Photoemission study of single-crystal faces of iron

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Energy-distribution curves (EDC's) of photoelectrons emitted normal to the surfaces of Fe(100), Fe(110), and Fe(111) have been measured using photon energies of 11.83, 16.85, and 21.22 eV. The results are interpreted by emission from electronic states of the corresponding symmetry lines in the three-dimensional Brillouin zone. The band structure of ferromagnetic Fe as computed by Singh *et al.* is found adequate to explain major features of the EDC's, whereas a band structure of the paramagnetic state cannot satisfactorily account for the results. The maximum of occupied states is observed at about 0.6 eV below the Fermi level in agreement with previous measurements of polycrystalline Fe films. Emission from surface states or resonances cannot be identified with certainty.

I. INTRODUCTION

In a previous paper Pessa *et al.* reported on a study of the electronic structure of polycrystalline Fe films by ultraviolet photoelectron spectroscopy[1] (UPS). Using a high-resolution photoelectron spectrometer[2] and applying photon energies of 11.83, 16.85, and 21.22 eV they concluded that characteristic properties of the density of occupied valence states can be derived from the experimental energy-distribution curves (EDC's) of the photoelectrons. One of the essential issues of Ref. 1 was the observation of a maximum of occupied states at 0.6 eV below the Fermi level E_F, which was assigned to the majority-spin electrons of the ferromagnetic band complex.[3] By considering the gross shape of the spectra it appeared also possible to give a qualitative explanation for discrepancies between results of spin-polarization measurements of photoemitted electrons[4] and requirements of the itinerant-electron theory of ferromagnetism.[3,5]

Although a general consistence of the photoemission data[1] with important features of the one-electron model of the electronic structure of Fe was thus obtained some problems still need a further clarification. (i) If one compares the position of the observed maximum of density of states with the band structure as computed by Singh *et al.*,[3] one finds it experimentally much closer to the Fermi level than it was predicted theoretically. (ii) The EDC's of the polycrystalline Fe films are characterized by an appreciable lack of pronounced fine-structure details. Results of x-ray-photoelectron-spectroscopy (XPS) work[6] show basically the same elements of structure as the UPS spectra of Ref. 1 although the instrumental resolution in the XPS investigation was worse by one order of magnitude. Höchst *et al.* have suggested[6] that lifetime effects probably cause dominant broadening of the EDC's and therefore smear out fine-structure details of the density of states.

To improve our understanding of the above-mentioned points we have continued our study of the electronic structure of Fe by measuring directional photoemission normal to the single-crystal surfaces of Fe(100), Fe(110), and Fe(111). We have recently applied this technique to other ferromagnetic transition metals[7,8] and to the noble metal[9–11] and found a clear correlation of the observed EDC's with properties of the bulk band structure of the corresponding symmetry direction. It can therefore be expected that also for Fe more-detailed information with respect to the three-dimensional band structure can be obtained by measurements of single crystals. In particular, we make an attempt to locate the flat d bands which mainly contribute to the maximum of the density of occupied majority-spin states in order to support the measurements of polycrystalline films. Another important question is whether consequences of the itinerant-electron theory of ferromagnetism, as for example the existence of an exchange splitting, may be evaluated from the experimental EDC's of the single crystals.

Finally, an exploration of the influence of the surface on the electronic structure seems to be interesting. By the presence of the surface the electronic states may strongly be modified when compared with the bulk as has been shown by Feuerbacher and Christensen for W in a similar photoemission experiment.[12] The occurrence of surface states at clean single-crystal faces of Fe has been theoretically predicted in a number of recent publications[13–18] and transitions from surface states might be visible in the EDC's of the single crystals.

II. EXPERIMENT

For the present work the same apparatus has been used as in Ref. 1 which has been described in some more details by Neddermeyer *et al.*[2] Therefore, only the basic characteristics of the instrument will be summarized here briefly.

The experimental setup consists of a main ultrahigh-vacuum chamber, which contains the electron energy analyzer and is connected via a bakeable gate-through valve with a second one, which is used as preparation chamber. The energy resolution of the photoelectron spectrometer is better than 0.06 eV for all energy regions of the EDC's and the acceptance cone of the photoelectrons amounts to an average value of $\pm 5°$ normal to the surfaces of the samples. Photon energies of 11.83 (Ar I), 16.85 (Ne I), and 21.22 eV (He I) are used for the excitation of the electrons. The working pressure in the spectrometer chamber during the measurements was in the low 10^{-8}-Pa range.

The samples were prepared by spark cutting a commercial strain-annealed single-crystal of bcc Fe (Materials Research Co.) in the desired orientation within an accuracy of $1° - 2°$. The purity of the single crystal was 99.9% as given by the manufacturer. After mechanical polishing the surfaces were electropolished in an aqueous solution of acetic anhydride and chromic acid as described by Tegart.[19] The samples were then introduced into the preparation chamber and further treated *in situ* by repeated anneal-sputter cycles. Annealing temperatures up to 800 K were used for a time of one to several hours. Sputtering was performed with Ar ions of 600-eV energy and a current density of approximately $2\mu A/cm^2$ in an Ar pressure of 6×10^{-3} Pa for a few minutes to approximately 1 h. Before the first sputtering the EDC's did not show any sharp structure but only two broad humps originating in photoemission from the contaminant layer. The first few heating periods after sputtering caused the reappearance of emission from impurity levels at about 5 eV below E_F, which gradually became less important with increasing number of anneal-sputter cycles. The final EDC's were measured at room temperature from surfaces where neither an additional sputtering nor heating produced distinct effects in the results. Although no direct control of surface cleanliness and geometry by means of Auger-electron spectroscopy and low-energy-electron diffraction was possible during the course of these measurements, we concluded from the low intensity of emission from impurity levels at $5 - 6$ eV below E_F and from the sharpness of the spectral features that the surfaces were of sufficient quality to represent clean and ordered Fe. It has to be mentioned that a similar surface treatment of noble-metal single crystals (where only a few and short anneal-sputter cycles were necessary to remove the contamination) produced surfaces, which showed pronounced emission from surface states.[20] The cleanliness and order of the Fe surfaces should therefore also suffice to allow the study of intrinsic surface states if they were present and their transition probability to unoccupied states large enough. From the measured EDC's a constant background was subtracted and the transmission function of the energy analyzer was considered. The spectra were further corrected for the doublet character of the Ar and Ne resonance radiation.

III. RESULTS

The EDC's obtained at different photon energies from Fe(100), Fe(110), and Fe(111) are shown in Figs. 1–3. They are plotted against the initial energy of electrons with the Fermi level chosen as $E_F = 0$ eV. The position of the Fermi level in the experimental EDC's could be determined and remained stable during the measurements within an accuracy of a few 0.01 eV.

Compared to the previous measurements of polycrystalline films,[1] where only a main peak and a few less pronounced shoulders could be observed, the large

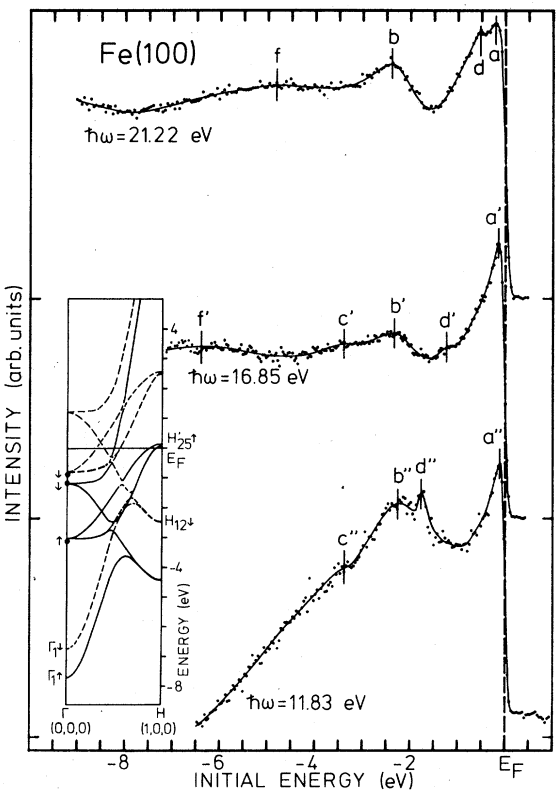

FIG. 1. Energy-distribution curves of photoelectrons emitted normal to the (100) face. The inset shows the ferromagnetic band structure of the ΓH line (Ref. 3) and the dots indicate possible surface states or resonances according to Ref. 15.

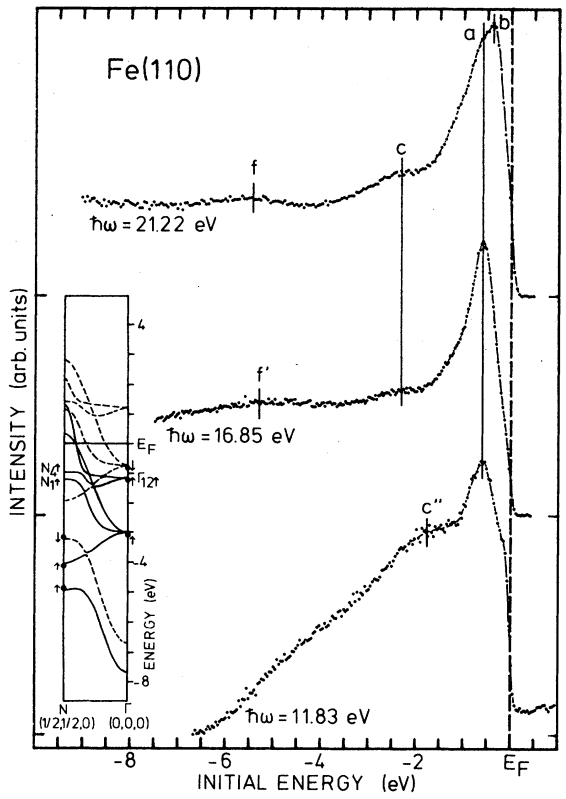

FIG. 2. Energy-distribution curves of photoelectrons emitted normal to the (110) face. The inset shows the ferromagnetic band structure of the ΓN line (Ref. 3) and the dots indicate possible surface states or resonances according to Ref. 16.

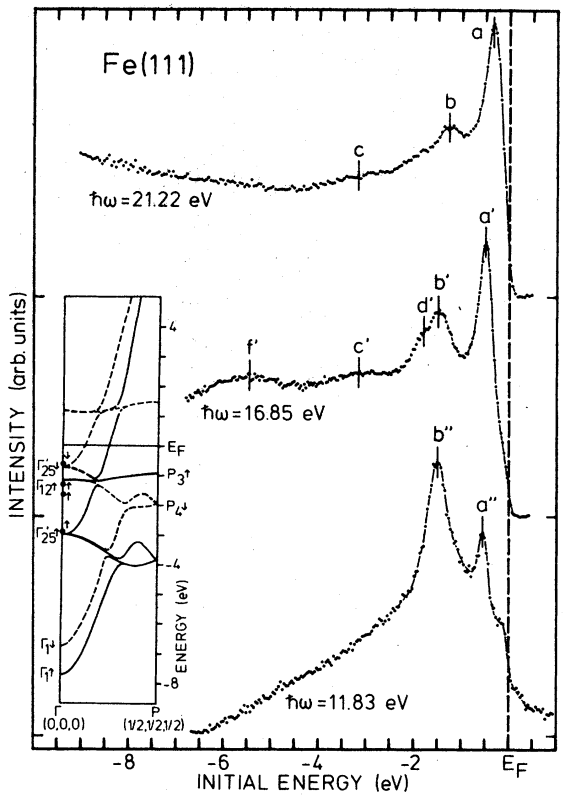

FIG. 3. Energy-distribution curves of photoelectrons emitted normal to the (111) face. The inset shows the ferromagnetic band structure of the ΓP line (Ref. 3) and the dots indicate possible surface states or resonances according to Ref. 17.

variety of well established spectral features is striking. It is obvious, however, that the sharpness of the structures decreases towards lower energies as well as their intensities. Since at a given photon energy for the individual single-crystal faces the fine-structure details have always different energy positions elastic scattering from high density-of-states regions of general points in the three-dimensional Brillouin zone into other directions seems to be negligible. We therefore expect a correlation of the measured EDC's with the energy bands of the corresponding symmetry lines in $\vec{k}$ space, which are included in the figures as insets.

We compare our results with the self-consistent band structure of ferromagnetic Fe as calculated by Singh *et al.*[3] The reasons that we have chosen a ferromagnetic band structure will be given in Sec. IV. In the band-structure insets the majority-spin bands are plotted as full lines and the minority-spin bands as broken lines. Positions of possible surface states or surface resonances as computed by Dempsey *et al.* for ordered ferromagnetic Fe films[15–17] are indicated by dots for the majority- (↑) and minority-spin (↓) electrons.

The only comparable investigation of a single-crystal face of Fe was reported recently by Brodén *et al.*,[21] who measured EDC's of Fe(110) with normal take-off of the photoelectrons for photon energies of 21.2 and 40.8 eV. The agreement between the experimental results obtained at 21.2 eV is fairly good. Only in the vicinity of the Fermi level our spectrum (Fig. 2) shows some additional fine structure details, namely, a shoulder labeled *a* and a weakly developed inflection point at the high-energy edge. The latter observation indicates the fact that the Fermi level has to be placed in the lower half of the high-energy edge and not in the middle part as in the results of Ref. 21. These small differences are probably due to a superior energy or eventually angle resolution of our photoelectron spectrometer. The weak features labeled *f* and *f'* in our EDC's of Fe(110) have possibly to be associated with emission from a small residual O_2 surface contamination. This structure is also present in the spectra of Brodén *et al.* for clean Fe(110) and was also

found with comparable intensity by Brucker and Rhodin in an UPS study of Fe(100).[22] Brucker and Rhodin concluded from Auger spectra that such minor emission correspond to a fraction of less than 0.01 of one monolayer of O_2, which therefore can be neglected in our discussion.

A comparison between our results of Fe(100) (Fig. 1) and those of Ref. 22 is not meaningful because in Ref. 22 an angle-integrating photoelectron spectrometer was employed. To our knowledge, photoemission studies of the (111) face are not reported in the literature.

Regarding the cleanliness of Fe(100) and Fe(111) a weak hump labeled f appears at -4.8 eV in the EDC of the (100) face for a photon energy of 21.22 eV and another one denoted f' at -5.5 eV in the EDC of the (111) face for a photon energy of 16.85 eV. These features could be due to emission from adsorbed species although their existence for only one photon energy may also indicate their origin from pure Fe states. We therefore believe that surface contamination for both the (100) and (111) faces is even smaller than for Fe(110).

IV. DISCUSSION

Our assignment of the observed elements of structure to the electronic states of Fe will be based on the ideas discussed, for example, in Refs. 9, 10, 12, and 20 and which may be summarized as follows. (i) Peaks due to direct $\vec{k}$-conserving transitions of the bulk band structure are recognized by the fact that they appear only for one photon energy at a certain initial energy position. In cases, where such transitions are possible from the same initial band for several photon energies, characteristic shifts according to the participating energy bands are observed. In addition, the shape of these transitions can often be described by a Lorentzian function, when they do not overlap too much with other transitions in the same energy region.[10] (ii) In some cases emission from bulk states may occur to unoccupied surface states. If these surface states lie in a gap of the bulk band structure the related mechanism is called "band-gap photoemission."[12] A participation of unoccupied surface resonances is also possible. In this case the surface states energetically overlap with bulk energy bands.[9] Experimental evidence for both kinds of transitions is obtained when elements of structure do not change their initial energy position for different photon energies. A definite relation of the observed structures to the one-dimensional density of states of the corresponding symmetry direction of the Brillouin zone might then be present.[9] This means that $\vec{k}_{\parallel}$ but not $\vec{k}_{\perp}$ is conserved for such transitions. (iii) Emission from surface states is experimentally verified in a similar way as for the transitions which have been described in (ii). The surface-states-related features appear at the same initial energy position for different photon energies and may therefore not easily be distinguished from those produced by mechanism (ii). Sometimes the intensity variation with photon energy may be helpful for an analysis of surface-state emission.[20] We note that for both surface photoemission processes (ii) and (iii) a sensitivity to surface contamination is expected.

A. Emission from the (100) face

The main features of the EDC's (Fig. 1) are structures a, a', a'', and b, b', b'', which practically do not change their initial energy position when the photon energy is varied.[23] In addition, there appears a weak hump labeled c' and c'' for photon energies of 11.83 and 16.85 eV, respectively, and some other small features, which are only observed at one photon energy (d, f, d', f', and d''). Peak a (a', a'') is certainly the most interesting structure of Fe(100). Its energy position immediately below $E_F = 0$ eV indicates the fact that the transitions contributing to a (a', a'') directly originate at E_F. Since the shape of peak a (a', a'') is approximately the same for each photon energy (for 21.22 eV the low-energy side of a is only superimposed by a small peak d) we conclude that a (a', a'') is strongly related to a rising part of the one-dimensional density of initial states, which is cut by the Fermi level before the maximum is reached. If one compares our observed spectra with the band-structure inset of Fig. 1 such rising part of the density of initial states starting approximately at -1 eV actually occurs and may be explained by the presence of the relatively flat majority spin bands ending at $H_{25'}\uparrow$. That the maximum of the one-dimensional density of states as represented by the levels near $H_{25'}\uparrow$ is found above E_F was already deduced from the existence of small electron hole pockets at symmetry point H.[3] We may therefore conclude that the location of $H_{25'}\uparrow$ above the Fermi level is also indicated by our photoemission results. It has to be noted that the other bands crossing the Fermi level in that direction do not contribute too much to the density of states because of their steep slope.

If our interpretation is correct we further may conclude that the use of a band structure of paramagnetic Fe for an explanation of peak a (a', a'') can be ruled out. In the self-consistent band structure for Fe in the paramagnetic state, which was computed by Yasui *et al.*,[24] no pronounced peak in the weighted one-dimensional density of states in the ΓH direction may be expected in the vicinity of the Fermi level.[25]

The rest of the structures obtained from Fe(100) cannot be related with certainty to transitions in the ferromagnetic band complex. We suggest that the pronounced structure b (b', b'') has to be associated via a surface photoemission process with a maximum of the one-dimensional density of initial states, which

for example exists at $H_{12}\downarrow$. However, a number of direct transistions could also explain peak b (b', b''). Structures f and f' may result from transitions of the sp-like bands starting at $\Gamma_1\uparrow$ and $\Gamma_1\downarrow$. Further theoretical work is needed for a reliable assignment of all these above-mentioned less-pronounced features.

According to the calculations of Dempsey *et al.*[15] surface states should exist at approximately −1 and −3 eV. At these energies only the weak humps c' and c'' could eventually be attributed to emission from surface states, since their energy positions remain practically unchanged for photon energies of 16.85 and 11.83 eV, respectively. In an *ab initio* calculation of paramagnetic Fe(001) films[18] surface states appear at −0.7 and −3.3 eV, which is not much different from the values of the ferromagnetic film.[15] However, due to the fact that assignments to candidates of surface states in our experimental EDC's are rather tentative we cannot conclude, whether one or the other theory is more appropriate.

B. Emission from the (110) face

The EDC's obtained from Fe(110) (Fig. 2) essentially show a structure a at −0.6 eV, whose initial energy position is independent from photon energy, shoulders c and c'', and for a photon energy of 21.22 eV, a peak b located at about −0.3 eV. Features f and f' have already been interpreted as due to a negligible amount of contamination on the surface. Compared to the EDC's of Fe(100) the intensity in the vicinity of the Fermi level is now reduced. A small density of initial states at E_F is also seen in the band-structure inset, since no flat bands are crossing the Fermi level in the ΓN direction.

As origin for the stationary structure a the rather flat majority spin bands running from $\Gamma_{12}\uparrow$ to $N_1\uparrow$ and $N_4\uparrow$ are possible. We suggest that a surface photoemission process gives rise to the experimental EDC's which therefore would correlate with the density of initial states. Such interpretation would explain the independence of the observed energy positions from photon energy. If, on the other hand, direct $\vec{k}$-conserving transitions were responsible for the occurrence of peak a, they should also originate in the flat majority-spin bands, since for the remaining steeper bands a certain observable shift with photon energy should be present.

The assignment of structure a to transitions from the flat majority-spin bands connecting $\Gamma_{12}\uparrow$ with $N_1\uparrow$ and $N_4\uparrow$ supports the localization of the maximum of the density of majority-spin electrons at −0.6 eV as has been reported in Ref. 1. Note that these flat bands considerably contribute to the maximum of the density of majority-spin electrons, which on the basis of the present single-crystal work has also to be placed at −0.6 eV, which is much closer to the Fermi level than obtained theoretically.[3]

The appearance of peak a at a constant and finite distance from the Fermi level further supports our conclusion that a ferromagnetic band structure is more adequate than a paramagnetic one for an explanation of our photoemission data. If, for example, a paramagnetic band structure had to be applied, the maximum of occupied states would be found immediately at the Fermi level[24] and a stationary peak very close to E_F as in the case of Fe(100) should be observed. If, however, direct transitions between energy bands of the paramagnetic band structure were responsible for a, the absence of any detectable shift could hardly be explained.

A large number of surface states and resonances should exist according to the theoretical work of Dempsey *et al.*[16] There is not much experimental evidence for any of these states, although a certain contribution to peak a by a majority-spin surface state below $\Gamma_{12}\uparrow$ cannot be excluded. It has to be mentioned, however, that the intensity of emission from the low-lying states is very small, in general, and the experimental details below −2 eV always appear rather broadened and structureless. Lifetime effects may indeed be responsible for this behavior[6] and therefore smear out also contributions from the predicted surface states.

C. Emission from the (111) face

The main features of the EDC's from Fe(111) (Fig. 3), namely, a, a', a'', and b, b', clearly show a small shift towards lower initial energies with decreasing photon energy. Such shifts have to be explained by the occurrence of direct transitions, which therefore are believed to be identified in the EDC's of the (111) face. The smallness of the shifts indicates the participation of rather flat initial energy bands. Actually the band structure shows a very flat degenerate majority-spin band running from $\Gamma_{12}\uparrow$ to $P_3\uparrow$, which could account for the observed energy differences of structures a, a', and a'' obtained at photon energies of 21.22, 16.85, and 11.83 eV, respectively.

An interesting point is the position of these degenerate majority-spin bands, which is found much closer to the Fermi level than was calculated by Singh *et al.*[3] This observation supports our previous conclusion that the maximum of the majority-spin electrons appears at −0.6 eV, since these bands significantly contribute to the maximum of the majority-spin states.

The origin of structures b, b', d', and b'' cannot be deduced with certainty. We suggest that these peaks are due to direct transitions from the flat parts of the minority-spin bands starting at $P_4\downarrow$, because the majority-spin band in that energy region (beginning at $\Gamma_{25'}\uparrow$) is rather steep and would cause more pronounced shifts of the measured structures when ob-

tained with different photon energies. If this interpretation is correct it seems possible to observe *separately* emission from both the majority- and minority-spin band system in one spectrum.

In the paramagnetic band structure of Ref. 24 a flat band is running immediately below E_F and is responsible for a high-density-of-states region. However, our spectra do not show appreciable intensity at the Fermi level and therefore do not confirm the existence of such a high-density-of-states region. In addition, in the paramagnetic band structure no flat energy bands are found in the energy region between -1.5 and -0.3 eV and could account for the occurrence of the observed direct transitions. We therefore conclude that also in this case a band structure of ferromagnetic Fe is more suitable for the interpretation of the measured EDC's.

Surface states are expected in the energy range between -2.8 and -0.6 eV.[17] At about -3.0 eV some weak structures (c and c') are obtained independent from photon energy. Whether they correspond to emission from low-lying surface states cannot be decided on the basis of our measurements. Emission from surface states may also be superimposed on b' and b'' but are not distinguishable from transitions of bulk states by the present experiment. The weak hump f' is only observed at a photon energy of 16.85 eV. Transitions from the low-energy sp bands starting at $\Gamma_1\uparrow$ or $\Gamma_1\downarrow$ are possible explanations for this structure.

V. CONCLUSION

In the present paper we have reported on the first systematic investigation of directional photoemission normal to the three low-index single-crystal faces Fe(100), Fe(110), and Fe(111). The results show a great variety of different spectral features and therefore demonstrate the improved capability of such measurements with respect to the determination of the structure of occupied valence states. In previous studies of polycrystalline Fe films only gross features of the density of initial states could be derived.

The results are compared with the electronic states of the corresponding symmetry directions of the three-dimensional Brillouin zone. We concluded that the band structure of ferromagnetic Fe as calculated by Singh *et al.*[3] is adequate for the interpretation of the experimental results. A band structure of the paramagnetic state cannot explain the measured EDC's in a satisfactory way.

A closer examination of our measurements revealed, however, that the position of the flat majority spin bands is located much nearer to the Fermi level than in the calculation. This conclusion was already reached by an analysis of measurements of polycrystalline films,[1] which are therefore confirmed by the present results.

The lack of fine-structure details in measurements of polycrystalline films was explained by Höchst *et al.* by dominant lifetime broadening.[6] Since, on the other hand, single-crystal spectra show pronounced fine structures especially in the neighborhood of the Fermi level down to -2 eV we believe that absence of sharp structures in measurements of polycrystalline films is essentially caused by the angle integration, which is inherent in measurements of polycrystals. However, weakness of features at low initial energies may still be explained by this effect.

Although a ferromagnetic band structure was necessary for an explanation of the EDC's an estimation of the exchange splitting was not possible by a consideration of the photoemission data alone. It is suggested, however, that in the EDC's distinct peaks may separately be attributed to transitions from majority- and minority-spin bands, respectively.

The influence of the surface on the electronic structure could not be separated from bulk effects in a definite way. No emission from surface states could be identified with certainty. A narrowing of energy bands in the surface region[15–17] could also not be deduced from the experimental results.

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[1] M. Pessa, P. Heimann, and H. Neddermeyer, Phys. Rev. B 14, 3488 (1976).
[2] H. Neddermeyer, P. Heimann, and H. F. Roloff, J. Phys. E 9, 756 (1976).
[3] M. Singh, C. S. Wang, and J. Callaway, Phys. Rev. B 11, 287 (1975).
[4] H. Alder, M. Campagna, and H. C. Siegmann, Phys. Rev. B 8, 2075 (1973).
[5] E. P. Wohlfarth, Rev. Mod. Phys. 25, 211 (1953).
[6] H. Höchst, A. Goldmann, and S. Hüfner, Z. Phys. B 24, 245 (1976)
[7] P. Heimann and H. Neddermeyer, J. Phys. F 6, L257 (1976).
[8] P. Heimann, E. Marschall, H. Neddermeyer, M. Pessa, and H. F. Roloff, Phys. Rev. B (to be published).
[9] P. Heimann, H. Neddermeyer, and H. F. Roloff, Phys. Rev. Lett. 37, 775 (1976).
[10] P. Heimann and H. Neddermeyer, J. Phys. F 7, L37 (1977).
[11] H. F. Roloff and H. Neddermeyer, Solid State Commun. 21, 561 (1977).
[12] B. Feuerbacher and N. E. Christensen, Phys. Rev. B 10, 2373 (1974).

[13]M. Tomasek and P. Mikusik, Phys. Rev. B 8, 410 (1973).
[14]M. C. Desjonquères and F. Cyrot-Lackman, J. Phys. F 5, 1368 (1975).
[15]D. G. Dempsey, L. Kleinman, and E. Caruthers, Phys. Rev. B 12, 2932 (1975).
[16]D. G. Dempsey, L. Kleinman, and E. Caruthers, Phys. Rev. B 13, 1489 (1976).
[17]D. G. Dempsey, L. Kleinman, and E. Caruthers, Phys. Rev. B 14, 279 (1976).
[18]E. Caruthers, D. G. Dempsey, and L. Kleinman, Phys. Rev. B 14, 288 (1976).
[19]W. J. McG. Tegart, *The Electrolytic and Chemical Polishing of Metals* (Pergamon , London and New York, 1959), p. 64.
[20]P. Heimann, H. Neddermeyer, and H. F. Roloff, J. Phys. C 10, L17 (1977).
[21]G. Brodén, G. Gafner, and H. P. Bonzel, J. Appl. Phys. (to be published).
[22]C. F. Brucker and T. N. Rhodin, Surf. Sci. 57, 523 (1976).
[23]The small shift of $a \rightarrow a' \rightarrow a''$ towards the Fermi level is due to a superior energy resolution at lower kinetic energies of the photoelectrons.
[24]M. Yasui, E. Hayashi, and M. Shimizu, J. Phys. Soc. Jpn. 34, 396 (1973).
[25]Under "weighted one-dimensional density of states" we understand a calculated density of states in one symmetry direction of the Brillouin zone, where the number of states is weighted by a factor equal to $\vec{k}^2$. This means that singularities in the vicinity of the Γ point are suppressed in the calculation. The reason for an introduction of a weighting factor in the one-dimensional density of states was found in a study of the (110) faces of the noble metals (Ref. 9), where the finite angle resolution of the photoelectron spectrometer should be considered in that way.