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Photoemission and electronic structure of iron

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Photoemission studies of the valence-band structure of iron are carried out in the photon energy range $11.8 \leqq \hbar\omega \leqq 21.2$ eV. A prominent peak at 0.58 ± 0.03 eV and a less pronounced maximum at 2.4 ± 0.2 eV below the observed Fermi level in the energy-distribution curve at $\hbar\omega = 21.2$ eV are shown to characterize the profile of the occupied states. Our results are compared with other experimental data and with band-structure calculations. Soft-x-ray appearance potential spectra, x-ray continuum isochromats, and the present ultraviolet-photoemission spectra, when taken together, suggest an upper limit of 1.9 eV for the exchange splitting of the spin-up and spin-down *d* bands. Finally, we have discussed the results of photoelectron spin-polarization measurements. Previous interpretations of these experiments indicated apparent contradiction with the Slater-Stoner-Wohlfarth itinerant-electron band theory of ferromagnetism.

I. INTRODUCTION

Theoretical density-of-states (DOS) and experimental photoelectron distribution curves (EDC) of the valence band of iron show great variety in their gross features as reported by different authors. Various approximations made in calculations[1–9] have caused substantial discrepancies in the details of the band structure. It is still not clear whether a one-electron approach is adequate for describing the photoemission spectra of the valence band or whether many-body effects play an important role. In experiments, continuing difficulties are encountered in preparation of clean surfaces. Even a relatively small amount of contamination on the surface gives rise to an anomalous structure at about -5 eV below the Fermi level[10] ϵ_F. The top of the band is also influenced by spurious surface effects; in particular ϵ_F of iron may become obscured by the broadening of the high-energy peak in the EDC as observed earlier.[10] Only a few successful ultraviolet-photoemission-spectroscopy (UPS) measurements[11,12] from clean surfaces of Fe have been published hitherto while several x-ray-photoemission-spectroscopy (XPS) works are available in literature.[13–16] Because the resolving power of the XPS technique is relatively low, it is difficult to determine the position of ϵ_F with sufficient accuracy. It will be shown below that the location of ϵ_F in the spectra is of great importance when interpreting the features of the valence band. The EDC's in the works by Eastman[11,12] were interpreted in terms of DOS calculations which, however, do not seem to explain recent XPS data. In particular, the EDC obtained at low photon energy[11] is often compared with the results of other valence-band measurements and considered to reflect the DOS profile of Fe. However, the shapes of the EDC's at high photon energies in the later work[12] are quite different from those shown in Ref. 11.

In the present article we attempt to construct a picture of the gross features of the electronic states of iron with the aid of our UPS data and the results of other experiments.[12,14,17,18] This work provides an experimental criterion for testing the degree of accuracy to which the electronic structure can be described by contemporary one-electron models. On the basis of the features of the valence band it seems possible to explain the results of photoelectron spin polarization (photo-ESP) measurements,[19,20] whereas previous interpretations of these experiments indicated apparent discrepancies with the Slater[21]-Stoner[22]-Wohlfarth[23] itinerant-electron-band theory of ferromagnetism.

II. THEORY

The energy distribution of the joint density-of-states (EDJDOS) of photoexcited electrons in the constant momentum matrix element approximation, within the framework of the three-step model, is given by

$$j(\epsilon, \hbar\omega) = (2\pi)^{-3} \sum_{i,f} \int_{\mathrm{BZ}} d\vec{k} \times \delta(\Omega_{fi}(\vec{k}))\, \delta(\epsilon - \epsilon_i(\vec{k})) \,. \quad (1)$$

In the direct-transition model, the initial state i and the final state f lies at the same point in $\vec{k}$ space. These transitions are then restricted to lie on the optical surfaces defined by

$$\Omega_{fi}(\vec{k}) = \epsilon_f(\vec{k}) - \epsilon_i(\vec{k}) - \hbar\omega \,, \quad (2)$$

where $\epsilon_f(\vec{k})$ and $\epsilon_i(\vec{k})$ represent the energy eigenvalues of the bands f and i at $\vec{k}$. To obtain the energy distribution of photoemitted electrons $\eta(\epsilon, \hbar\omega)$ from the EDJDOS one must multiply $j(\epsilon, \hbar\omega)$ by the escape probability function $T(\epsilon^*, \hbar\omega)$ of the excited electrons in the scheme of the random-$\vec{k}$ approximation, where $T(\epsilon^*, \hbar\omega)$ is independent of $\vec{k}$. Thus

$$\eta(\epsilon, \hbar\omega) = CT(\epsilon^*, \hbar\omega) j(\epsilon, \hbar\omega) \tag{3}$$

and C is a normalizing constant. Here

$$T(\epsilon^*, \hbar\omega) = \begin{cases} \frac{1}{2}[1 - (e\phi/\epsilon^*)^{1/2}]R & \text{if } \epsilon^* > e\phi \ , \\ 0 & \text{if } 0 < \epsilon^* < e\phi \ , \end{cases} \tag{4}$$

where $\epsilon^* = \hbar\omega + \epsilon$ is the kinetic energy of electrons with respect to the Fermi level $\epsilon_F = 0$ eV, and $0.5 \leq R \leq 1.0$ is a correction factor[24] ($e\phi$ is the work function).

With increasing photon energy, the EDC samples the DOS

$$D(\epsilon) = (2\pi)^{-3} \sum_i \int_{BZ} d\vec{k}\, \delta(\epsilon - \epsilon_i(\vec{k})) \ . \tag{5}$$

Several authors[16,25-29] have discussed the phenomena which tend to smooth out a characteristic EDJDOS profile and cause a resemblance between the EDJDOS and DOS. The change from the low-energy regime [Eq. (1)] to the high-energy regime [Eq. (5)] is well presented by Eastman *et al.*[26,27] in their synchrotron radiation induced photoelectron spectra. The details of the assumptions made in Eqs. (1)–(5) can be found, e.g., in Ref. 25.

III. EXPERIMENTS

Samples were prepared from a 99.998%-pure iron wire by means of electron-gun evaporation. A special gun was constructed to bombard directly one end of a 2.5-cm-long specimen wire; the other end of the wire was fixed to the gun framework.

Several films of 50–150 Å thickness were deposited at evaporation rates of 2–3 Å/sec upon a polycrystalline silver foil. The thickness of a film was monitored by a quartz crystal oscillator.

The photoemission spectrum from each film was obtained by using rare-gas resonance lines 21.2 (He), 16.8 (Ne), and 11.8 eV (Ar). The base pressure in the preparation chamber was 5×10^{-10} and in the analyzer chamber 8×10^{-11} Torr. During the evaporation the pressure increased to about 10^{-8} Torr. The sample was introduced through a gate valve into the analyzer chamber immediately after the evaporation. The working pressure with the gas lamp on was $1-4\times10^{-10}$ Torr.

The spectra at photon energies 21.2 and 16.8 eV, when recorded from the first evaporated film with a thickness about 50 Å, showed a small peak at -5.4 eV which was obviously due to oxygen contamination. In the subsequent evaporations the intensity of this peak in the EDC's gradually decreased and eventually stabilized at the height shown in Fig. 1. Since the partial pressure of oxygen was below the sensitivity limit (10^{-13} Torr) of our quadrupole residual gas analyzer and the partial pressure of CO gas was $3\times10^{-11}-5\times10^{-11}$ Torr,

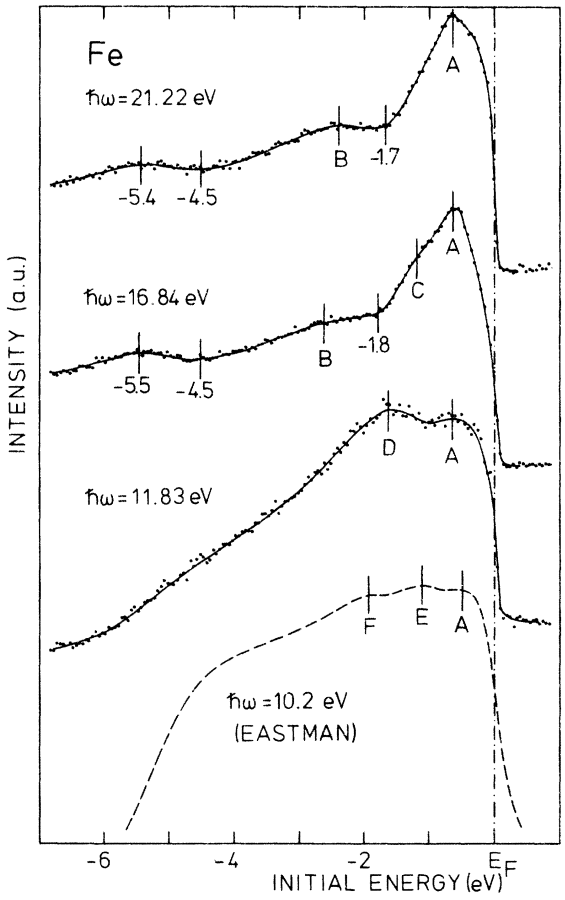

FIG. 1. Photoemission spectra (EDC) from evaporated iron surfaces for different photon energies. Details of the spectra are listed in Table I.

we have concluded that the presence of oxygen observed on the film was most likely due to contamination of the iron wire itself. We found no difference between the spectra run from a freshly evaporated surface and from the same surface 15 h later.

The spectra were obtained by sweeping the potential between the electrodes of the analyzer. The instrumental resolution was better than 0.06 eV for all measurements. In the subsequent discussion we will concentrate mainly on the EDC structure observed in the energy range of -5 eV to ϵ_F. In this interval $T(\epsilon^*, \hbar\omega)$ changes by less than 20%. The reduction in the analyzer transmission function is about 25% when going from ϵ_F to -5 eV for $\hbar\omega = 21.2$ eV. These corrections would only enhance the intensity of the low-energy tail of the measured EDC but would not influence the structure itself. Therefore, except for a constant background subtraction, no corrections were made in the recorded spectra.

Technical details of the apparatus have been described elsewhere.[30]

IV. RESULTS

In Fig. 1 our UPS spectra are presented together with the UPS ($\hbar\omega = 10.2$ eV) of Eastman.[11] At photon energy 21.2 eV two resolved structures, labeled A and B, characterize the EDC down to -4.5 eV. It is not possible to determine accurately the bottoms of the d and sp bands. Instead, the onset of the occupied states is clearly observable. The accuracy in the location of ϵ_F is ± 0.02 eV in this spectrum. The position of the leading peak A relative to ϵ_F remains stationary in all spectra. Peak B is also indicated in the EDC at $\hbar\omega = 16.8$ eV. However, this EDC exhibits an additional shoulder C which we believe not to reflect the band DOS but to be associated with a structure of the EDJDOS at the given photon energy. An influence of the optical surfaces [Eq. (2)] on the low-energy photon excited spectra is further demonstrated in the shapes of the EDC at $\hbar\omega < 16.8$ eV, which display nonstationary structures D, E, and F varying in position, shape, and intensity. None of these structures are present in the EDC obtained at the highest photon energy. Accordingly, we are left only with the two peaks, A and B, on which the discussion and conclusions in Sec. V are based. The measured characteristics of the UPS and XPS spectra are summarized in Table I.

A discussion of the broad maximum at -5.4 eV seen in the EDC's at $\hbar\omega = 21.2$ and 16.8 eV is in order here. This maximum does not likely belong to the genuine band structure of Fe. UPS and XPS spectra from clean nickel surfaces[14,16,31] always exhibit a weak structure between -5 and -6 eV. This fact cannot be explained by assuming the presence of residual amounts of chemisorbed oxygen on the surface. Conrad *et al.*[31] showed by means of the Auger-electron technique that in their experiment the oxygen coverage on the Ni surface was certainly less than 0.01 but this structure persisted in their EDC with an intensity of (4–5)% relative to the main d-peak intensity ($\hbar\omega = 40.8$ eV). Therefore they concluded that the peak was not due to oxygen. Hüfner and Wertheim[14,32] have suggested that the peak is attributable to a satellite effect originating from a double d-hole state. A trace of the low-energy structure in the XPS of clean Fe is also reported.[14,16] The possibility that a satellite of this type could contribute to the intensity of the peak at -5.4 eV cannot be ruled out in our case. A study of the energy of Auger transitions $L_3M_{4,5}M_{4,5}$ which yield localized two-hole states shows that a satellite arises in this energy range. The energy of the $L_3M_{4,5}M_{4,5}$ transition is 701.2 eV,[33] in agreement with the energy difference 701.9 eV between the $2p_{3/2}$ level[17] (707.3 eV) and the assumed two-hole state (i.e., 5.4 eV). Furthermore, the intensity of this peak with respect to the intensity of peak A is 3% which is nearly equal to the corresponding ratio for Ni.[31] Accordingly, the structure could originate from this satellite and, perhaps, from residual oxygen which corresponds to at most a small fraction of an atomic monolayer and which has no effect on the iron band structure itself. Even the EDC from the slightly oxidized first film showed exactly the same shape as the EDC's from the other films in the energy range from ϵ_F to -4 eV.

V. DISCUSSION

A. Comparison with other experiments

In Fig. 2 our EDC at $\hbar\omega = 21.2$ eV is compared with the EDC at $\hbar\omega = 40.8$ eV reported by Eastman[12] and with the XPS (Al $K\alpha$) by Hüfner and Wertheim.[14] Within the limitations imposed by instrumental resolutions 0.06, 0.25, and 0.5 eV, respectively, the spectra reveal qualitatively the same features. Our UPS and the XPS bear a strong resemblance to the DOS as will be shown later. This means that the square of the momentum matrix element does not vary markedly for the transitions in question. In the EDC of Eastman[12] a tentative correction was made for inelastically scattered electrons which explains the difference between the spectra in the low-energy region.

The most pronounced difference is found in the location and the sharpness of the Fermi edge. This

TABLE I. Peak positions of energy distribution curves of iron obtained by using different photon energies and Al $K\alpha$ x rays for excitation.[a]

Peak	$\hbar\omega = 21.2$ eV	$\hbar\omega = 16.8$ eV	$\hbar\omega = 11.8$ eV	$\hbar\omega = 40.8$ eV[b]	$\hbar\omega = 10.2$ eV[c]	$\hbar\omega = 1486$ eV[d]
A	-0.58 ± 0.03	-0.60 ± 0.07	-0.65 ± 0.10	-0.6	-0.5	-0.6
B	-2.4 ± 0.2	-2.6 ± 0.2	...	-2.4	...	-2.2
C	...	-1.2 ± 0.1	...	...	...	...
D	...	...	-1.6 ± 0.2	...	...	...
E	...	...	...	...	-1.1	...
F	...	...	...	...	-2.1	...

[a]The energies of peak B of Refs. 12 and 14 are estimated from the reproduced curves in Fig. 2.

[b]Reference 12.

[c]Reference 11.

[d]Reference 14.

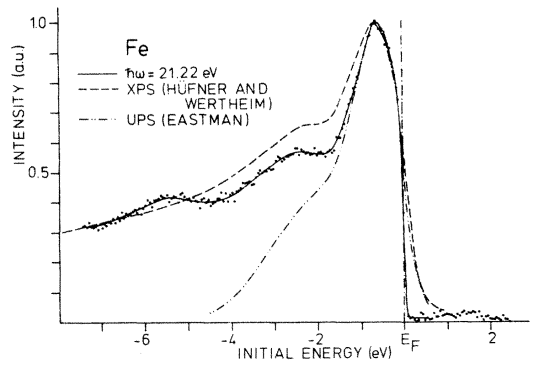

FIG. 2. Comparison of the EDC of Fe at photon energies 21.2 and 40.8 eV (Ref. 12) with the XPS (Ref. 14) (Al $K\alpha$). ϵ_F of the three spectra are adjusted to coincide.

does not appear at the intensity maximum of the DOS, as one could conclude from the XPS curve, but at a position where the DOS is already decreasing. The observation of ϵ_F in our spectrum at photon energy 21.2 eV (for more details, see the insert of Fig. 3) allows us to determine precisely the position of the maximum of the EDC (and DOS) which occurs at 0.58 ± 0.03 eV.

Very recent XPS results[16,34] concerning the iron valence band seem to sustain the continuous controversy surrounding the question of the location of ϵ_F. Ley *et al.*[16] have placed ϵ_F at the onset of peak A in their spectrum; this leads to different conclusions about the iron band structure deduced in the works by Ley *et al.*[16] and by us. In the XPS of Goldmann[34] ϵ_F is quoted at a position which approximately corresponds to $\frac{1}{3}$ of the maximum intensity of peak A. Our result confirms Goldmann's suggestion.

A further note on the shape of the Fermi edge and the leading peak may be worthwhile. In the EDC at $\hbar\omega = 21.2$ eV the total width of the edge is approximately 0.15 eV, in close agreement with the value 0.135 eV observed by Neddermeyer *et al.*[35] for gold. In the EDC at $\hbar\omega = 16.8$ and 11.8 eV the sharp Fermi edge is smoothed out simply because these photon radiations consist of two components with slightly different energies and intensities. A broadening of the Fermi edge in the EDC's by Eastman[11,12] (Figs. 1 and 2) is probably due to a lower instrumental resolving power.

McAlister *et al.*[36] have studied the soft-x-ray $M_{2,3}$ emission spectrum of iron. They extracted the M_3 emission profile from a measured $M_{2,3}$ spectral complex by a computational data analysis. The main emission bandwidth of 5 eV agrees satisfactorily with our result but the over-all triangular shape of the M_3 band, showing at least six distinct shoulders but no Fermi edge at all, contradicts the UPS, XPS, and recent band calculations.[7,8] Since all structures in the SXS appear with considerable amplitudes, it is hard to decide what features are attributable to the DOS.

B. Comparison with calculated DOS's

Wakoh and Yamashita[4] applied the Korringa-Kohn-Rostoker (Green's function) method to their calculation of the valence band and DOS of ferromagnetic Fe. To improve the accuracy of the DOS obtained by these authors, Connolly[5] used the linear combination of atomic orbitals (LCAO) method and derived the total DOS by doing two separate calculations for the majority- and minority-spin bands of Wakoh and Yamashita.[4] This profile shows two peaks emerging at -0.5 and -1.0 eV and several other peaks with almost comparable strengths in the region -2.2 to -4 eV. A deep minimum was predicted to occur around -2 eV. These structures are so prominent that, if real, they should be detectable in UPS measurements. Eastman[11] compared his EDC with this DOS and found general agreement (see Table I). However, Fig. 1 shows that the EDC's vary markedly with low photon energy indicating that these spectra should be interpreted in terms of initial and final state properties [Eq. (1)]. Hence, the EDC at $\hbar\omega = 10.2$ eV does not lend any straightforward support to the existence of such an initial DOS in iron. As a matter of fact, the major peak in the EDC's at $\hbar\omega = 21.2$ and 40.8 eV, as well as in the XPS (Fig. 2) is structureless, and no significant valley is seen between this single peak and the shoulder at -2.4 eV. Consequently, the over-all agreement of the theoretical DOS of Connolly[5] with our data is only approximate.

A tight-binding method for calculating the d band and the OPW method for the sp band were applied by Yasui *et al.*[9] They obtained an extremely low intensity of the DOS at ϵ_F and the first maximum at -1.2 eV. Duff and Das[6] have also used a composite LCAO-OPW method. Their calculation predicts peaks in the DOS at about -2.6, -5.3, and -7.3 eV and a d bandwidth as broad as 10.9 eV. The experimental peak at -0.58 eV has no counterpart in these theories.

It should further be noted here that calculations for paramagnetic iron[2,5] are at even greater variance with the experimental results. These calculations predict a deep valley at -1 to -1.5 eV where we observe a high intensity in the EDC.

Recently, Tawil and Callaway[7] and Singh, Wang, and Callaway[8] have carried out extensive calculations on the band structure of iron within the framework of a self-consistent LCAO approximation. They incorporated the exchange splitting according to the $X\alpha$ method and included the spin-orbit coupling.[8] As the most accurate calculation available today, this DOS deserves a more detailed consideration here. The DOS[8] and EDC are shown in

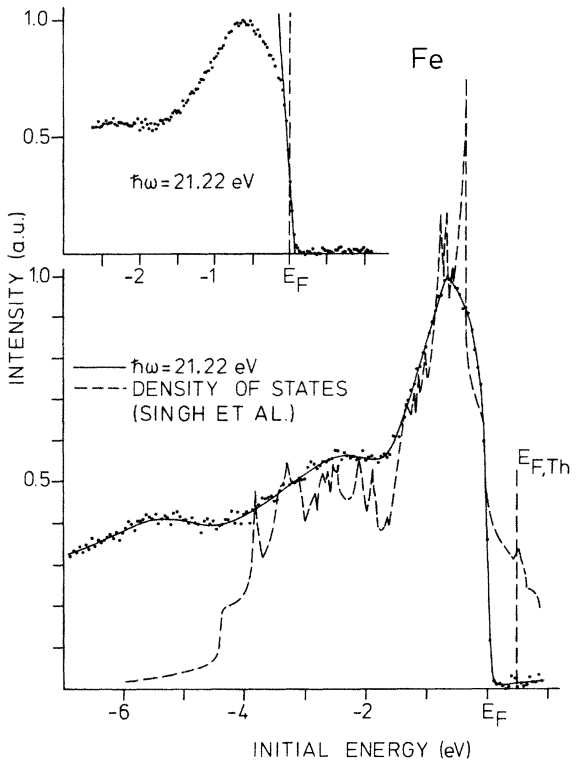

FIG. 3. Comparison of the EDC at $\hbar\omega = 21.2$ eV with the density of states by Singh *et al.* (Ref. 8). The peak intensity of the histogram is lined up with the maximum of the EDC curve. The high-energy part of the EDC showing the onset of the occupied states is inserted for clarity.

Fig. 3. The leading peaks of the DOS and EDC have been lined up for an easy comparison of the shapes of the curves. This shift causes the difference of 0.5 eV between the theoretical Fermi level $\epsilon_{F,\mathrm{Theor}}$ and the experimental one. The peak at -1.1 eV mainly results from nearly flat bands of the majority-spin states in the directions $\Gamma_{12} \rightarrow \Sigma_4 \rightarrow N_4 \rightarrow D_4 \rightarrow P_3$ and $\Gamma_{12} \rightarrow \Lambda_2 \rightarrow P_3$. An occupied section of minority-spin states fills up the valley in the DOS of majority spin around -2 eV when the two states are superimposed.

The good agreement between the shapes of the EDC and DOS indicates the unlocalized character of d-hole states created in the excitation; in other words, the interaction between the hole and the surrounding electrons should be small. We do not see any evidence that many-body effects are unexpectedly large in the case of iron.

An objection to our results that might be raised is the fact that only electrons generated within a distance 10–15 Å of the surface can escape from the sample without losing their kinetic energy through scattering processes, and that the surface-like states may differ from the bulk states. We refer to recent estimates by Desjonquères and Cyrot-Lackmann[37] on the local DOS of low-index surfaces of bcc Fe. Both the surface and bulk DOS's have sharp peaks just at ϵ_F which should contribute to the EDC of a polycrystalline film. We do not observe any corresponding peak in the EDC. It seems that more calculations are needed for quantitative estimates of the contribution of the surface states to the photoemission.

On the basis of the above comparisons we draw the conclusion that our EDC at photon energy 21.2 eV samples the initial bulk DOS to a high accuracy.

C. On relations between theoretical DOS, photo-ESP, and UPS results

In the calculations by Callaway *et al.*[7,8] the coefficient of the Slater-exchange parameter $\alpha = 0.64$ was found optimum. By employing this value a close agreement was obtained between the calculated saturation magnetic moment ($2.29\ \mu_B$) and the experimental value (2.1–$2.2\ \mu_B$). The areas of the majority-spin hole pockets observed experimentally around the H_{25}' symmetry point are also reproduced in a satisfactory manner. Including the spin-orbit coupling, Singh *et al.*[8] obtained a detailed description for many properties of cross sections of the Fermi surface which are consistent with the results of measurements of the de Haas–van Alphen effect. Soft-x-ray appearance potential measurements[17] and x-ray continuum isochromats[18] of Fe show that there does exist a sharp maximum in the density of unoccupied states ranging from 1 to 1.3 eV above ϵ_F as predicted by the theory.[7,8] Apart from this agreement, there is still the question of the difference of about 0.5 eV between the energy positions of the main peak of the occupied states in the calculated DOS and the measured EDC. The exchange splitting $\delta\epsilon_{ex}$ of the two spin states is thus no larger than 1.9 eV as opposed to the theoretical value of 2.35 eV,[8] below the Curie temperature.[38]

Photo-ESP results show that the electrons expelled from the range of ϵ_F to[19] -0.1 eV have a polarization which agrees with theory. However, the measured polarization (54%) of electrons originating at depths of ϵ_F to[20] 1 eV is larger than theoretical predictions. Moreover, the wavelength dependence of the photo-ESP has not been understood in the light of any calculated band structure.[20] These findings have been claimed to place constraints on interpretation of the Slater-Stoner-Wohlfarth theory.

We believe that the large ESP value (54%) is due to the narrow majority-spin d bands which fall into the probed ESP range between ϵ_F and at most -1 eV, i.e., just the energy region where peak A appears in the EDC. Accordingly, the calculated distance between ϵ_F and peak A is too large. This

fact can completely account for the difference between the observed and calculated ESP values.

Finally, the depth of 3 eV, where the saturation ESP of 28% was reached,[20] was interpreted to be smaller than the estimated d band width in the UPS[12] and XPS.[13] This may be true, but clearly the main structure (peaks A and B) lies above -3 eV. Only a low-energy tail extends further and this tail should not contribute significantly to the photo-ESP.

Thus, there seems to be no need to question the basic principles of the Slater-Stoner-Wohlfarth theory on the grounds of these ESP results.

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[38]The SSW theory postulates that $\delta\epsilon_{ex}$ of d bands for a ferromagnetic transition metal vanishes as one passes through the Curie point T_C. The corresponding shift of the occupied d bands should be large enough, roughly half of $\delta\epsilon_{ex}$, to be verified experimentally. However, XPS[13] investigations on Fe do not indicate any change in the position or in the amplitude of the peak below and above T_C. Sokoloff [J. Phys. F 5, 528; 1946 (1975)] has accounted for this absence of the band shift.