it furthermore turns out that the contribution of all higher tensors except ρ_{10} can be neglected.[10,17] This approximation reduces the number of terms in Eq. (1) to 1 [for $k_0=1$ only the set $(k_0kk_\gamma)=(122)$ is allowed]. We can further omit the quantities ρ_{10} and F_{122}, which do not depend on the quantum numbers characterizing the final ionic state: they are constant over the whole photoelectron spectrum. The shape of the LMDAD curve is therefore solely determined by the coefficients B_{122} and independent of the experimental geometry. We thus find

$$\text{LMDAD}=I(\uparrow\downarrow)-I(\uparrow\uparrow)\propto\frac{d\sigma}{d\Omega}(\uparrow\downarrow)-\frac{d\sigma}{d\Omega}(\uparrow\uparrow)\propto B_{122}. \tag{2}$$

We determined the dipole matrix elements given above for the Cr $2p$ photoionization within a Hartree-Fock (HF) calculation performed in the single-configuration approximation in intermediate coupling. We only considered the configuration $\text{Cr}^+\ 2p^5\ 3d^5\ 4s$. The Slater integrals have been scaled down to 85% to take into account the influence of electron correlation effects. Inserting the matrix elements in the expression for B_{122} given in Ref. 16 we calculated the LMDAD for the different final ionic states according to Eq. (2). The result of these calculations is shown in Fig. 1(c) and referred to in the following as the ''HF calculation.''

The relative intensities of the bars in Fig. 1(c) are given by the calculated values of the coefficients B_{122}. The solid curve was obtained by replacing the bars by Lorentzian profiles of full width at half maximum (FWHM) of 0.3 eV, reflecting the lifetime of the $2p$ hole states.[18] The sum of the Lorentzian profiles was convoluted with a Gaussian profile of FWHM$=1.4$ eV to account for our instrumental broadening.

The HF calculation well reproduces the experimental spectrum. Two patterns with each one positive and one negative lobe and inverted with respect to each other are predicted for the two spin-orbit partners. Also the weak and broad dichroic signals stemming from satellite structures discernible between the $2p_{1/2}$ and the $2p_{3/2}$ lines and on the high binding energy side of the $2p_{1/2}$ line are reproduced.

The bars in Fig. 1(c) reflect the atomic multiplet splitting of the final ionic states of $\mathrm{Cr}^+\ 2p^5\ 3d^5\ 4s$. The lowest levels at binding energies around 580 eV can be described by a coupling where the $2p$ hole is jj coupled to $j=3/2$ and the valence electrons $3d^5\ \ 4s$ are LS coupled to ^7S according to Hund's rule. This is justified by the HF calculation which gives for the spin-orbit interaction in the $2p$ shell $\zeta(2p)=5.7$ eV and for the $3d$ intrashell Coulomb interactions $F^2(3d,3d)=8.8$ eV and $F^4(3d,3d)=5.5$ eV. The strong $2p$-$3d$ intershell Coulomb interactions $G^1(2p,3d)=3.5$ eV, $G^3(2p,3d)=2.0$ eV, and $F^2(2p,3d)=4.9$ eV couple the $2p$ hole and the valence electrons. This leads to four levels $J_f=9/2$, 7/2, 5/2, and 3/2 for the $2p_{3/2}$ hole. Three of these levels show a strong LMDAD as can be seen in Fig. 1(c) (one positive, two negative). They mainly lead to the $+/-$ pattern observed in the measured spectrum in Fig. 1(b). The 7/2 level is barely visible in Fig. 1(c) like two weak levels stemming from a spin flip of the $4s$ valence electron. Except this the interactions with the $4s$ electron are negligibly small. Likewise the spin-orbit interaction in the $3d$ shell is negligible. van der Laan and Kirkman calculated similar values for the Slater integrals and spin-orbit parameters as given here in their study of the $2p$ absorption spectra of various $3d$ transition metal ions.[19] In a recent theoretical investigation of the $2p$ core hole states of Mn^{2+} ions a similar angular momentum coupling scheme has been used as presented above.[20]

The satellite structures around 585 eV in Figs. 1(a)–1(c) can be attributed to $2p_{3/2}$ states with a recoupled $3d$ shell (^4P,^4D) as the result of a spin flip of one of the $3d$ valence electrons. In the $2p_{3/2}$ main line in contrast the spins of all $3d$ electrons are aligned parallel ($3d^5\ \ ^6S$).

The situation in the second main line at 590 eV in Figs. 1(a)–1(c) is more complicated because in this binding energy region the levels of $2p_{1/2}$ states with parallel $3d$ spins (^6S) overlap with the levels of $2p_{3/2}$ states and a recoupled $3d$ shell with two flipped $3d$ spins (^2L). This results in a strong mixture of states which makes an assignment very difficult. Furthermore, there are considerably more energy levels than the two with $J_f=7/2$ and 5/2 obtained by the coupling of the $j=1/2$ core with ^7S valence electrons. As a consequence the negative LMDAD signal is suppressed compared to the positive one in this line as observed in the experimental spectrum.

The weak and broad positive LMDAD signal at around 593 eV in Figs. 1(b) and 1(c) can be attributed to satellite lines with a $2p_{1/2}$ hole and a recoupled $3d$ shell with a flip of one $3d$ spin (^4L). These lines therefore can be seen as the spin-orbit partners of the satellites around 585 eV: they accordingly contribute with an inverted (positive) signal in contrast to the negative one of the $2p_{3/2}$ satellites. This is comparable to the inverted patterns of the two main lines.

The satellite lines with recoupled $3d$ valence shell unambiguously are the reason for the deviation of the shape of the LMDAD curve from the simple standard pattern showing positive and negative signals of equal size. The LMDAD does therefore not vanish neither when integrated over the binding energy region of the two main lines nor when integrated over the whole measured binding energy region. This holds for the experimental and for the calculated spectrum.

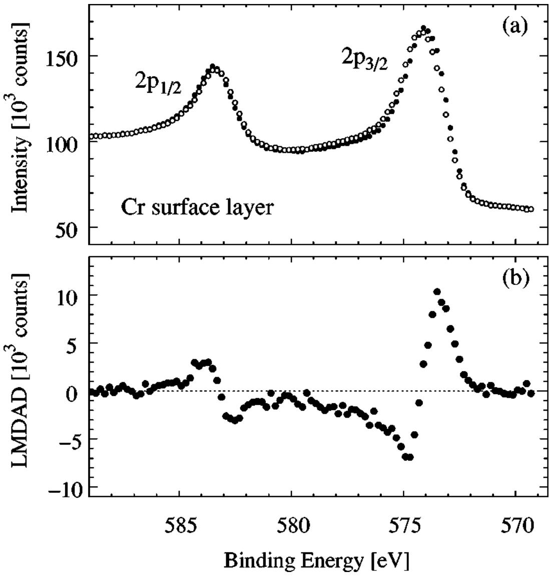

FIG. 2. The $2p$ photoelectron spectra of a magnetized Cr surface layer excited with linearly polarized undulator radiation ($h\nu=705$ eV) for two opposite magnetizations are depicted in the upper (a) and their difference (LMDAD) is displayed in the lower part (b).

In the following the $2p$ photoelectron spectra of free Cr atoms are compared to the corresponding spectra of Cr atoms bound at a surface. The $2p$ photoelectron spectra of the Cr surface layer excited at a photon energy of 705 eV for two opposite magnetizations are shown in Fig. 2(a). Their difference, i.e., the LMDAD, is displayed in Fig. 2(b). The $2p$ photoelectron spectra of the Cr surface layer clearly display the ‘‘$2p_{1/2}$’’ and the ‘‘$2p_{3/2}$’’ line. The spectrum of the $2p$ photoemission for adsorbed Cr shows less fine structure than that of the free atom. This in part is caused by many-body electron hole excitations leading to asymmetric photoemission lines,[21] as well as by the influence of secondary electrons which always accompany photoemission spectra of solids. The reduced multiplet splitting expected for the bound Cr atoms also contributes to the loss of fine structure. This is consistent with the smaller half-width and smaller energy separation of the two main lines observed in the spectrum of the Cr surface layer and can be explained by a reduction of the Coulomb and exchange interactions in the bound Cr atoms to 70% of the (scaled) free atom value as verified by HF calculations. The LMDAD of the surface layer in Fig. 2(b) shows the characteristic pattern of a LMDAD in both lines. In addition a negative dichroic signal between the two lines is clearly discernible.

A detailed comparison of the LMDAD in $2p$ photoelectron spectra of free Cr atoms and a Cr surface layer is done with the aid of Fig. 3. We replotted the dichroism curves from Fig. 1(b) and Fig. 2(b) along the binding energy axis of the free atom. The spectrum of the surface layer had therefore to be shifted by approximately 5.5 eV towards higher binding energies to account for the atom-to-solid binding

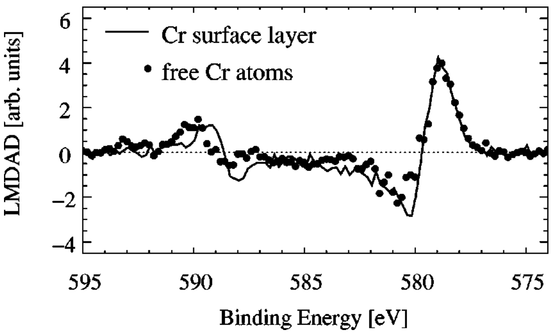

FIG. 3. Comparison of the LMDAD of a magnetized Cr surface layer [taken from Fig. 2(b)] and the LMDAD of free oriented Cr atoms [taken from Fig. 1(b)]. Both curves are displayed along the binding energy axis of the free atoms and normalized to each other in the maximum. The spectrum of the Cr surface layer has been shifted by 5.5 eV towards higher energies.

energy shift. The binding energies and the intensities of the two curves have been matched in the strongest positive lobe. The contraction of the spectrum of the Cr surface layer discussed above clearly manifests itself also in the LMDAD. Figure 3 demonstrates the close similarity of the LMDAD in the $2p$ photoelectron spectra of free and bound Cr atoms. This observation is convincing proof of the atomic nature of the effect. Intra-atomic interactions determine the structure and shape of the LMDAD of the Cr surface layer. Atomic multiplet splitting like in the free Cr atoms due to the Coulomb interactions of the $2p$ core hole and the $3d$ valence electrons in the final ionic state is the origin of the $+/-$ LMDAD patterns of the Cr surface layer. This implies that the $3d$ valence electrons of the $2p$ excited Cr surface atoms are of localized atomic character. The experimental data for the surface layer can be described by assuming a $2p^5\ 3d^5$ ionic configuration though some admixture of $2p^5\ 3d^4$ cannot be excluded.

The dichroism of crystalline samples can be influenced by photoelectron diffraction.[22] For high kinetic energies >300 eV, forward scattering dominates the diffraction effects, while for the low kinetic energies (~ 100 eV) of our experiment also large-angle scattering is important,[23] so that in principle the dichroism could be affected by diffraction even for emission from an adsorbed monolayer. However, it is known that diffraction influences primarily the magnitude of the dichroism while leaving the line shape of the dichroism spectrum essentially unaffected.[24] Therefore, for a discussion of the dichroism line shape, diffraction can be neglected.

The similarity of the $2p$ LMDAD of the free and bound Cr atoms indicates that the effects of the high background of secondary electrons in the spectra of the Cr layer and the asymmetric Doniach-Sunjic line shapes nearly cancel out in the difference spectrum of the surface layer. This is supported by model calculations. Spin-dependent transmission effects can be neglected as the photoelectrons were collected under normal emission.[25] In their study of the dichroism in the Ni $2p$ spectrum van der Laan *et al.* reached a similar conclusion.[8]

The $2p$ LMDAD spectrum of the Cr surface layer displays a strong negative signal between the two main lines. From the comparison to the atomic spectrum we conclude that satellite lines with a spin flip of one of the $3d$ valence electrons are the reason for this dichroic signal in the surface layer spectrum. Like in the free atom spectrum these satellites are the reason why the LMDAD of the Cr surface layer integrated over the measured binding energy region is not equal to zero. In the $2p$ LMDAD of a thin Fe layer a strong and broad signal between the two main lines has also been observed[1,11] and may have the same origin as in the Cr surface layer investigated here. In agreement with our assignment the authors excluded solid-state effects and suggested an origin of atomic nature to be responsible for this structure.

The close resemblence of the $2p$ photoabsorption spectra of Mn layers recorded by Dürr *et al.*[26] and the $2p$ photoabsorption spectra of free Mn atoms[27] is consistent with our observation of the close similarity of the $2p$ LMDAD of free and bound Cr atoms. Dürr *et al.* also assumed a strong localization of the $3d$ valence electrons. In other recent investigations indications for localized $3d$ valence electrons of $3d$ metal atoms bound in thin layers and in clusters have been found.[28–32]

Dichroism in the $2p$ photoelectron spectra of magnetized metallic systems[33] is commonly described with the aid of one-electron models.[1,14,15,34–43] These go back to the theoretical investigations of Ebert *et al.*,[2] Cherepkov and Kuznetsov,[3] and van der Laan[4] and are based on the assumption of an itinerant character of the $3d$ metal valence electrons. In addition Thole and van der Laan have developed theoretical many-electron approaches for localized systems (see, e.g., Ref. 5). In the one-electron model it is assumed that the exchange interaction of the $2p$ core electrons and the bandlike spin-polarized $3d$ valence electrons in the ground state causes a Zeeman-like splitting of $2p_{1/2}$ and $2p_{3/2}$ into the sublevels $m_j=-1/2,+1/2$ and $m_j=-3/2,-1/2,+1/2,+3/2$, respectively. The dichroism is described by a polarization-dependent photoionization probability of these sublevels. The origin of the dichroism is thus explained in the one-electron model by the ground-state properties. This is inconsistent with our observation of the similarity of the $2p$ LMDAD of free and bound Cr atoms. We demonstrated that the local intra-atomic interactions in the final ion, causing atomic multiplet splitting and satellite emission, are crucial for the description of dichroism. Detailed studies (see, e.g., Refs. 44–47) have shown that the $2p$-$3d$ Slater integrals of $3d$ metal atoms bound in metals or compounds are only reduced by up to 30% from the (scaled) free atom values consistent with our findings. The free atom values typically are of the order of 3–8 eV for the different $3d$ metal atoms.[47,19] The $2p$–$3d$ Coulomb interactions thus are comparable in magnitude to the $2p$ spin-orbit interaction and can certainly not be neglected in the interpretation of the $2p$ photoelectron spectra of $3d$ metals. The suitability of the ground-state one-electron model has been questioned earlier in the investigation of the magnetic dichroism in $2p$ photoelectron spectra of thin Fe films.[1,37] van der Laan *et al.* demonstrated the complete breakdown of the one-electron model for the description of the magnetic dichroism in the $2p$ photoelectron spectra of thin Ni layers which are dominated by satellite emission.[38] The Ni spectra are therefore described using a final-state impurity model[6–8] or a small-cluster model,[9] both accurately taking into account the final-state interactions of the ions.

IV. CONCLUSIONS

Our investigations on the linear magnetic dichroism in the $2p$ photoelectron spectra of free Cr atoms prove that the Coulomb interaction of the $2p$ core hole and the $3d$ valence electrons in the final ionic state is crucial for the description of the dichroism. The corresponding spectra of a Cr surface layer clearly display the atomic signature of the effect. The origin of the $+/-$ LMDAD patterns for the two spin-orbit split main lines can be traced back to the multiplet splitting in the final ion. This demonstrates the importance of the $2p$-$3d$ Coulomb interaction in the $2p$ photoionization of $3d$ metal thin films. The influence of satellite lines with recoupled $3d$ shell leads to additional weak and broad LMDAD signals and to a redistribution and/or partial suppression of the LMDAD in the main lines.

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