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FIRST PRINCIPLE CALCULATIONS OF MCD SPECTRA FOR SANDWICHED Co(110) SYSTEMS

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Abstract- X-ray magnetic-circular-dichroism (MCD) spectra, orbital ($\langle L_z \rangle$) and spin magnetic moments ($\langle S_z \rangle$) for Co(110) monolayers a free standing mode or sandwiched between Pd (Pd/1Co/Pd) and Cu layers (Cu/1Co/Cu) are calculated using the thin film full potential linearized augmented plane wave energy band method. In contrast to the double peak structure predicted for the Co(0001) surface, only a minor side peak is found in the MCD spectra for Cu/Co/Cu, while MCD spectra for the other systems show a single peak structure. The MCD sum rules originally derived from a single ion model are found in the band approach to be valid for the systems investigated. However, for the spin sum rule, the magnetic dipole term ($\langle T_z \rangle$) is not negligible and needs to be included.

I. INTRODUCTION

Magnetic overlayer and multilayer systems have received great attention from the fundamental and technological points of view. Besides their potential applications as magnetic sensors and media, these systems attract much interest because of the novel and exotic properties they exhibit when compared to the bulk properties of their constituents. In particular, some Co/X multilayers have perpendicular magnetic anisotropy and large Kerr rotation, which are highly desirable for high density recording media. Since the magnetic anisotropy is related to the spin-orbit coupling, it is expected that separate measurements of spin and orbit angular momenta will give fundamental information on its origin. In principle, the recent development of magnetic circular dichroism (MCD) technique makes possible their separate measurement with sum rules.

In the present study, we report first principle calculations of the x-ray MCD spectra, $\langle L_z \rangle$, and $\langle S_z \rangle$ for Co monolayers sandwiched between Pd(110) and Cu(110) layers in order to discuss the interface and strain effects on the magnetism of Co monolayers. We use the highly precise FLAPW method based on the local spin density approximation (LSDA). The (110) plane may effectively exhibit low dimensional properties since it has the lowest atom density of the low index planes of the fcc structure. Some calculations on free standing monolayers with Cu ($1Co_{Cu}$) and Pd ($1Co_{Pd}$) 2D lattice constants are also presented in order to separate, by comparison, the effects of the band hybridization between Pd–Co and Cu–Co atoms from those of two dimensionality and strain.

II. COMPUTATIONAL METHODS

The Pd/1Co/Pd and Cu/1Co/Cu sandwich systems are assumed as Co monolayers sandwiched by bilayers of Pd(110) and Cu(110) on each side, respectively. The lattice constants of the systems are taken as the bulk values of Pd(110) and Cu(110), respectively. The same Co MT radius of 2.2 a.u. is taken for both systems. Surface relaxations are not included in the present calculations since minor effects on the magnetism are expected.

The FLAPW method [1] is employed to obtain self-consistent solutions of the Kohn-Sham [2] equations. The valence states are treated semi-relativistically (i.e., including all relativistic terms but the spin-orbit coupling(SOC)) while the core ones are calculated fully relativistically. The exchange-correlation potential is taken in the explicit form of von Barth and Hedin [3]. About 100 basis functions per atom and 64 uniformly distributed k-points in the 1/4 irreducible 2D BZ are used. Within the muffin-tin (MT) spheres, lattice harmonics

with angular momentum l up to 8 are employed to expand the charge density, potential and wave functions. Self-consistency is assumed when root mean square differences between input and output charge and spin densities are less than 2×10^{-4}e/(a.u.)^3. Using a second variational method [4], the SOC is included to calculate the orbital magnetic moment and MCD spectra.

III. RESULTS

1. Spin and Orbital Magnetic Moments

First of all, we discuss the charge distribution since charge and spin densities are fundamental physical quantities in LSDA and may give some physical intuition on interface formation. Table 1 exhibits the electronic configurations and work functions of Cu/1Co/Cu and Pd/1Co/Pd. The number of electrons within the MT sphere of Co are 7.714 and 7.506 for Cu/1Co/Cu and Pd/1Co/Pd, respectively. Notice that the number of electrons within the MT sphere of the interface Cu is larger compared to the surface Cu, while for Pd/1Co/Pd the interface atom has fewer d electrons than the surface one even though the difference is very small. These results may imply that some weak charge transfer occurs from Cu to Co and from Co to Pd. Spin magnetic moments of Cu/1Co/Cu and Pd/1Co/Pd are calculated to be 1.542 and 2.102 μ_B, respectively. The Cu layer reduces the magnetic moment of the Co layer while the Pd layer keeps it. These results agree with previous calculations for Co/Cu and Co/Pd systems [5] and can be understood through d-band hybridization. The single particle energy spectra (LDOS and energy bands) for Cu/1Pd/Cu and Pd/1Co/Pd [5] show that there are strong Co–Pd and Co–Cu d-band hybridizations. The Cu d-band is located farther below the Fermi level, compared to Co and Pd d-bands. The Co-Cu hybridization pushes up some of the Co majority spin states and makes some majority spin holes on Co sites. Meanwhile, minority spin bands gain electrons to maintain the charge neutrality, which results in a decrease of spin moment on Co, of course. By contrast, the d-band of Pd is spread over a wide range from +0.5 eV to -5 eV around the Fermi level. The Pd-Co hybridization does affect the center of Co band strongly.

Table 1. Number of electrons of Cu/1Co/Cu and Pd/1Co/Pd within each MT sphere decomposed by orbital and spin angular momenta

		s	p	d	total
Cu/1Co/Cu					
Cu(S)	↑	0.228	0.115	4.634	4.984
	↓	0.222	0.113	4.622	4.964
Cu(I)	↑	0.234	0.185	4.626	5.057
	↓	0.238	0.198	4.568	5.015
Co	↑	0.168	0.139	4.311	4.628
	↓	0.160	0.133	2.785	3.086
Pd/1Co/Pd					
Pd(S)	↑	0.119	0.057	4.077	8.258
	↓	0.126	0.058	3.804	8.258
Pd(I)	↑	0.137	0.092	4.072	8.273
	↓	0.143	0.102	3.704	8.273
Co	↑	0.154	0.114	4.532	4.809
	↓	0.147	0.117	2.425	2.697

The calculated orbital magnetic moments for Cu/1Co/Cu, Pd/1Co/Pd, $1Co_{Cu}$, and $1Co_{Pd}$ are 0.123, 0.136, 0.166, and 0.322 μ_B, respectively. The values are enhanced significantly compared to that (0.079 μ_B) of clean Co(0001) [7]. The large enhancement may come from the low atom density of the fcc(110) surface. It is found that $< L_z >$ is more sensitive to environmental change than $< S_z >$.

2. The Orbital and Spin Sum Rules

The power of MCD spectra is the ability to derive the average spin and orbital moments of the ground state by employing recently developed orbital and spin sum rules. They are expressed as

$$\frac{I_m = \int_{L_3+L_2} \sigma_m dE}{I_t = \int_{L_3+L_2} \sigma_t dE} = \frac{l(l+1)+2-c(c+1)}{2l(l+1)N_h}\langle L_z \rangle \quad (1)$$

$$\frac{I_s = \left[\int_{L_3} \sigma_m dE - \frac{c+1}{c}\int_{L_2} \sigma_m dE\right]}{I_t = \int_{L_3+L_2} \sigma_t dE}$$

$$= \frac{l(l+1)-2-c(c+1)}{6cN_h}\langle S_z \rangle$$

$$+\{l(l+1)[l(l+1)+2c(c+1)+4]$$

$$-3(c-1)^2(c+2)^2\}\{6lc(l+1)N_h\}^{-1}\langle T_z \rangle \quad (2)$$

where c, l, and N_h denote the angular momentum of core and valence states and number of valence holes, respectively and $T_z = S_z(1-3\cos^2\theta)/2$ for S aligned along the z direction.

The calculated total absorption and MCD spectra for Pd/1Co/Pd are plotted in Fig. 1(a). The two peak structure, shown for the clean Co(0001) surface, is not found in the MCD spectrum for Pd/1Co/Pd. Probably, the two

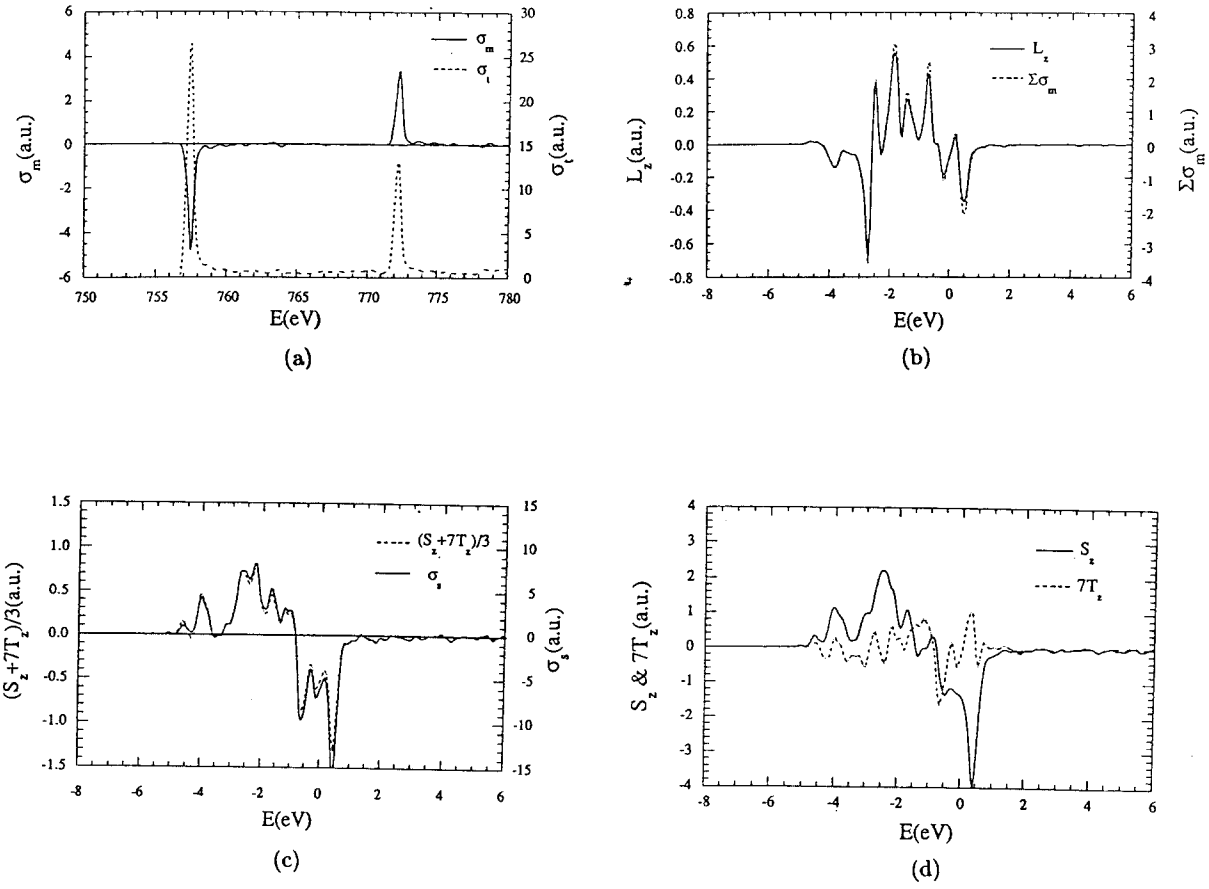

Fig. 1. (a)The calculated total absortion and MCD spectra and the energy distributions of (b) L_z and $\sum_{L_3,L_2}\sigma_m$ and (c) $S_z + 7T_z/3$ and σ_s, (d) S_z and $7T_z$ for Pd/1Co/Pd.

peaks may be related to the surface states inherent in the clean Co(0001) surface. In Figs. 1(b) and (c) we plot $\langle L_z\rangle$ and $\sum_{L_2,L_3}\sigma_m$, and $(S_z+7T_z)/3$ and $\sigma_s(=\sigma_{m,L_3}-2\sigma_{m,L_2})$ to investigate the validity of the MCD orbital and spin sum rules. The orbital sum rule is quite valid in real materials while the spin sum rule becomes valid including the dipole term. The energy distributions of S_z and $7T_z$ for Pd/1Co/Pd are shown in Fig. 1(d). This figure shows clearly that the dipole term is not negligible compared to the spin magnetic moment term.

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