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Surface electronic structure of ferromagnetic Fe(001)

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A thorough investigation of the surface electronic structure of ferromagnetic Fe(100) films, epitaxially grown on single-crystal W(100), has been conducted using spin- and angle-resolved photoemission combined with *state-of-the-art* density-functional theory slab computations. The dispersion of the surface emission close to the Fermi level has been assessed quantitatively. The experimental results are in a good agreement with the calculations and, in particular, the presence of a minority surface state with d_{xz+yz} character along the $\overline{\Gamma X}$ high-symmetry direction is unambiguously established. Additionally, the calculations predict the existence of a different unoccupied surface state localized at $\bar{\Gamma}$. The existence of the related minority interface resonance near the Fermi edge and outside of the surface-Brillouin-zone center $\bar{\Gamma}$ is believed to control the tunneling magnetoresistance in Fe/MgO/Fe(001) for very thin MgO spacers thus our results serve as indirect confirmation to these predictions.

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I. INTRODUCTION

Surface electronic states in thin magnetic films have received considerable attention in recent times. This is due to recognizing the primary role of the electronic structure in determining the performance of advanced magnetic devices, such as magnetic tunnel junctions (MTJs) or spin-transfer systems. Although the role of surface and interface phenomena in magnetic multilayer structures extends beyond any specific example, the present study has been motivated by our interest in MTJs based on the epitaxial Fe/MgO/Fe(001) trilayer structure and similar material systems.[1] In this system, exceptionally high values of the magnetoresistance have been achieved,[2,3] whereby the excellent degree of crystallinity and high quality of the metal-oxide epitaxial interface are believed to be principal key factors of this success. Upon deposition of epitaxial MgO on Fe(001), in the region close to the Fermi edge, a strongly polarized Fe minority surface state is transformed into an interface resonance state and the performance of the Fe/MgO/Fe-MTJ system strongly depends on this state[4,5] especially for very thin MgO spacers. Additionally, the influence of an interfacial FeO layer on the interface resonance state[6] and tunneling properties have also been extensively investigated.[1,7]

The investigation of the nature of Fe surface states has been an area of intense research spanning several decades. Due to their high localization, surface states of magnetic materials have been closely scrutinized for signs of surface-enhanced electronic correlation, surface-dominated magnetic anisotropies, and surface-enhanced magnetism.[8,9] Methods of choice to investigate these surface states have been angular-resolved photoemission spectroscopy (ARPES) and its spin-polarized version SP-ARPES, yielding detailed insights into the spin-split electronic structure and the symmetry of the occupied and unoccupied electronic states.[10] In spite of these efforts, the determination of the surface photoemission contribution from a seemingly simple system like ferromagnetic Fe(001) is still somewhat unclear. One of the reasons for this is the interplay of exchange and spin-orbit interaction, which tend to split and mix states particularly in the vicinity of the Fermi level. Another reason for this is the insufficient description of electronic correlations in standard density-functional theory (DFT) approaches.

Early studies,[11,12] based on nonrelativistic tight-binding electronic structure calculations and ARPES experiments, found a surface state, filling a prominent gap located along the $\overline{\Gamma X}$ high-symmetry line of the Fe(001) surface. In particular, both the minority and majority components were found to be occupied at $\bar{\Gamma}$, the minority state lying just below the Fermi level. This early evidence was first put in question experimentally and ARPES measurements—this time spin resolved—revealed that the emission close to the E_F has actually a majority rather than a minority-spin character.[13] Later, additional experimental evidence was collected by scanning tunneling microscopy (STM) studies,[14] suggesting that the minority surface state is actually unoccupied, lying just above the E_F at $\bar{\Gamma}$. Furthermore, first-principles calculations, performed in order to interpret the STM results, found no evidence of the occupied surface states—both minority or majority—just below the E_F at $\bar{\Gamma}$. Instead, the occupied minority surface band, which fills the symmetry gap along the $\overline{\Gamma X}$ line is found to disappear in the proximity of $\bar{\Gamma}$ point while an unoccupied surface state emerges only exactly at $\bar{\Gamma}$.[14] Being only a single point in these calculations, it is not clear if these two surface emission signatures are actually originating from the same band. Finally, indirect confirmation of the presence of an empty minority state at $\bar{\Gamma}$ was found by spin-polarized photoemission, exposing the Fe(001) surface to potassium, thereby forcing the minority surface state to become occupied.[15] Other experimental work by Sawada *et al.*[16] does not contain convincing results while the recent theoretical work by Chantis *et al.*[17] still points out the lack of the direct experimental confirmation to the spin character of the surface states near the E_F in Fe(001).

In this study we examine the Fe(001) surface emission by using SP-ARPES. Although being limited to sampling occupied states—contrary to STM studies—these types of measurements probe the k dependence and spin character of the occupied electronic bands directly together with their energy distribution. Furthermore, by adjusting the photon energy and emission angle, several distinct points in the bulk Brillouin zone (BZ) can be sampled. In this paper, a set of experimental data is compared to a state-of-the-art band-structure computation. The minority surface state is observed to cross the Fermi level and to become unoccupied in the proximity of $\bar{\Gamma}$ as predicted by the calculations.

Furthermore, our calculations confirm the presence of an empty minority surface state at $\bar{\Gamma}$, however, its orbital symmetry is different from the occupied surface state away from $\bar{\Gamma}$, which implies a different electronic origin. Finally, we also examine the effects of oxygen adsorption on the relative intensities of various features in valence-band spectra, which provide an additional evidence whether they are bulk or surface related.

II. EXPERIMENT

The experiments were performed at beamline U5UA of the National Synchrotron Light Source (NSLS). This beamline, equipped with a planar undulator and a high-resolution spherical-grating monochromator, is dedicated to SP-ARPES studies.[18] The incident light is linearly polarized in the horizontal plane. A commercial hemispherical electron energy analyzer,[19] originally equipped with seven channeltrons, has four channeltrons removed and replaced with home-designed transfer optics, coupling the electron spectrometer to a mini-Mott spin polarimeter.[20] The three remaining channeltrons are left in place and are used for standard high-resolution spin-integrated photoemission. The spectrometer was operated in angular-resolved mode ($\pm 1°$ angular acceptance) and experiments were performed in a geometry where the incoming photons and emitted (detected) electrons were lying in the horizontal plane with the angle between them fixed at 45°. The sample surface plane was always vertical and various emission angles were sampled by rotating the sample around its vertical axis. The typical overall resolution was approximately 80 meV for spin integrated and 120 meV for spin-polarized spectra. The Sherman function of the mini-Mott spin detector is estimated to about 0.2.

Relatively thick Fe(001) films (~30 Å) were grown on a W(001) single crystal at 100 K at a rate of ~8 Å per minute by electron-beam evaporation. The base pressure in the chamber was 5×10^{-11} Torr and rose to about 1×10^{-10} Torr during Fe deposition. After deposition the sample was flashed to 400 K to improve crystallinity and subsequently cooled down again to 100 K. Low-energy electron-diffraction (LEED) observations indicate that above a few monolayers, such procedure yields epitaxial films with a relaxed bulk-Fe lattice constant. We neither observed LEED patterns related to three-dimensional structures[21] nor traces of tungsten core levels in wide range photoemission spectra at $h\nu=128$ eV (not shown here). All presented spectra were measured on the sample held at 100 K.

III. DENSITY-FUNCTIONAL THEORY SLAB CALCULATIONS

Our slab computations were performed within the DFT scheme[22] and an unusually large number of k points (100 k points between $\bar{\Gamma}$ and $\bar{X}$) was used with the intent of reproducing the details of the surface state crossing the Fermi level. Previous calculations for the Fe(001) surface[14] showed the sudden appearance of an empty surface state at $\bar{\Gamma}$ located approximately at 0.3 eV above E_F. However, these calculations displayed eigenvalues only for a few points along the $\overline{\Gamma X}$ direction and could not really address the relationship (if any) between the two surface emission features.

Surface states depicted in this paper decay exponentially into the bulk but they are actually not lying in the gaps of the bulk band structure projected onto the (001) surface. The occupied state lies in the gap of the projected states of *even* symmetry[14] while there is no gap in the *odd-symmetry* states. However, in our experimental geometry we can only measure states with even symmetry.[23] On the other hand, these states cannot be considered *surface resonances* either because they are not only strongly localized in the surface atomic layer but also their orbital character is different from the bulk states of similar energies.[14]

In Fig. 1 one can see that there actually exist two distinct surface states near the Fermi edge. An occupied state lies between a binding energy of ~0.2 eV and E_F and extends for most of the $\overline{\Gamma X}$ line but disappears near $\bar{\Gamma}$ and near $\bar{X}$—this surface state is a principal object of the present investigation—while an unoccupied state at $\bar{\Gamma}$ lies ~0.3 eV above E_F.

An important aspect of electronic states is their orbital symmetry. In Fig. 1 the orbital symmetry of the occupied and unoccupied surface states is identified. The empty state at $\bar{\Gamma}$ has exclusively d_{z^2} ($d_{3z^2-r^2}$) symmetry while the occupied state between $\bar{\Gamma}$ and $\bar{X}$ has a different symmetry, being mostly a sum of d_{xz} and d_{yz}-like orbitals (d_{xz} and d_{yz} are equivalent due to the symmetry of the bcc (001) surface and actually only one of the two is even with respect to the emission plane in our experimental geometry). Additionally, the surface state around 2.5 eV binding energy, which is often used as a check of the surface quality,[24] is a mixture of s and $d_{x^2-y^2}$ orbitals while the unoccupied surface state around 1.5 eV above the Fermi edge has mostly d_{z^2} character with some mixing of $d_{x^2-y^2}$.

The orbital characters of the relevant surface states close to E_F are further visualized in Fig. 2, where the charge contours for the unoccupied surface state at $\bar{\Gamma}$ and for the occupied surface state at 37% of the distance between $\bar{\Gamma}$ and $\bar{X}$ are plotted. Note that the present results, which confirm the earlier finding for an unoccupied state at $\bar{\Gamma}$ by Stroscio *et al.*,[14] add the information of the different orbital symmetry for the occupied state along the $\overline{\Gamma X}$ line. This fact should certainly

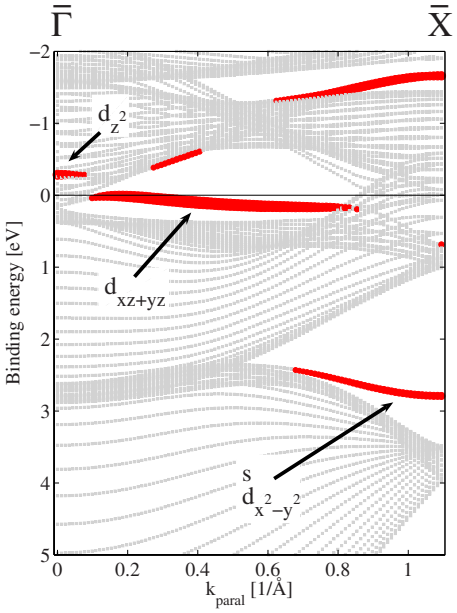

FIG. 1. (Color online) Minority-spin band structure of Fe(001) along $\bar{\Gamma}\bar{X}$ calculated using WIEN2K (Ref. 22) for a 30 atoms slab. Adjacent slabs were separated by 29.8 Å of vacuum. States with more than 20% charge located on the surface atom are emphasized as thicker (red) lines, with the thickness of the line related to the percentage of charge on the surface atom and there is up to 72% of charge lying on the surface atom for the most surface-related part of the d_{xz+yz} band. Only even states with respect to the emission plane are plotted since only these states are accessible in our experimental geometry (Ref. 23).

be considered in realistic estimations of the tunneling probabilities in Fe/MgO/Fe(001)-based MTJs.[25]

IV. EXPERIMENTAL RESULTS AND DISCUSSION

Normal-emission spectra from Fe(001) sample bands along ΓH in the bulk Brillouin zone. Figure 3 compiles normal-emission data taken at 64 eV photon energy for the clean and oxygen exposed Fe(001) surface. Adopting the usual free-electronlike final state, bulk states close to the Γ point are excited at this photon energy. In order to test for any surface-related emission in these spectra, experiments with carefully controlled oxygen exposures were performed. The sample was continuously held at 100 K during these exposures. Note that by applying a proper evaporation procedure and keeping strict ultrahigh vacuum conditions we were able to minimize the oxygen contamination and obtain an extremely clean initial Fe(001) surface to perform this study. This is evident from the total absence of any oxygen $2p$ feature at 6 eV in the clean Fe spectra (see left panel in Fig. 3). The region near the Fermi edge is dominated by a strong minority feature, which, however, is not influenced by oxygen exposure. This indicates that the electronic origin of this feature is rather of a bulk than surface nature. Furthermore, no indication of the majority counterpart to the unoccupied d_{z^2} minority surface state, expected at around 2 eV binding energy,[14] is present in these normal-emission spectra.

In order to find the occupied surface state described in the calculations above, we have continued the search by mapping the band structure along ΓH in off-normal emission. As seen in Fig. 4, separate sharp emission features near the Fermi edge were observed especially for 67 eV, 12° and 72 eV, 20° (actually both having minority character). The latter parameters have been chosen for more detailed spin-polarized measurements. It is also clear that near the $\bar{X}$ point (67 eV, 16°) the sharp peak at the Fermi edge is absent.

Figure 5 presents the results of the oxygen absorption test for the off-normal-emission condition. This time the minority emission close to the Fermi level is strongly suppressed by the presence of adsorbed oxygen, clearly indicating its surface origin. It should, however, be noted that in order to completely quench this state relatively high oxygen exposures (1.4 L) are needed. By contrast, for smaller doses (up to 0.4 L) it remains practically unaffected. Oxygen is known to form epitaxial crystalline overlayers on the Fe(001) surface[26,27] and this can be seen, for example, by comparing the oxygen $2p$ emission between 5 and 9 eV binding energy in Figs. 3 and 5. A single broad feature is observed in normal emission while two distinct features are seen in the spectra 20° off-normal emission. This dispersive behavior is suggestive of a (1×1) overlayer[28] and such oxygen-related features are known to be spin polarized.[26,29] Possibly the surface state is pushed above the Fermi level only when a certain fraction of the surface is covered with oxygen.[6]

Surface states are two-dimensional entities and their binding energy does not depend on the perpendicular component $k_\perp$ of the **k** vector. This can be used to confirm the surface origin of the state by photoemission, as long as a variable energy light source, such as a synchrotron, is available. Figure 6 presents a test in which photon energies and emission angles were chosen to keep the $k_\parallel$ component constant while $k_\perp$ is changed. Related BZ points are presented graphically in Fig. 7. Clearly the feature near the Fermi edge appears in all spectra in Fig. 6 and its binding energy is nearly constant, thus confirming the surface origin of this photoemission contribution. Note that the small changes in binding energy are most likely to occur because spin-integrated spectra are a mixture of minority and majority states, and bulk majority states are, in general, not expected to have constant binding energy along the probed line in the BZ (as mentioned before, the surface state lies in the symmetry gap of the minority states).

It is convenient to use lower photon energies in order to measure the energy dispersion of the minority surface state along the $\bar{\Gamma}\bar{X}$ line of the surface Brillouin zone with a high degree of accuracy. Performing the band mapping at $h\nu=16.6$ eV also allows a direct comparison with the results in the literature, mentioned in the introduction above.[11,13] Our new spectra are shown in Fig. 8 where a strong and sharp feature appears near the Fermi edge for all angles. However, its spin character clearly reverses as a function of emission angle. The feature at the Fermi edge in the normal-emission spectra is of majority-spin type,[13] however, at off-normal angles it quickly disperses away from the Fermi edge, reaching 0.3 eV at 18° emission angle while a new minority-spin feature appears at the Fermi edge.

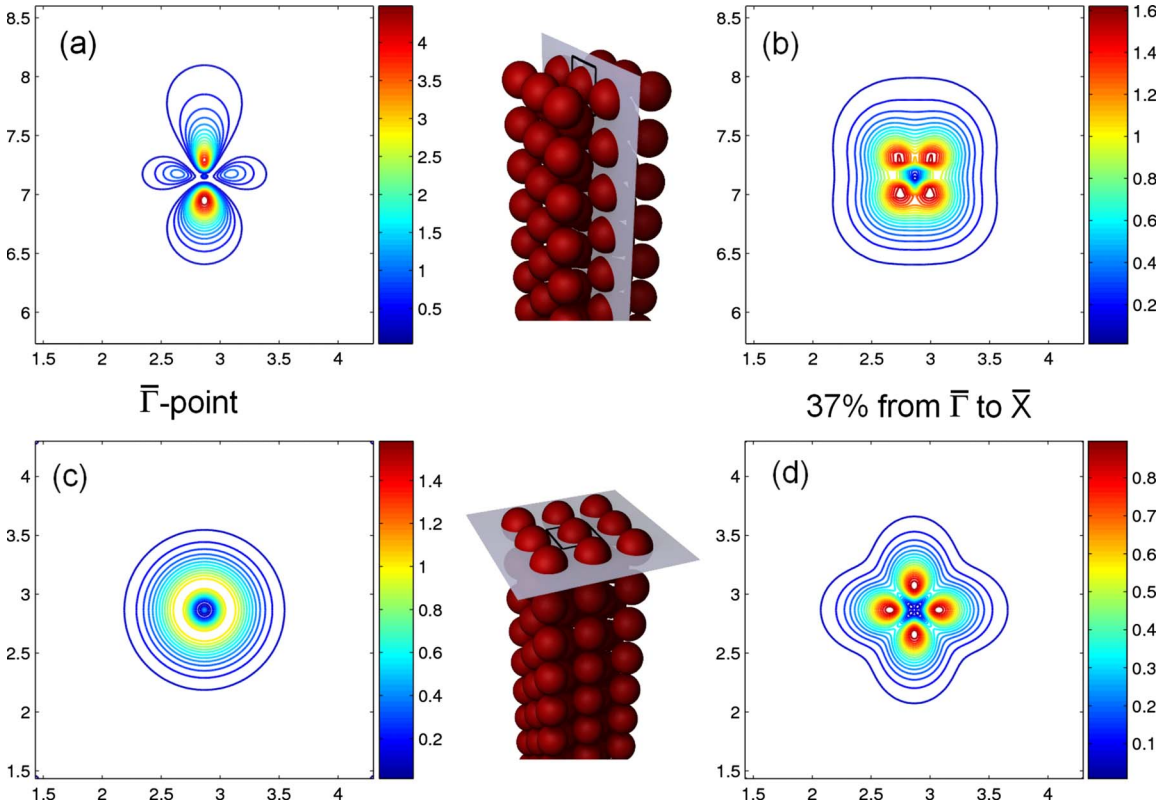

FIG. 2. (Color online) Charge densities for minority surface states on the Fe(001) surface: (a) and (b) show cuts in the [1 0 0] plane while (c) and (d) show cuts in the surface plane. Figures (a) and (c) refer to the unoccupied surface state at $\bar{\Gamma}$ (0.3 eV above the Fermi edge) while (b) and (d) show the occupied surface state at ~0.1 eV below the Fermi edge at 37% of the distance between $\bar{\Gamma}$ and $\bar{X}$. Additional graphics, included for convenience, show three-dimensional slab model with cut surfaces as explained above. Distances are in Å and charge-density scales are in electrons per Å^3.

According to the free-electron final-state model at $h\nu$=16.6 eV states near the H point, roughly along HΓ, are probed, see Fig. 7. From the Fe bulk band structure[1,11,30] no minority-spin states near the Fermi edge exist up to midway of the HΓ distance while in our experiment a minority-spin peak at the Fermi edge is already clearly visible at the first quarter of HΓ. This again indicates that this feature is indeed of a surface-related origin. Going beyond the free-electron final-state model, we extract from calculated unoccupied band structures[31] that there is a gap in unoccupied states at the Γ point extending from zero up to above the final-state energy of 20 eV. Thus, at least in normal emission no states from around Γ will be observed at $h\nu$=16.6 eV. This, however, does not determine which states can be observed in off-normal emission.

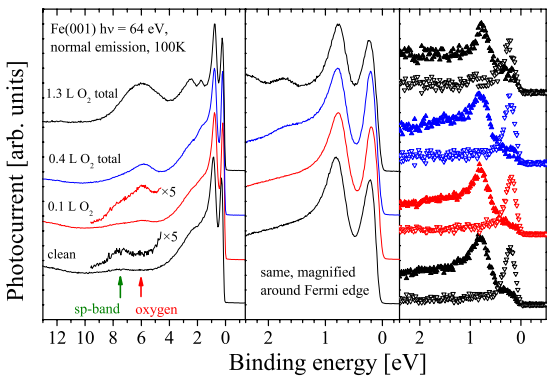

FIG. 3. (Color online) Oxygen adsorption on Fe(001): normal-emission spectra at $h\nu$=64 eV. Both spin-integrated (left and center panels) and spin-polarized (right panel) spectra are shown; ▲—majority states and ▽—minority states.

In the initial work of Butler *et al.*,[4] which was further developed by Belashchenko *et al.*,[5] it was pointed out that a minority resonance localized in the Fe layer of MgO/Fe(001) interface is the reason for the decrease in TMR for very thin MgO spacer layer in Fe/MgO/Fe(001) MTJs. It seems that the minority surface state in clean Fe(001) is very similar to the resonance in MgO/Fe(001) junction, basically being the surface state of Fe(001), slightly influenced by the MgO overlayers.[25] Such an interpretation agrees with the theoretical work by Li and Freeman[32] for 1 or 2 monolayers of Fe on MgO(001), where very little interaction between Fe and MgO was found. MgO is a wide band-gap insulator and in the MgO/Fe(001) interface the Fe Fermi level lies within this gap (which is the intrinsic feature of tunnel junctions based on such interfaces) certainly promoting limited hybridization between MgO and Fe at the interface. In this paper we have directly proven the existence of the important Fe(001) surface state and its disappearance at $\bar{\Gamma}$, which is in accord with

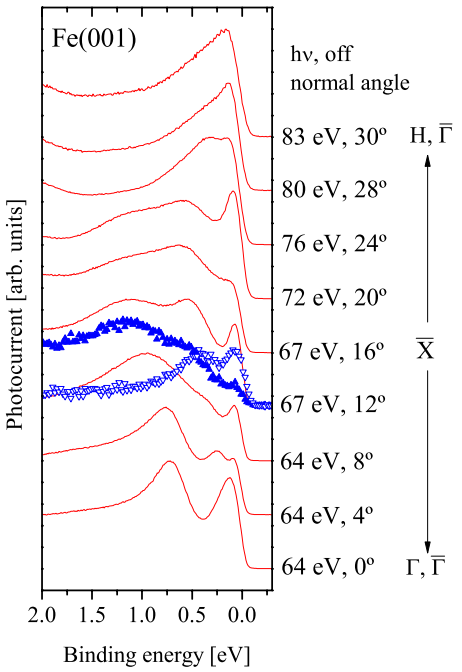

FIG. 4. (Color online) Set of spin-integrated spectra with photon energies and emission angles adjusted to probe ΓH high-symmetry direction in the bulk BZ according to the free-electron final-state model. Related positions in the BZ are shown in Fig. 7. Additionally spin-polarized data is shown for 67 eV and 12° spectrum indicating that the feature at the Fermi edge has a minority character. Detailed data for 72 eV and 20° is shown in Fig. 5.

the theoretical predictions and thus at least indirectly confirms TMR models presented in Refs. 4 and 5.

V. SUMMARY

With our recent investigations we have established details of the occupied minority-spin surface state in Fe(001). On the basis of our data we have been able to unify previous results[11,13–15] into one interpretation, which is fully consistent with our dedicated theoretical DFT calculations. The minority-spin surface state of d_{xz+yz} symmetry lies in the gap of the projected bulk spin-down band structure of even symmetry. It is occupied for the major part of the $\bar{\Gamma}\bar{X}$ distance and disappears both near $\bar{\Gamma}$ and near $\bar{X}$. Around $\bar{\Gamma}$ there exists another unoccupied surface state of d_{z^2} character, which was previously observed.[14,15] Adsorption of an ordered monolayer of oxygen quenches the surface state, however, without removing the surface ferromagnetism.

Our results provide an important information regarding the details of the electronic states which are believed to play

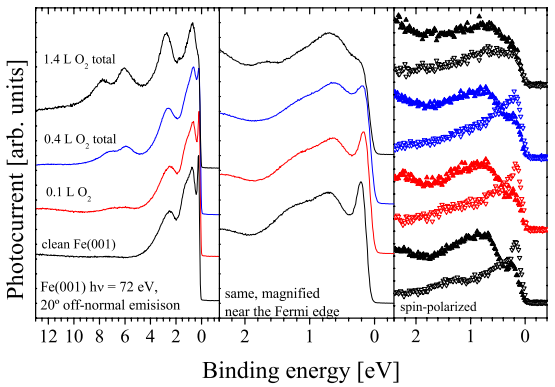

FIG. 5. (Color online) Oxygen adsorption on Fe(001): 20° off-normal-emission spectra at $h\nu$=72 eV probing states in the bulk BZ where a strong minority peak appears near the Fermi edge, as evident from Fig. 4. See caption of Fig. 3 for details.

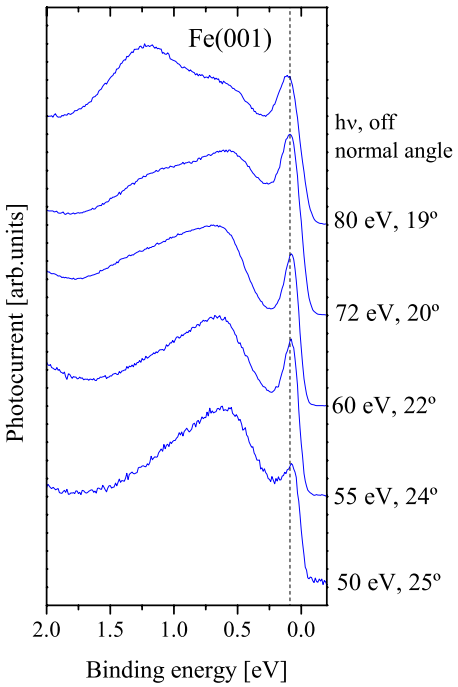

FIG. 6. (Color online) Set of spectra with photon energies and emission angles adjusted to probe states with the same $k_{\parallel}$ but different $k_{\perp}$. Related positions in the BZ are shown in Fig. 7).

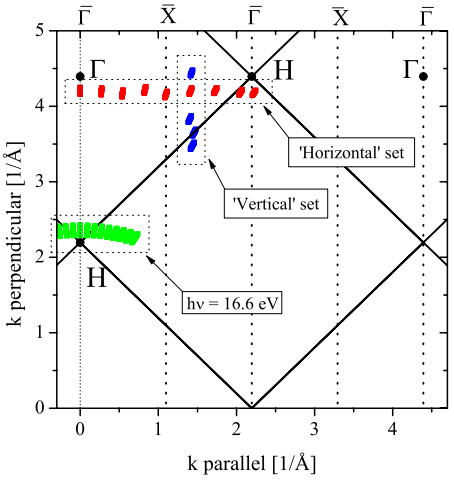

FIG. 7. (Color online) Emission plane probed in our photoemission experiment (cut through the bulk BZ). Surface normal (001) is vertical in this figure. Energy distribution curve spectra shown in other figures are plotted here in the k space according to the free-electron final-state model. "Horizontal" set of spectra is presented in Fig. 4, "vertical" set in Fig. 6, and $h\nu$=16.6 eV set in Fig. 8.

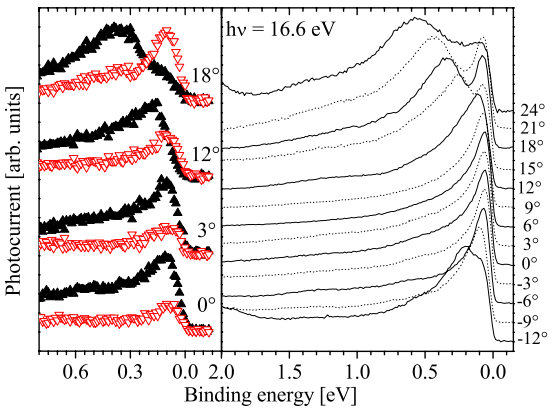

FIG. 8. (Color online) Set of angle-resolved spectra at $h\nu = 16.6$ eV. Spin-polarized spectra are shown in left panel for selected angles; ▲—majority states and ▽—minority states.

an essential part in the functionality of Fe/MgO/Fe(001)-based MTJs. Further off-normal-emission experimental results and detailed theoretical calculations are needed to establish how MgO overlayers influence the minority surface state of Fe(001).

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