PHYSICAL REVIEW B VOLUME 50, NUMBER 9 1 SEPTEMBER 1994-I

Photoelectron-diffraction effects and circular dichroism in core-level photoemission

C. Westphal and A. P. Kaduwela
Materials Sciences Division, Lawrence Berkeley Laboratory, Berkeley, California 94720

C. S. Fadley
Materials Sciences Division, Lawrence Berkeley Laboratory, Berkeley, California 94720
and Department of Physics, University of California-Davis, Davis, California 95616

M. A. Van Hove
Materials Sciences Division, Lawrence Berkeley Laboratory, Berkeley, California 94720

(Received 15 April 1994)

We have calculated the circular dichroism associated with core-level photoemission using multiple-scattering photoelectron-diffraction theory. For C 1*s* emission in a chiral geometry from CO adsorbed on Pd(111), photoelectron-diffraction calculations predict the dichroism found in experimental results due to Bansmann *et al.* and also agree well with prior free-molecule calculations by McKoy and Stephens. Backscattering from the Pd substrate is also found to alter the dichroic asymmetries for different adsorption geometries. Analogous calculations for Fe 2*p* emission from a small Fe cluster also indicate that dichroism due to a chiral geometry can strongly affect measurements of magnetic circular dichroism in systems with net magnetization. With generalization to include spin-orbit and multiplet splittings in the initial state and spin-dependent scattering of the outgoing electrons, photoelectron-diffraction theory thus should provide a general method for modeling dischroism in core-level photoemission from both nonmagnetic and magnetic systems.

INTRODUCTION

In recent years, the availability of circularly polarized synchrotron radiation has stimulated considerable interest in spectroscopic studies in the vacuum ultraviolet and/or soft-x-ray and hard-x-ray regimes.[1-19] Most of the experiments[1-4] and calculations[5-8] have been directed to simple photoabsorption measurements. However, in a smaller number of cases the intensities of the photoelectrons emitted have been calculated[9-12] and observed,[13-19] including, for a few systems, also their angular variations.[14,15,17-19] In the photoelectron experiments, up to ±100% differences have been observed between photoelectron intensities obtained with left and right circularly polarized (LCP and RCP) light, provided that the experiments were performed in a chiral geometry.[15,17]

We will concentrate here on the simplest case of *core-level photoelectron emission,* which has been measured with circularly polarized excitation from absorbed molecules,[18(a)] ferromagnetically ordered atoms,[4,16] and most recently, a semiconductor surface.[19] For the case of emission from an adsorbed diatomic molecule, a chiral geometry results if the direction of the incoming light, the direction of molecular orientation, and the direction of the outgoing electron wave are not coplanar. This we shall term "normal" circular dichroism (CD) to distinguish it from the magnetic circular dichroism to be discussed later. The normalized difference in the photoelectron intensities I_{LCP} and I_{RCP} excited with LCP and RCP light, respectively, measured as a function of the direction of the outgoing electron, has also been termed circular dichroism in the angular distribution of photoelectrons (CDAD).[14,15] For a magnetic system, analogous core-level experiments have involved measuring differences in I_{LCP} and I_{RCP} when the magnetization axis of the specimen was charged with respect to the incidence direction of the light (e.g., from parallel to antiparallel); in only a couple of such magnetic circular dichroism (MCD) studies to data have angular variation measurements been made.[20] Prior theoretical treatments of circular dichroism in core-level photoemission have, furthermore, not considered fully the effects of photoelectron scattering and diffraction from the atoms neighboring the emitters. For diatomic adsorbates, only the effect of the other atom in the molecule and perhaps one underlying substrate atom on the photoelectron final state have been considered[18(b)] and for ferromagnets, no influence of near-neighbor scattering has been considered.[10,20]

In this paper, we consider such core-level dichroism in angle-resolved photoemission for the first time from a multi-atom photoelectron diffraction viewpoint. This approach is, in principle, a more versatile method for treating the effects of all atoms surrounding the emitter, and it can be applied in a rigorous fashion including fully converged multiple scattering.[21,22] We first present a theoretical analysis of recent experimental C 1*s* CDAD data from CO adsorbed on Pd(111) obtained by Bansmann *et al.*,[18(a)] taking into account the scattering of photoelectrons from the substrate lattice. Then we consider the potential influence of such normal CDAD effects on recent MCD measurements on Fe(110) by Baumgarten *et al.*[16]

0163-1829/94/50(9)/6203(6)/$06.00

C 1*s* EMISSION FROM CO/Pd(111)

Figure 1(a) shows a schematic diagram of the experimental geometry used in performing the CO/Pd(111) experiments.[17] Left and right circularly polarized radiation was obtained by going above and below the plane of the Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. storage ring in Berlin.[23] Figure 1(a) indicates the chiral geometry that results if the direction of the incoming light **q**, the direction of the molecular orientation **n** (here assumed to be parallel to the [111] surface normal), and the direction of the outgoing electron **k** are not coplanar. The electron detector was moved in the plane defined by **n** and **k**, and the scanning angle θ was measured from the [111] surface normal. For the special case of $\theta=0$, the geometry is thus not chiral, and I_{LCP} should equal I_{RCP}. Prior studies have shown that the axes of the CO molecules are aligned with the surface normal and that the C atoms are bound to the surface,[24–27] while the precise adsorption site depends on CO coverage. The apparatus and the experimental method are described in detail elsewhere.[17,18(a)]

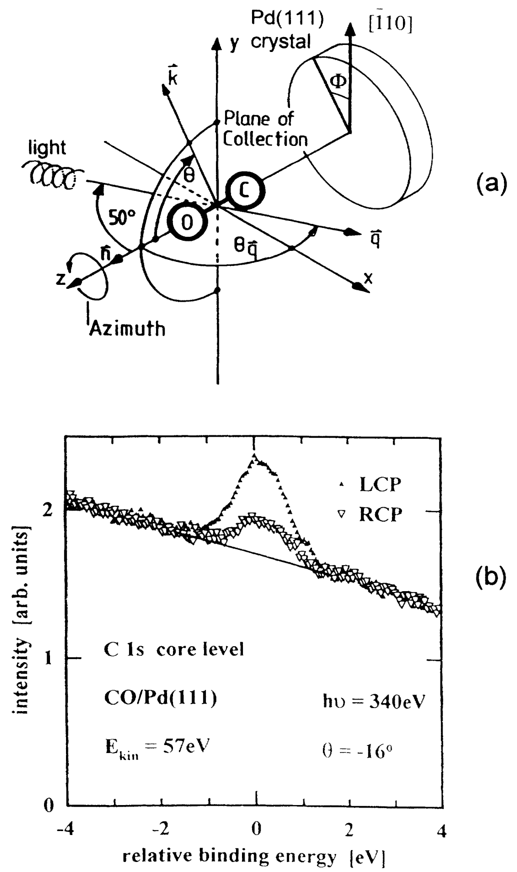

FIG. 1. (a) Schematic diagram of the experimental geometry and by Bansmann *et al.* [Ref. 18(a)] to measure circular dichroism in C 1*s* emission from CO/Pd(111). (b) Typical energy-resolved C 1*s* photoelectron spectra obtained in this experiment with left circularly polarized light (LCP) and right circularly polarized light (RCP), are shown as filled and open triangles, respectively. The solid line represents the photoelectron intensity from the clean Pd(111) surface.

Figure 1(b) shows a typical set of C 1*s* photoelectron spectra obtained with LCP and RCP light at the room-temperature saturation coverage of approximately $\frac{1}{2}$ of a monolayer.[18(a)] The photon energy used was $h\nu=340$ eV, corresponding to a kinetic energy of 57 eV, and the angle of observation was $\theta=-16°$. The solid line in Fig. 1(b) indicates the spectrum for the clean Pd(111) surface. The very strong dichroism is evident here in the difference between the data for RCP and LCP. The intensities from such spectra were used to calculate an angle-dependent asymmetry $A_{\mathrm{CDAD}}(\theta)$ in the usual way

$$A_{\mathrm{CDAD}}(\theta)=[I^{\mathrm{RCP}}(\theta)-I^{\mathrm{LCP}}(\theta)]/[I^{\mathrm{RCP}}(\theta)+I^{\mathrm{LCP}}(\theta)]\ . \tag{1}$$

This normalized quantity is convenient for comparing experiment and theory, since it is independent of the spectrometer transmission function and the free-atom differential photoelectric cross section (which would show no dichroism).

Figure 2 compares experimental results for $A_{\mathrm{CDAD}}(\theta)$ (solid points) with various theoretical calculations at kinetic energies of $E_{\mathrm{kin}}=22$, 37, 57, 77, and 97 eV. The solid lines in Figs. 2(a)–2(e) represent the results of prior calculations by McKoy and Stephens[18(b)] for a single oriented CO molecule with no substrate atoms present. These curves are based on accurate Hartree-Fock photoelectron states calculated in the full potential of the CO molecule by the Schwinger variation method.[18(b)] There is in general good agreement with experiment, including the symmetry-based zeros in asymmetry for $\theta=0°$, although experiment shows lower peak asymmetries for three of the five energies and also falls off more sharply than theory for $|\theta|$ greater than about 30° at the four highest energies.

We have theoretically simulated these same CO/Pd(111) results using the separable Green's-function method of Rehr and Albers[21(a)] as implemented in a multiple-scattering cluster algorithm by Kaduwela, Friedman, and Fadley.[21(c)] This approach has previously been found to be very accurate for describing photoelectron diffraction results obtained with both unpolarized and linearly polarized excitation sources.[21,22] The existing algorithm for calculating intensities with linear polarization[21(c)] (with operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ for radiation propagation along $\hat{\mathbf{z}}=\mathbf{q}$) has been modified so as to be applicable to circular polarization (with operators $\hat{\mathbf{x}}\pm i\hat{\mathbf{y}}$). $I^{\mathrm{RCP}}(\theta)$, $I^{\mathrm{LCP}}(\theta)$, and then $A_{\mathrm{CDAD}}(\theta)$ were computed for both a single oriented CO molecule (with the C-O distance assumed to be that in the free molecule, as in the calculations by McKoy and Stephens) and a single CO molecule adsorbed in various possible sites on a Pd(111) surface consisting of clusters of approximately 20 atoms in three layers. Matrix elements were calculated for the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ operators, and these are then added with appropriate complex phase to yield the matrix elements for $\hat{\mathbf{x}}\pm i\hat{\mathbf{y}}$. Finally, these matrix elements were squared to obtain the intensities I^{RCP} or I^{LCP}. This procedure automatically leads to satisfying the selection rule for circularly polarized light for each transition from a given orbital: $\Delta m=m_f-m_i=\pm 1$.

The dashed lines in Figs. 2(a)–2(e) represent our computed $A_{\mathrm{CDAD}}(\theta)$ for a single oriented CO molecule in the gas phase. In general, our results are in very good agreement with those calculated using the more accurate Schwinger variation method,[18(b)] especially for the three highest energies for which the approximations inherent in photoelectron diffraction theory become more accurate.[21,22] Our calculations are overall closer to experiment over the region $-30° \leq \theta \leq 30°$ for the two highest and two lowest energies, but they do not decrease as rapidly outside of this range as experiment and the variation method results, particularly at lower kinetic energies. This discrepancy could be due to the principal additional approximation made in all electron diffraction calculations that the electron scattering can be described through spherically symmetric muffin-tin potentials centered on each atom. This approximation is expected to be worse for energies below about 50 eV, but to be quite accurate above this point.[28] Thus, the present cluster diffraction approach should be sufficiently accurate for higher energies, and in addition permits easily adding in the effects of more scatterers at or near the surface, as we now illustrate.

From prior low-energy electron diffraction[25] (LEED) and infrared reflection spectroscopy investigations[26,27] it has been suggested that CO is adsorbed in threefold hollow sites on the Pd(111) surface up to a third of a monolayer, on bridge sites up to half a monolayer, and on both bridge and on-top sites at higher coverages. At the experimental conditions of Ref. 18(a), we thus might expect a mixture of adsorption sites, and we have thus investigated all three of these sites at each experimental energy, with comparisons of experiment and theory appearing in panels (f)–(j) of Fig. 2. Although the precise azimuthal orientation of the Pd(111) crystal was not known in the experiment, we have in our calculations arbitrarily chosen to scan the detector in the [$\bar{1}$10] azimuth in order to get some idea as to the sensitivity of the results to adsorption site. Back scattering from the substrate is found to produce noticeable differences in the asymmetries compared to equivalent results for the case of a single oriented CO molecule in the dashed curves of Figures 2(a)–2(f). These differences are most pronounced for the highest three energies and for adsorption in the atop

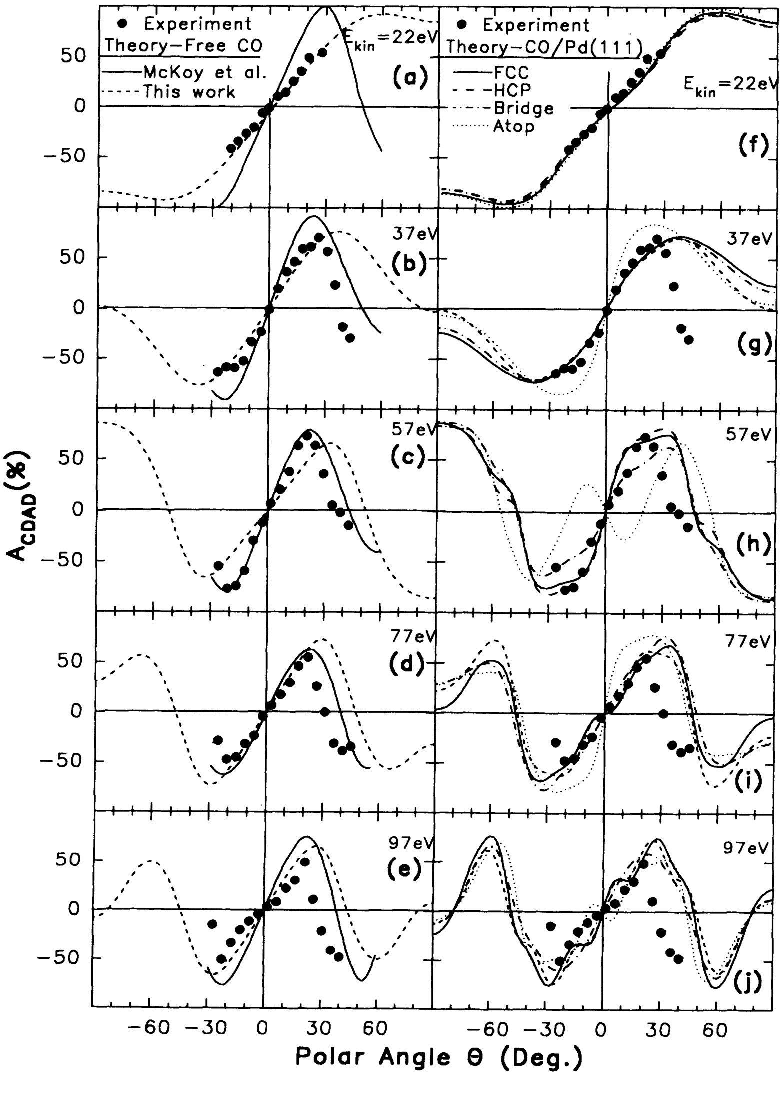

FIG. 2. Experimental and theoretical circular dichroism asymmetries A_{CDAD}. The experimental data (solid points) are for CO/Pd(111). The theoretical calculations for a single oriented CO molecule (a)–(e) and for a single CO molecule adsorbed in different sites on a Pd(111) cluster of about 20 atoms (f)–(j). In (a)–(e), the solid curve has been calculated by McKoy and Stephens [Ref. 18(b)] using the Lippman-Schwinger variation method to determine Hartree-Fock photoelectron states. All other theoretical curves are from multiple scattering photoelectron diffraction calculations in this work.

geometry. As might be expected, results for the two different threefold hollow sites (fcc and hcp) are nearly identical because the difference between these two sites begins only in the second Pd layer whose contribution to the diffraction pattern is reduced by the short inelastic attenuation lengths of about 2.5–5.0 Å appropriate over this energy range. The atop and bridge sites have different atomic arrangements in the first layer and the A_{CDAD} curves for them show greater differences. The difference among these curves for different adsorption sites might permit determining the adsorption site (although probably not distinguishing between fcc and hcp based on this data alone). However, an extensive experimental data set would be required, including a precise specification of the crystal azimuthal orientation(s).

One type of discrepancy between experiment and theory seen in Figures 2(b)–2(e) and 2(g)–2(j) deserves further comment: the sharp decrease and sign change occurring over $\theta=25°-35°$ in experiment for the four highest energies that is systematically found at higher angles in theory, with or without substrate scattering. The first nonzero polar angle at which the sign of the experimentally determined A_{CDAD} changes falls between 25° and 35°, and the value of this intersection angle decreases with increasing photon energy. By contrast, the calculated asymmetries for the free CO molecule and for the CO molecule adsorbed on a Pd(111) cluster show analogous sign changes over $\theta=37°-47°$. One physical parameter that could affect the angle of the sign change in A_{CDAD} is the C—O bond distance, which was fixed in the calculations of Fig. 2 at the gas-phase value of 1.15 Å. In the Blyholder model of bonding in CO adsorption, electron charge is donated from the highest occupied 5σ CO molecular orbital to the metal and back donated from the metal d bands to the unoccupied 2π molecular orbitals. As a consequence of this back donation, the C—O bond length can be increased for adsorbed CO compared to free CO. We have thus performed theoretical calculations for various bond lengths, and these, in fact, show that the angle of the sign change shifts towards smaller θ values with increasing bond length. For example, the intersection point moves towards lower angles by 8° when the CO bond length is increased to 1.35 Å. Thus an increase in the CO bond length could explain this particular difference between the measured and calculated asymmetries.

We have also investigated the influence of crystal azimuthal orientation on A_{CDAD} by calculating a set of curves at $E_{\mathrm{kin}}=97$ eV for ϕ values from 0° (along $[\bar{1}10]$) to 120° (along $[0\bar{1}0]$) in 10° steps using a more rapid single-scattering version of the same algorithm.[21(b)] For this energy, single-scattering calculations are found to differ by only a few percent from fully converged multiple-scattering calculations. Figure 3 shows such azimuthal scans for the four high-symmetry adsorption sites. For reasons given above, the curves for threefold fcc and hcp hollow sites are nearly identical for all azimuthal angles. Curves for atop and bridge adsorption sites show greater differences from one another and from fcc≈hcp, which could be useful in determining the adsorption site. However, the differences over all the

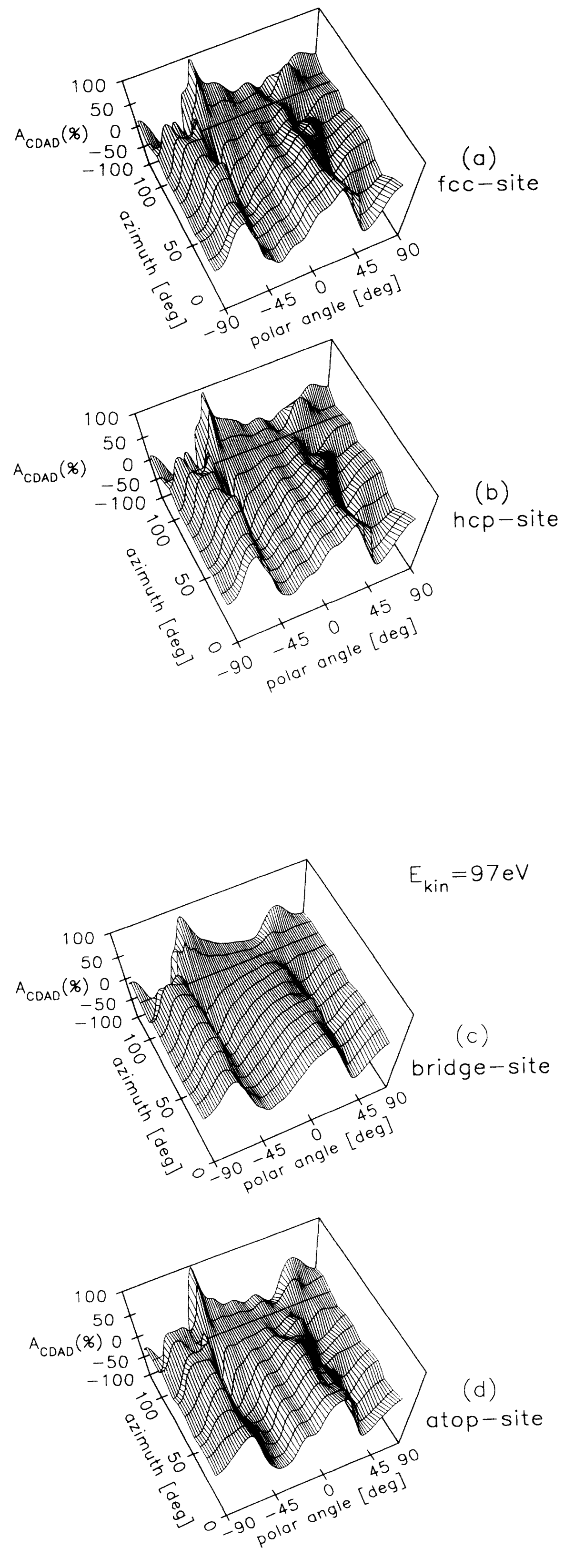

FIG. 3. Calculated asymmetries A_{CDAD} at $E_{\mathrm{kin}}=97$ eV for a single CO molecule adsorbed on a Pd(111) cluster in four possible adsorption sites (fcc, hcp, bridge, and on top) as a function of the polar and azimuthal angles of emission defined in Fig. 1(a).

curves are not pronounced enough to determine the experimental azimuthal angle from the limited data set available.

Fe 2*p* EMISSION FROM Fe(110)

Finally, we discuss the influence of such normal CD effects on magnetic circular dichroism (MCD) measurements using photoelectrons. As a quantitative example, we consider a system investigated previously experimentally: ferromagnetic Fe.[16] Baumgarten *et al.*[16] have measured the magnetic circular dichroism in Fe 2*p* emission from Fe(110) with the axis of magnetization along the easy [100] direction and aligned parallel or antiparallel to the direction of the incoming light, and with the direction of observation lying in a plane containing the direction of magnetization and the [110] surface normal [see Fig. 4(a)]. The MCD effects they observed were of the order of ±2%. In this coplanar geometry CDAD effects must vanish for reasons of symmetry.[10,11,13,14] However, if there is a slight misalignment of the azimuthal orientation of the sample or the detector, then normal CD effects may occur simultaneously with MCD effects, adding an additional element to the interpretation of such data.[17]

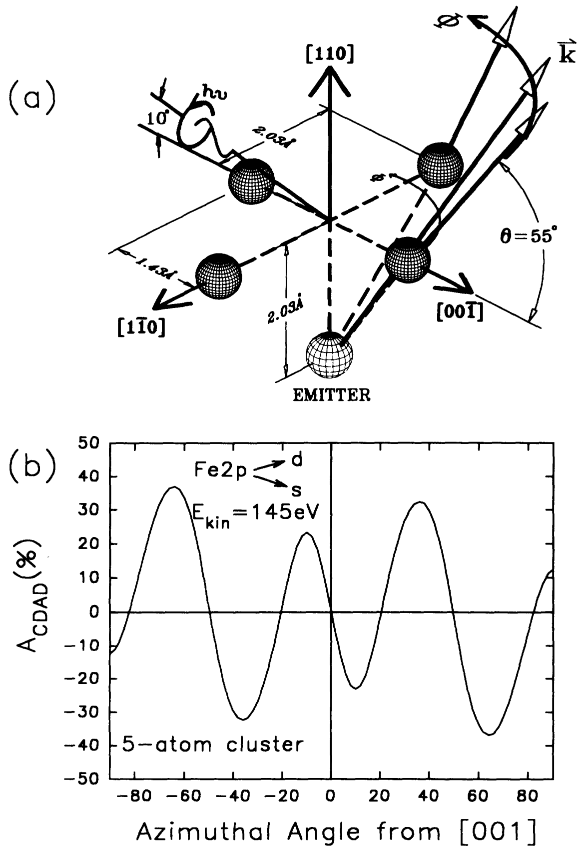

FIG. 4. (a) Cluster of Fe atoms simulating a Fe(110) surface. For $\phi=0°$ in the [00$\bar{1}$] azimuth, the emission geometry is identical to that used by Baumgarten *et al.* (Ref. 3) in studying MCD for this system. (b) Calculated normal dichroism asymmetries A_{CDAD} for the cluster in (a) as a function of the azimuthal angle ϕ.

To assess the degree of such CD-MCD interference effects, Fig. 4 displays the asymmetry A_{CDAD} calculated for a small cluster of Fe atoms simulating the system studies by Baumgarten *et al.*[16] The direction of the incoming light in the calculation is taken to be 10° away from the surface of the cluster, with the electrons being emitted at a takeoff angle of 55° with respect to the surface. The azimuthal direction of observation was varied so as to move out of the plane defined by the incoming light and the normal to the cluster. The angle $\phi=0°$ thus corresponds to a nonchiral geometry with $A_{\mathrm{CDAD}}=0$, but for all $\phi\neq0$ the geometry is noncoplanar and thus chiral. Our results for A_{CDAD} are shown in Fig. 4(b), and it is clear that it rapidly increases on moving away from $\phi=0°$, reaching a maximum of around 25% by $\phi=\pm10°$. Thus, a misalignment of the sample of a few degrees, while performing a MCD experiment could lead to a normal CD asymmetry of around 5% that is even larger than the MCD effects. Switching the magnetization direction from parallel to antiparallel to the light incidence direction for a fixed light polarization (LCP or RCP) and then measuring *I* (parallel) and *I* (antiparallel), as has been done by Baumgarten *et al.* should tend to cancel these normal CD effects, as the actual emission geometry relative to the light incidence direction then does not change, but such effects remain as an important consideration in the quantitative analysis of all MCD phenomena.

CONCLUSIONS

In conclusion, we have considered for the first time from a photoelectron diffraction perspective the circular dichroism in angular distributions associated with core photoemission (CDAD). Quantitative multiple-scattering calculations for C 1*s* emission from a single oriented CO molecule in the gas phase and for a CO molecule adsorbed on a Pd(111) cluster are found to agree well with prior experimental CDAD results and single-molecule theoretical calculations. Substrate backscattering induces differences in the dichroism for different adsorption sites, and may permit using them for structure determinations. Calculations on a small Fe cluster also indicate that such CDAD effects could complicate magnetic circular dichroism (MCD) measurements, as minor misalignments in the experimental geometry could result in both sources of dichroism being of the same general magnitude. The model we have used here could also easily be generalized to fully describe MCD by including spin-orbit and multiplet splittings in the initial state, spin resolution of the outgoing photoelectrons, and spin-dependent scattering from surrounding atoms. For example, spin-dependent scattering has already been included in the modeling of spin-polarized photoelectron diffraction from multiplet-split levels.[22,29] Photoelectron diffraction theory thus should provide a general approach for predicting dichroism in core-level photoemission.

ACKNOWLEDGMENTS

This work was supported in part by the Office of Naval Research (Contract Nos. N00014-90-5-1457 and N00014-94-1-0162), by the Director, Office of Energy Research, Office of Basic Energy Science, Materials Sciences Division of the U.S. Department of Energy (Contract No. DE-AC03-76SF00098), by the San Diego Supercomputer Center, and by the National Energy Research Supercomputing Center.

---

[1] G. Schütz, W. Wagner, W. Wilhelm, P. Kienle, R. Zeller, R. Frahm, and G. Materlik, Phys. Rev. Lett. **58**, 737 (1987); G. Schütz, M. Knülle, R. Wienke, W. Wilhelm, W. Wagner, P. Kienle, and R. Frahm, Z. Phys. B **73**, 67 (1988); G. Schütz, R. Frahm, P. Mautner, R. Wienke, W. Wagner, W. Wilhelm, and P. Kienle, Phys. Rev. Lett. **62**, 2620 (1989).

[2] C. T. Chen, F. Sette, Y. Ma, and S. Modesti, Phys. Rev. B **42**, 7262 (1990); C. T. Chen, N. V. Smith, and F. Sette, *ibid.* **43**, 6785 (1991); L. H. Tjeng, P. Rudolf, G. Meigs, F. Sette, C. T. Chen, and Y. Idzerda, SPIE Proceedings **1548**, 160 (1991); L. H. Tjeng, Y. U. Idzerda, P. Rudolf, F. Sette, and C. T. Chen, J. Magn. Magn. Mater. **109**, 288 (1992).

[3] (a) J. G. Tobin, G. D. Waddill, and D. P. Pappas, Phys. Rev. Lett. **68**, 3542 (1992); (b) G. D. Waddill, J. G. Tobin, and D. P. Pappas, Phys. Rev. B **46**, 552 (1992).

[4] J. Stöhr, Y. Wu, B. D. Hermsmeier, M. G. Samant, G. R. Harp, S. Koranda, D. Dunham, and B. P. Tonner, Science **259**, 658 (1993); Y. Wu, J. Stöhr, M. G. Samant, and D. Weller, IBM Research Report No. RJ 8782 (78912), 1992.

[5] S. Imada and T. Jo, J. Phys. Soc. Jpn. **59**, 3358 (1990).

[6] T. Jo and G. A. Sawatzky, Phys. Rev. B **43**, 8771 (1991).

[7] N. V. Smith, C. T. Chen, F. Sette, and L. F. Mattheis, Phys. Rev. B **46**, 1023 (1992).

[8] B. T. Thole, G. van der Laan, and G. A. Sawatzky, Phys. Rev. Lett. **55**, 2086 (1985).

[9] B. Ritchie, Phys. Rev. A **12**, 567 (1976); **13**, 1411 (1976).

[10] N. A. Cherepkov, Chem. Phys. Lett. **87**, 344 (1982).

[11] R. L. Dubs, S. N. Dixit, and V. McKoy, Phys. Rev. Lett. **54**, 1249 (1985).

[12] G. Van der Laan, Phys. Rev. Lett. **66**, 2527 (1991); B. Thole and G. Van der Laan, *ibid.* **67**, 3306 (1991); Phys. Rev. B **44**, 12 424 (1991); Phys. Rev. Lett. **70**, 2499 (1993).

[13] J. R. Appling, M. G. White, R. L. Dubs, S. N. Dixit, and V. McKoy, J. Chem. Phys. **87**, 6927 (1987).

[14] C. Westphal, J. Bansmann, M. Getzlaff, and G. Schönhense, Phys. Rev. Lett. **63**, 151 (1989).

[15] G. Schönhense, Phys. Scr. T **31**, 255 (1990).

[16] L. Baumgarten, C. M. Schneider, H. Petersen, F. Schäfers, and J. Kirschner, Phys. Rev. Lett. **65**, 492 (1990).

[17] C. Westphal, J. Bansmann, M. Getzlaff, G. Schönhense, N. A. Cherepkov, M. Braunstein, V. McKoy, and R. L. Dubs, Surf. Sci. **253**, 205 (1991).

[18] (a) J. Bansmann, Ch. Ostertag, G. Schönhense, F. Fegel, C. Westphal, M. Getzlaff, F. Schäfers, and H. Petersen, Phys. Rev. B **46**, 13 496 (1992); (b) V. McKoy and J. A. Stephens (private communication).

[19] H. Daimon, T. Nakatani, S. Imada, S. Suga, Y. Kogoshima, and T. Miyahara, Jpn. J. Appl. Phys. **32**, L1480 (1993).

[20] C. M. Schneider, M. S. Hammond, P. Schuster, A. Cebollada, R. Miranda, and J. Kirschner, Phys. Rev. B **44**, 12 066 (1991); C. M. Schneider, D. Venus, and J. Kirschner, *ibid.* **45**, 5041 (1991); D. Venus, L. Baumgarten, C. M. Schneider, C. Boeglin, and J. Kirschner, J. Phys. Cond. Matter **5**, 1239 (1993); J. Bansmann, Ph.D. thesis, University of Bielefeld (unpublished).

[21] (a) J. J. Rehr and R. C. Albers, Phys. Rev. B **41**, 8139 (1990); (b) D. J. Friedman and C. S. Fadley, J. Electron Spectrosc. **51**, 689 (1990); (c) A. P. Kaduwela, D. J. Friedman, and C. S. Fadley, J. Electron Spectrosc. Relat. Phenom. **57**, 223 (1991).

[22] C. S. Fadley, in *Synchrotron Radiation Research: Advances in Surface and Interface Science,* edited by R. Z. Bachrach (Plenum, New York, 1992).

[23] F. Schäfers, W. Peatman, A. Eyers, Ch. Heckenkamp, G. Schönhense, and U. Heinzmann, Rev. Sci. Instrum. **57**, 1032 (1986).

[24] R. J. Smith, J. Anderson, and G. J. Lapeyre, Phys. Rev. Lett. **37**, 1081 (1976).

[25] H. Othani, M. A. Van Hove, and G. A. Somojai, Surf. Sci. **187**, 372 (1987).

[26] A. M. Bradshaw and F. M. Hoffmann, Surf. Sci. **72**, 513 (1978).

[27] F. M. Hoffmann and A. Ortega (unpublished).

[28] S. Nagano and S. Y. Tong, Phys. Rev. B **32**, 6562 (1985).

[29] B. Sinkovic and C. S. Fadley, Phys. Rev. B **31**, 4665 (1985); B. Sinkovic, B. D. Hermsmeier, and C. S. Fadley, Phys. Rev. Lett. **55**, 1227 (1985); B. D. Hermsmeier, J. Osterwalder, D. J. Friedman, T. Tran, and C. S. Fadley, Phys. Rev. B **42**, 11 895 (1990); B. Sinkovic and D. J. Friedman, J. Magn. Magn. Mater. **92**, 301 (1991).