Theoretical study of resonant x-ray emission spectroscopy of Mn films on Ag

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We report a theoretical study on resonant x-ray emission spectra (RXES) in the whole energy region of the Mn L2,3 white lines for three prototypical Mn/Ag(001) systems: (i) a Mn impurity in Ag, (ii) an adsorbed Mn monolayer on Ag, and (iii) a thick Mn film. The calculated RXES spectra depend strongly on the excitation energy. At L3 excitation, the spectra of all three systems are dominated by the elastic peak. For excitation energies around L2, and between L3 and L2, however, most of the spectral weight comes from inelastic x-ray scattering. The line shape of these inelastic “satellite” structures changes considerably between the three considered Mn/Ag systems, a fact that may be attributed to changes in the bonding nature of the Mn-d orbitals. The system-dependence of the RXES spectrum is thus found to be much stronger than that of the corresponding absorption spectrum. Our results suggest that RXES in the Mn L2,3 region may be used as a sensitive probe of the local environment of Mn atoms.

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I. INTRODUCTION

With the advent of 3rd generation sources of synchrotron radiation, resonant x-ray emission spectroscopy (RXES) has recently been used to investigate the nature of localization of the 3d orbitals of transition metal (TM) compounds. The fundamental and technological interest of these systems, in particular their magnetic properties, is well known (Ref. 5-11). An accurate mapping of these two types of excitations is very useful for a better understanding of these systems. In 2p → 3d → 2p RXES spectra of typical TM compounds such as MnO, the features of the CT excitation are clearly separated from those of the dd excitation, because in these systems the CT energy Δ is large. This separation obviously greatly simplifies the analysis of the spectra. It is, however, important to explore the behavior of these two types of excitations also in the less favorable case where a clear separation of dd and CT features in the RXES spectra is impossible. It is the first aim of this paper to present such a study.

The second aim is to make predictions for RXES spectra of Mn films on Ag(001), which is an interesting and well characterized example of supported ultra thin transition metal films. The fundamental and technological interest of these systems, in particular their magnetic properties, is well known (Ref. 5-11).

Recently, we have presented calculations of the 2p x-ray photoemission (XPS), 2p x-ray absorption (XAS), and (a few) resonant x-ray emission spectra (RXES) of several Mn/Ag thick film structures (Ref. 13, 14). By combining band structure, atomic multiplet and impurity Anderson model calculations, we constructed a realistic impurity model that includes full intra-atomic multiplet interaction and inter-atomic coupling to the Mn-3d and Ag-4d bands. The calculated Mn 2p XPS spectra reproduced well the experimental ones in the whole range of structures from Mn impurities in Ag to bulk bct Mn. These calculations indicate that the satellite structure observed in the ultra-thin films is due to a final state charge transfer process, mainly from the Mn-d majority spin state on the neighboring atoms to the empty minority spin state of the emitter atom. As an interesting "by-product" of these studies we found that the CT energy Δ is much smaller in Mn/Ag than in MnO. This fact suggests that in Mn/Ag, CT and dd excitations coexist in the same energy range. Mn/Ag is therefore an interesting case for our purpose, all the more that in these thick film systems, two parameters relevant for the CT excitation (CT energy and hybridization) can, to some extent, be controlled by the Mn coverage.

In order to vary these parameters, we have selected the following three Mn/Ag(001) systems for the present study: (i) a Mn impurity atom featuring weak hybridization to the Ag d-band with moderate CT energy, (ii) an adsorbed Mn monolayer featuring weak and moderate hybridization to Ag and Mn d-bands, respectively, with moderate and small CT energy, and (iii) a thick Mn film characterized by strong hybridization to the Mn d-band with small CT energy.

Our previous paper in Ref. 14 was devoted to a comparative study of XPS, XAS, RXES of Mn/Ag in order to construct a single model that is valid for all these spectroscopies. In the RXES part, only a few examples of spectra were shown. The present paper, in contrast, is devoted to a systematic study of the Mn 2p → 3d → 2p RXES in a wide range of the incident photon energy for the three above mentioned Mn/Ag systems. We analyze
the competition between CT and dd excitations in RXES and compare the different systems among them and with MnO. We also study the dependence of the RXES line shape on the hybridization strength. One main result is that the Mn 2p \rightarrow 3d \rightarrow 2p RXES line shape varies appreciably as a function of hybridization and CT energy and the RXES spectra differ, accordingly, strongly between the three different Mn/Ag systems. This suggests that 2p \rightarrow 3d \rightarrow 2p RXES may be used as a sensitive probe for the local environment of transition metal atoms.

The paper is organized as follows. In section II, we discuss the theoretical model. The results and discussion are given in section III and VI, respectively.

II. METHOD OF CALCULATION

Here we give a brief description of the model. Further details may be found in Refs. [13] and [14]. For the system one Mn monolayer on Ag, a schematic diagram of our impurity model is given in Fig. 1 which is based on the results of ab initio calculation [13]. We take into account the Mn 3d orbital of a central Mn atom (core hole site, which has a 3d⁶ configuration) together with appropriate linear combinations of Mn 3d orbitals (while the Mn 3d band is filled for locally majority spin, which is denoted as Mn⁺, and empty for locally minority spin, which is denoted as Mn⁻) on neighboring sites and Ag 4d filled orbitals of the Ag substrate.

The thick Mn film is modeled as bulk bct Mn. A single impurity Mn atom in Ag is hybridized to the Ag 4d-band only.

![Central Mn atom and Neighboring site](image)

**FIG. 1:** (Color online) Schematic diagram of the impurity model for Mn/Ag system. The Fermi level (E_F) separates the occupied density of states from the unoccupied density of states.

| Central Mn atom | Neighboring site |
|-----------------|------------------|
| Minor Spin      | Majority Spin    |

The Hamiltonian is given by

\[
H = \sum_{\Gamma, \sigma} \varepsilon_{3d}(\Gamma)d_{\Gamma \sigma}^\dagger d_{\Gamma \sigma} + \sum_{m, \sigma} \varepsilon_{2p}d_{m \sigma}^\dagger p_{m \sigma} + U_{dd} \sum_{(\Gamma', \sigma) \neq (\Gamma, \sigma)} d_{\Gamma' \sigma}^\dagger d_{\Gamma' \sigma}^\dagger d_{\Gamma \sigma}^\dagger d_{\Gamma \sigma} - U_{dc} \sum_{\Gamma, m, \sigma, \sigma'} d_{\Gamma \sigma}^\dagger d_{\Gamma \sigma}^\dagger (1 - p_{m \sigma}^\dagger p_{m \sigma'}) + H_{\text{multiplet}} + \sum_{X, k, \sigma} \varepsilon_X(k)a_{Xk \sigma}^\dagger a_{Xk \sigma} + \sum_{X, k, \Gamma, \sigma} \frac{t_X(\Gamma)}{\sqrt{N}} (d_{\Gamma k \sigma}^\dagger a_{Xk \sigma} + a_{Xk \sigma}^\dagger d_{\Gamma \sigma}) .
\]

The first five terms of the total Hamiltonian \( H \) are the atomic part describing the central Mn atom. The sixth term represents the X band (X = Mn⁺, Mn⁻ and Ag) and the last term describes the hybridization between the atomic Mn 3d states and the X band. The \( \varepsilon_{3d}(\Gamma) \), \( \varepsilon_{2p} \), and \( \varepsilon_X(k) \) represent the energies of Mn 3d, Mn 2p, and X band states, respectively, with the irreducible representation \( \Gamma \) ( = \( t_{\sigma} \), \( t_{\sigma'} \)) of the \( O_h \) symmetry. The indices \( m \) and \( \sigma \) are the orbital and spin states. \( V_X(\Gamma) \), \( U_{dd} \), and \( U_{dc} \) are the hybridization between the central Mn 3d and X band states, the Coulomb interaction between Mn 3d states, that between Mn 3d and 2p core-hole states, respectively. The term \( H_{\text{multiplet}} \) describes the intra-atomic multiplet coupling between Mn

### TABLE I: Energy parameter values (in eV) used in the calculations.

| System independent impurity model parameters | \( \Delta \) | \( U_{dd} \) | \( U_{dc} \) | \( \varepsilon_{Mn^+} \) | \( \varepsilon_{Mn^-} \) | \( \varepsilon_{Ag} \) | \( N \) | \( 10Dq \) |
|---------------------------------------------|-------------|-------------|-------------|----------------|----------------|----------------|--------|--------|
| \( -3.012 \) | 3.0         | 4.123       | \(-2.5\)    | 0.5           | \(-5.0\)       | 4              | 0.5    |

| System dependent impurity model parameters | \( W(\text{Ag}) \) | \( t_{Ag}(c_g) \) | \( W(Mn) \) | \( t_{Mn}(c_g) \) |
|---------------------------------------------|-------------------|-----------------|--------------|-----------------|
| impurity in Ag                             | 3.0               | 0.866           | 0.0          | 0.0             |
| ML                                          | 3.0               | 0.5             | 1.0          | 0.8             |
| Mn bct                                      | 0.0               | 0.0             | 3.0          | 2.0             |
3d states and that between Mn 3d and 2p states. The spin-orbit interactions for Mn 3d and 2p states are also included. The Slater integrals and the spin-orbit coupling constant are calculated by Cowan’s Hartree-Fock program [17] and then the Slater integrals are rescaled by 80%, as usual [17]. We assume rectangular bands $X$ of width $W(X)$, and we approximate them by $N$ discrete levels $\varepsilon_X(k) = \varepsilon_X + \frac{W(X)}{N}(k - \frac{N+1}{2})$, $(k = 1, ..., N)$. For the hybridization, we use the empirical relation: $V_X(e_g) = -2V_X(i_{2g})$. The charge transfer energy $\Delta$ is defined as $\Delta = \varepsilon_{3d} + 5U_{dd}$.

The main contribution to Mn $2p \rightarrow 3d \rightarrow 2p$ RXES corresponds to the process $2p^53d^n \rightarrow 2p^53d^{n+1} \rightarrow 2p^53d^n$ where $n$ is the 3d occupation number in the ground state. Mn $2p \rightarrow 3d \rightarrow 2p$ RXES is calculated on the basis of the formula of a coherent second order optical process as

$$F(\Omega, \omega) = \sum_f \sum_m \frac{|\langle f | T^\dagger | m \rangle \langle m | T | g \rangle|^2}{E_g + \Omega - E_m - i\Gamma_L} \times \delta(E_g + \Omega - E_f - \omega) \ ,$$

where $| g \rangle$, $| m \rangle$ and $| f \rangle$ are the ground, intermediate and final states of the Hamiltonian $H$ with energies $E_g$, $E_m$ and $E_f$, respectively. The incident and emitted photon energies are represented by $\Omega$ and $\omega$, respectively. The core-hole lifetime broadening is denoted by $\Gamma_L$ for the $2p$ core-hole in the intermediate states. The operators $T$ represents the optical dipole transition. The polarization of the incident photon is neglected, for simplicity.

Unless stated explicitly, the parameter values are the same as in Ref. [14] and are also summarized in Table I.

### III. Calculated Results

We recall that we are considering the following three systems: (i) a Mn impurity in Ag (labelled "impurity" in the figures below) (ii) an adsorbed Mn monolayer on Ag (labelled "ML"), and (iii) a thick Mn film (labelled "bct").

A schematic energy diagram of the initial (and RXES final) states for the three considered systems is shown in Fig. 2. The configuration averaged energies of the ionic configurations have been used which means that multiplet, crystal field and hybridization effects are neglected in the diagram, which would otherwise become too complex. It should be kept in mind, however, that all these

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**FIG. 2:** Schematic energy diagram of the ground state configurations for the different systems (see text).

**FIG. 3:** Calculated RXES spectra (b) for a Mn impurity in Ag. (a): the absorption spectrum in the Mn $L_{2,3}$ region with the indication of the excitation energies used in the RXES calculation. All RXES spectra have been rescaled to the same amplitude.
FIG. 4: Calculated RXES spectra (b) for a Mn monolayer on Ag. (a): the absorption spectrum in the Mn L$_{2,3}$ region with the indication of the excitation energies used in the RXES calculation. X stands for Mn$^+$ and Ag. All RXES spectra have been rescaled to the same amplitude.

FIG. 5: Calculated RXES spectra (b) for bulk bct Mn. (a): the absorption spectrum in the Mn L$_{2,3}$ region with the indication of the excitation energies used in the RXES calculation. All RXES spectra have been rescaled to the same amplitude.

effects shift and spread the levels. If we had represented, for example, the lowest lying multiplet energy of each configuration instead of the configuration averaged energies, the level ordering would be changed in several cases. In particular, the (3d$^5$ 6S) term is lowest in energy for all systems including bct Mn and ML rather than a 3d$^6$(Mn$^+$) term as suggested by the configuration averaged energies. Despite these subtleties, it is instructive to look at this simplified diagram in order to get an idea about the CT excitation energies in the different systems.

Let us start with the simplest system considered here: a Mn impurity in Ag. The calculated Mn 2p XAS is shown in Fig. 3(a). Note that in contrast to Ref. [14] we have now used an artificially reduced core hole lifetime broadening $\Gamma_L$ of 0.3 eV. This was done merely to enhance the resolution of spectral features for easier comparison. The calculated Mn 2p $\rightarrow$ 3d $\rightarrow$ 2p RXES spectra are shown in Fig. 3(b) at various excitation energies across the L$_{2,3}$ energy region shown by arrows on the XAS spectra in Fig. 3(a). The Gaussian broadening is taken to be $\sigma = 0.5$ eV. Two main inelastic peaks can be seen around, respectively, 4 eV and 5.5 eV below the elastic peak. At excitation energies on the L$_3$ white line (labelled 1 and 2), the elastic peak clearly dominates. For excitation energies increasing from L$_3$ to L$_2$ (excitation 3-5), most of the spectral weight shifts to the inelastic peaks before it goes partly back to the elastic one (excitation 6-7). On the spectra 4-7 a weak and broad feature at 7-13 eV can also be distinguished.

The RXES features are divided into three groups named as 3d$^5$, 3d$^6$(Ag) and 3d$^7$(Ag)$^2$ as is depicted in the left panel in Fig. 2 and also in Fig. 3(b). The enhancement of 3d$^5$ state mainly occurs well above the L$_3$ edge region (from excitations 3 to 7) with an intensity maximum just in between the L$_3$ and L$_2$ edges (excitation 6-7).
FIG. 6: RXES spectra (b) from atomic multiplet calculation with crystal field for the 3d\(^5\) configuration. (a): the absorption spectrum in the Mn \(L_{2,3}\) region with the indication of the excitation energies used in the RXES calculation. All RXES spectra have been rescaled to the same amplitude.

This feature is assigned to the on-site \(dd\) excitations in the 3d\(^6\) configuration. On the other hand, with further increasing the excitation energy, the 3d\(^5\)(Ag) feature is enhanced and has maximum intensity at excitation 4-7. Since the 3d\(^5\)(Ag)\(^2\) configuration lies far above 3d\(^5\) and 3d\(^6\)(Ag) (see Fig. 2), it has a very small weight in the ground state, which explains the weakness of the corresponding feature in the RXES.

Next we consider the monolayer (ML) system. Since CT can occur both from the Ag and the Mn\(^+\) band, its electronic structure is more complicated than the "impurity" system (see the middle panel in Fig. 2). The calculated RXES spectra are shown in Fig. 4. The most simple interpretation of these spectra would be to superimpose CT satellites originating from 3d\(^6\)(Mn\(^+\)) onto the "impurity" spectra with some weighting factor. This approach neglects, however, configuration mixing in the final state, which strongly modifies the spectral shape, especially the relative peak intensities. For the RXES spectra at excitations 4-6, the inelastic peaks dominate over the elastic one, a feature that is common to all three systems. At excitation 3, there is one broad inelastic structure centered at 3-4 eV with a weight comparable to the elastic peak. This inelastic peak is mainly due to the anti-bonding state that is formed by the hybridization between 3d\(^5\) and 3d\(^6\)(Ag\(^+\)), together with its multiplet structure. On the other hand, the spectra at excitation 4 has one more inelastic peak around 6 eV which we assign to the 3d\(^6\)(Ag) configuration. The reason for this is that excitation 4 corresponds to a XAS final state energy equal to that of the 2p\(^5\)3d\(^5\)(Ag) configuration. For higher excitation energies (5-7), weak and broad structures appear.

FIG. 7: Calculated RXES spectra (b) as a function of hybridization \(t_{Ag}\) for a Mn impurity in Ag. (a): the absorption spectrum in the Mn \(L_{2,3}\) region with the indication of the excitation energies used in the RXES calculation. RXES spectra are presented with a somewhat artificially reduced broadening in order to show some fine structure. All RXES spectra are normalized for the maximum intensity of the inelastic satellites.
at 7-10 eV energy shift, in addition to the strong inelastic peak already mentioned. These structures are mainly due to the $3d^6(Mn^-)(Mn^+)$ and $3d^7(Mn^+)^2$ states. At excitation 7, the $3d^6(Ag)$ peak around 6 eV appears again for the same reason as in the case of excitation 4.

Finally, we move to the bct thick films where there is no charge transfer from the Ag substrate but a considerably strong hybridization (nearly two times larger than that of the ML system) from the neighboring Mn atoms exists. The calculated Mn 2p → 3d → 2p RXES spectra for bct thick films are shown in Fig. 5. As depicted in the right panel in Fig. 2, the ground state is described by $3d^6$, $3d^6(Mn^+)$, $3d^7(Mn^+)^2$, $3d^4(Mn^-)$, $3d^7(Mn^-)(Mn^+)$. Due to the comparable energy of the $3d^6$ and $3d^7(Mn^+)$ states and the enhanced hybridization strength as compared to ML, the ground and RXES final states have strong configuration mixing. This results in more complicated RXES spectral shapes. We divide the RXES features into four groups named as $3d^6(Mn^+)$, $3d^5$, $3d^7(Mn^+)^2$ and $3d^4(Mn^-)(Mn^+)$. In contrast to a Mn impurity in Ag, the inelastic peaks with the lowest energy shift are assigned to a CT excitation from $3d^6(Mn^+)$ states, rather than to a dd excitation. This is because, as we mentioned just before, the configuration-averaged energy of $3d^6(Mn^+)$ is slightly lower in energy than that of the $3d^5$ state and they are strongly hybridized with each other.

On the other hand, the $3d^5$ feature lies around 5-8 eV which is enhanced at excitation 4 and 7. Note that this $3d^5$ feature is not due to the dd transitions but to anti-bonding states which are formed by hybridized $3d^6(Mn^+)$ and $3d^5$ configurations. Since the Mn$^+$ bands are rather strongly hybridized with the central Mn atom, the $3d^7(Mn^+)^2$ feature around 8-12 eV and broad $3d^5(Mn^-)(Mn^+)$ features are also seen in the RXES spectra at excitations 3, 6 and 7.
IV. DISCUSSION

As shown above, the spectral shape of the inelastic satellites changes considerably among the three considered systems. For a Mn impurity in Ag, the two main inelastic peaks are essentially due to dd excitations, but the one at higher energy shift (5-6 eV) is modified by a CT excitation from the Ag band. For the ML system, on the other hand, the lowest satellite is a mixture of dd excitations and CT satellite from the Mn$^+$ band, while the part with higher energy shift (≥6 eV) is affected by CT satellites from the Ag band. For the bct system, finally, the CT satellite from the Mn$^+$ band has the lowest excitation energy, whereas the dd structure is hard to see in this system. Since the spectral shapes are considerably complicated, explaining their dependence is not a trivial task from a general point of view. In this section, we show the hybridization strength dependence of RXES spectra to clearly distinguish between dd structure and CT satellite and to understand how CT excitations modify the dd structure.

For this purpose, we start by considering the atomic limit to view the original dd structure of 3$d^5$. In Fig. 6, we have performed atomic multiplet calculations including the crystal field with O$_h$ symmetry (10Dq=0.5 eV). The dd excitation has basically three structures at -3 eV, -4 eV, and -5.5 eV, while their relative intensities depend on the excitation energy. Qualitatively, the atomic RXES spectra resemble those of Mn impurity in Ag and ML, but there are some discrepancies. In Mn impurity in Ag, the intensity of the lower part of dd structure (around 5-6 eV) is decreased and the peak become broad in contrast to the atomic calculation. In ML, new structures can be seen around 2.5 eV in addition to the lower part changes as well as the case of Mn impurity in Ag.

Next we study the dependence of RXES spectra as a function of hybridization. Figure 7 summarizes a qualitative study of the effect of increasing the hybridization $t_{Ag}$ for impurity system with respect to fixed parameters ($U_{dd}$, $U_{dc}$, $\varepsilon_{Ag}$, $\Delta$ and 10Dq). As can be seen from Fig. 7, a CT satellite originating from 3$d^6$(Ag) appears when switching on the hybridization to the Ag band: its energy position almost coincides with the left-most of the three dd-peaks (at 5-6 eV). This is due to the small charge transfer energy $\Delta_{Ag} \equiv \Delta - \varepsilon_{Ag} \approx 2.0$ eV with the notation of Ref.[2].

In a typical TM compound such as MnO, CT and dd excitations are clearly separated in the RXES spectra as shown in Fig. 8. The dd structure is then hardly affected by the CT satellite even with some moderate hybridization strength. This is also indicated in the upper part of Fig. 9. In the present system, Mn impurity in Ag, the CT and dd excitation energy regions partly overlap (at 5-6 eV) as shown in the middle part of Fig. 9. The two types of excitations can therefore easily mix. This leads to a deformation of the dd structure at 5-6 eV which increases with hybridization strength. On the other hand, the hybridization dependence of the upper part of dd structure (around 3-4 eV) is similar to the crystal field dependence (i.e. increasing the crystal field results in the change of the relative peak intensity and the peak shift only) and also to the hybridization dependence for MnO like parameters as shown in Fig. 8.

Let us next look at the hybridization dependence in the ML system. We show in Fig. 10 the RXES of ML for the hybridization $t_{Ag}$ varied between 0 eV and 0.5 eV with keeping the ratio $t_{Ag} = 5/8t_{Mn}$. Figure 10 clearly shows that the inelastic structures with lowest energy shift (2-3 eV) are due to the hybridization with the Mn$^+$ bands. Since the averaged configuration energy of 3$d^6$(Mn$^+$) is very close to 3$d^5$ configuration ($\Delta_{Mn} \approx -0.5$ eV), the corresponding CT satellite is lower than the dd excitation.
energy as is shown in the middle panel in Fig. 9. However, since the actual hybridization strength is not so big in the Mn/Ag system ($t_{Ag} = 0.5$ eV and $t_{Mn} = 0.8$ eV) the $dd$ structure can still be recognized in the spectrum.

Finally, let us consider the $t_{Mn}$ dependence of RXES spectra for bct thick film. As shown in Fig. 11, the RXES spectra strongly depends on $t_{Mn}$. This is partly due to the fact that the hybridization strength is much bigger than in ML. In this case the original $dd$ peaks are drastically modified and the spectra have a much richer structure.

We have shown that CT screening from the Ag and Mn bands strongly modifies the $2p \rightarrow 3d \rightarrow 2p$ RXES line shape. In contrast to typical TM compounds, there is a strong mixing between $dd$ excitations and CT satellites, which is mainly due to the much smaller CT energies involved.

**V. CONCLUDING REMARKS**

In summary we have presented calculations of Mn $2p$ XAS and $2p \rightarrow 3d \rightarrow 2p$ RXES spectra for three kinds of Mn/Ag thick film structure. We have used an impurity model including full multiplet interaction and coupling to the Mn 3$d$ and Ag 4$d$ bands. This allowed us to investigate the interplay between on-site $dd$ excitations and charge transfer screening from neighboring Mn and Ag atoms. The calculated RXES line shapes are very sensitive to the hybridization strength of Mn 3$d$ and Ag 4$d$ orbitals. Since our results show that in systems with small charge transfer energy the $dd$ excitation structure is considerably modified by charge transfer screening, it would be interesting to verify it experimentally.

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