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Energy bands of a (110) iron thin film*

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We have performed a tight-binding calculation of the energy bands of a 29-layer (110) ferromagnetic iron thin film. The matrix parameters were obtained by fitting a bulk calculation of Tawil and Callaway with the diagonal surface matrix elements shifted by a constant amount to obtain surface charge neutrality. The energy bands were calculated at 117 points in the irreducible (one fourth) two-dimensional Brillouin zone. The planar and total densities of states are also reported and compared to previous results. A discussion of the surface states and energy bands is given and the structure of the energy bands is correlated to structure seen in the planar density of states and the effects of s-d hybridization.

I. INTRODUCTION

In a previous paper,[1] we reported a calculation of the energy bands and densities of states for a 41-layer (100) film of ferromagnetic iron using s, p, and d basis functions and a tight-binding-approximation scheme. We now present a similar calculation for a 29-layer (110) ferromagnetic iron film. Because the method is basically the same as was used for the (100) face, we will indicate only the differences in the new calculation. The two-dimensional lattice is centered rectangular which has a parallelogram-shaped primitive unit cell. The alternate planes of atoms in the (110) film are located at the center and corners of the parallelogram respectively. (See Fig. 1). Also shown in Fig. 1 are rectangular and hexagonal alternate choices for the primitive unit cell. The film was taken to have 29 layers; with an interplanar spacing of $a/\sqrt{2}$, this is the same thickness as the 41-layer (100) film[1] with its $\frac{1}{2}a$ interplanar spacing. With nine (one $4s$, three $4p$, and five $3d$) planar Bloch basis functions per plane this gives 261×261 Hamiltonian matrices which are reduced to 132×132 and 129×129 matrices for solutions even and odd under reflection through the central plane. The matrices are further reduced at symmetry points or lines by using the basis functions shown in Table I.

The two-dimensional Brillouin zone (2DBZ) is an irregular hexagon (reciprocal to the hexagonal unit cell) with the symmetry directions and points as indicated in the bottom part of Fig. 1. (See Caruthers and Kleinman[2] for the relationships between the two-dimensional reciprocal-lattice vectors and the three-dimensional cubic coordinates.) Using the bulk matrix element parameters previously obtained[1] by fitting the calculation of Tawil and Callaway[3] and modifying the surface layer zeroth-neighbor parameters by an identical -0.022 Ry shift to obtain surface charge neutrality, the energy bands for the majority and minority spins were calculated at 47 points in the quarter 2DBZ to produce the energy bands shown in Figs. 2–4 and discussed in detail in Sec. II. For the calculation of the densities of states and the determination of the surface parameter shift required for surface charge neutrality (discussed in Sec. III) the energy levels were calculated on a 14×20 grid inside the rectangular reciprocal-lattice unit cell, i.e., at 70 interior nonsymmetry points in the irreducible quarter rectangle. This sampling required an equal weighting of each point which is a simplification over sampling points in the hexagonal 2DBZ. Because our method includes the effects of s-d hybridization, the results overcome the limitations of those[4,5] whose calculations have been limited solely to d basis functions. The effects of this on the planar den-

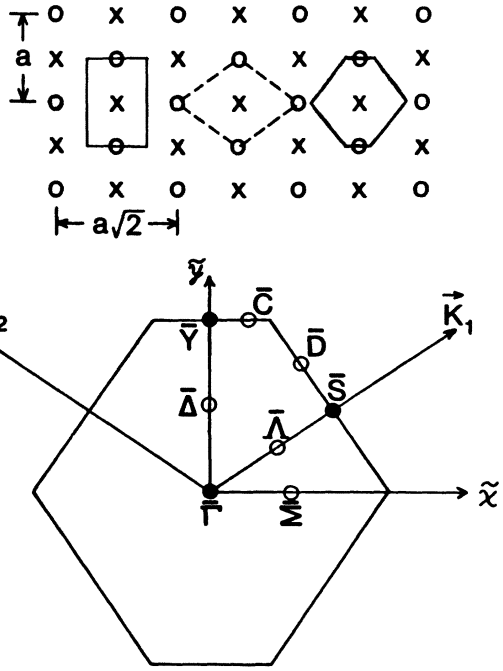

FIG. 1. Two-dimensional unit cells and Brillouin zone for a (110) slab of a bcc crystal.

TABLE I. Symmetrized basis functions at points of higher symmetry. The basis set for $\bar{S}$ symmetry depends on whether the plane has atoms at the cell centers (A planes) or atoms at the cell corners (B planes). The basis is chosen to make the Hamiltonian matrix real and application of relfection symmetry may further reduce the basis set on the center or 0 plane. The $\bar{\Lambda}$ and $\bar{D}$ lines have no special symmetry and use the complete basis set.

Symmetry	Functions
$\bar{\Gamma}_1$, $\bar{Y}_1$	s, z, x^2-y^2, $3z^2-r^2$
$\bar{\Gamma}_2$, $\bar{Y}_2$	xy
$\bar{\Gamma}_3$, $\bar{Y}_3$	ix, ixz
$\bar{\Gamma}_4$, $\bar{Y}_4$	iy, iyz
$\bar{S}_1$	(A) s, z, xy, x^2-y^2, $3z^2-r^2$ (B) ix, iy, ixz, iyz
$\bar{S}_2$	(A) ix, iy, ixz, iyz (B) s, z, xy, x^2-y^2, $3z^2-r^2$
$\bar{\Delta}_1$, $\bar{C}_1$	s, iy, z, iyz, x^2-y^2, $3z^2-r^2$
$\bar{\Delta}_2$, $\bar{C}_2$	ix, xy, ixz
$\bar{\Sigma}_1$	s, ix, z, ixz, x^2-y^2, $3z^2-r^2$
$\bar{\Sigma}_2$	iy, xy, iyz

sity of states (PDS) is also discussed in Sec. III.

II. ENERGY BANDS

Figure 2 shows the energy bands along the various directions in the 2DBZ for the majority and minority spin electrons. The bulk states are dashed lines in these energy-band figures. The surface states are drawn without dashes to facilitate their identification. As on the (100) face of iron previously reported, the minority spin bands, aside from the upward shift of about 0.07 Ry, are similar to the majority spin bands.

The majority spin bands have five large absolute gaps with one or more surface states appearing in three of these gaps. Starting at $\bar{\Gamma}$, an unoccupied gap extends upward from -0.24 Ry to above the vacuum level. Another $\bar{\Gamma}$ gap, from -0.63 to -0.69 Ry, extends along $\frac{1}{3}$ of the $\bar{\Sigma}$ line before pinching off. This gap opens as we move to the $\bar{\Lambda}$ direction and extends along $\bar{\Lambda}$ to $\bar{S}$ where it becomes the lowest gap in $\bar{D}$ at -0.64 Ry. (The $\bar{D}$ bands are symmetric about $\bar{S}$.) Moving toward the $\bar{\Delta}$ line, the gap slopes upward and shortens to pinch off midway along the $\bar{\Delta}$ line. At the bottom of this gap, a surface state extends from $\bar{\Gamma}$ along $\bar{\Sigma}$ and $\bar{\Delta}$ until the gap closes. However, in the $\bar{\Lambda}$ direction, this surface state disappears into the band bottom by $\frac{1}{4}$ the distance to $\bar{S}$. In $\bar{\Sigma}$ and $\bar{\Delta}$, the state possesses $\bar{\Sigma}_1$, and $\bar{\Delta}_1$ symmetry, respectively, and $\bar{\Gamma}_1$ symmetry at $\bar{\Gamma}$. At the gap top around $\bar{\Gamma}$, a second surface state belonging to $\bar{\Sigma}_2$, $\bar{\Delta}_2$, and $\bar{\Gamma}_2$, respectively, extends only briefly in any direction before vanishing into the bands at the gap's top. Along $\bar{\Delta}$, this surface state reappears briefly from $\frac{1}{3}$ to $\frac{5}{12}$'s the distance to $\bar{Y}$ as a $\bar{\Delta}_2$ surface state. At $\bar{S}$, we find two large gaps in addition to the $\bar{\Gamma}$ gap just discussed. The first opens from -0.1 Ry upward to the vacuum level. This gap contains one surface state, with energy of -0.094 Ry at $\bar{S}$, that extends upward in the $\bar{D}$ and $\bar{\Lambda}$ directions and has $\bar{S}_2$ symmetry at $\bar{S}$. The second large gap at $\bar{S}$ runs from -0.25 to -0.31 Ry at $\bar{S}$. The gap opens in the $\bar{D}$ direction to extend from -0.35 Ry to just below the vacuum level at the $\bar{\Sigma}$-$\bar{D}$ and $\bar{D}$-$\bar{C}$ intersections. It pinches off along $\bar{\Sigma}$ by $\frac{7}{12}$'s the distance to $\bar{\Gamma}$ with this pinch-off point moving closer to the $\bar{D}$ line as we go from $\bar{\Sigma}$ to $\bar{\Lambda}$ where the gap pinches off and reopens $\frac{1}{5}$ the distance from $\bar{S}$ to $\bar{\Gamma}$ and finally pinches off $\frac{2}{5}$ of the distance to $\bar{\Gamma}$. The gap opens as we move from $\bar{S}$ toward $\bar{Y}$, then closes down along the $\bar{C}$ line and pinches off along the $\bar{\Delta}$ line $\frac{1}{6}$ of the distance from $\bar{Y}$ to $\bar{\Gamma}$. For the majority spin this gap contains no surface states.

The fifth large majority spin gap runs from the center of $\bar{\Sigma}$ at -0.5 Ry through $\bar{\Lambda}$ at the same energy to $\bar{\Delta}$ where it appears at an energy of -0.53 Ry $\frac{5}{12}$ the distance from $\bar{\Gamma}$ to $\bar{Y}$. At $\bar{\Sigma}$, the gap contains a $\bar{\Sigma}_1$ surface state in the lower right $\frac{2}{3}$'s of the gap. At $\bar{\Lambda}$ we find 3 surface states: one V-shaped surface band in the bottom half of the gap which extends the length of the gap, a second in the top right half of the gap, and a third in the top right third of the gap running along the very top edge of the gap. The first (lowest) of these $\bar{\Lambda}$ surfaces states connects with the $\bar{\Sigma}_1$ surface state at $\bar{\Sigma}$ and with the $\bar{\Delta}_2$ surface state which runs through the center of the gap at $\bar{\Delta}$. At $\bar{\Delta}$, this gap also contains a $\bar{\Delta}_1$ surface state that runs along the top left edge of the gap. Because these surface states, with their large extent across the 2DBZ and their relatively flat energy range, have significant effects on the surface PDS which we will discuss in Sec. III, we have examined their properties on the $\bar{\Lambda}$ line $\frac{6}{10}$ of the distance from $\bar{\Gamma}$ to $\bar{S}$ in detail. At this $\bar{k}$ point, all three surface states are present. The bands immediately above the gap are very d-like with very little s or p hybridization. For example, the ratio of the largest coefficient of the surface layer d orbitals to the coefficient of the surface s orbital is 12.5 to 1. In the interior layers, this state is even more d-like with the ratio of the same coefficients increasing to as much as 440 to 1 on the intermost planes. The upper most and middle surface states are also very d-like with the ratios of their respective d and s coefficients being 57 and 79 to 1, respectively. These two surface states are Tamm surface states and are pulled out of the top of the band by our attractive surface potential shift. The lowest surface state, however, is strongly s-d hybridized with s and maxi-

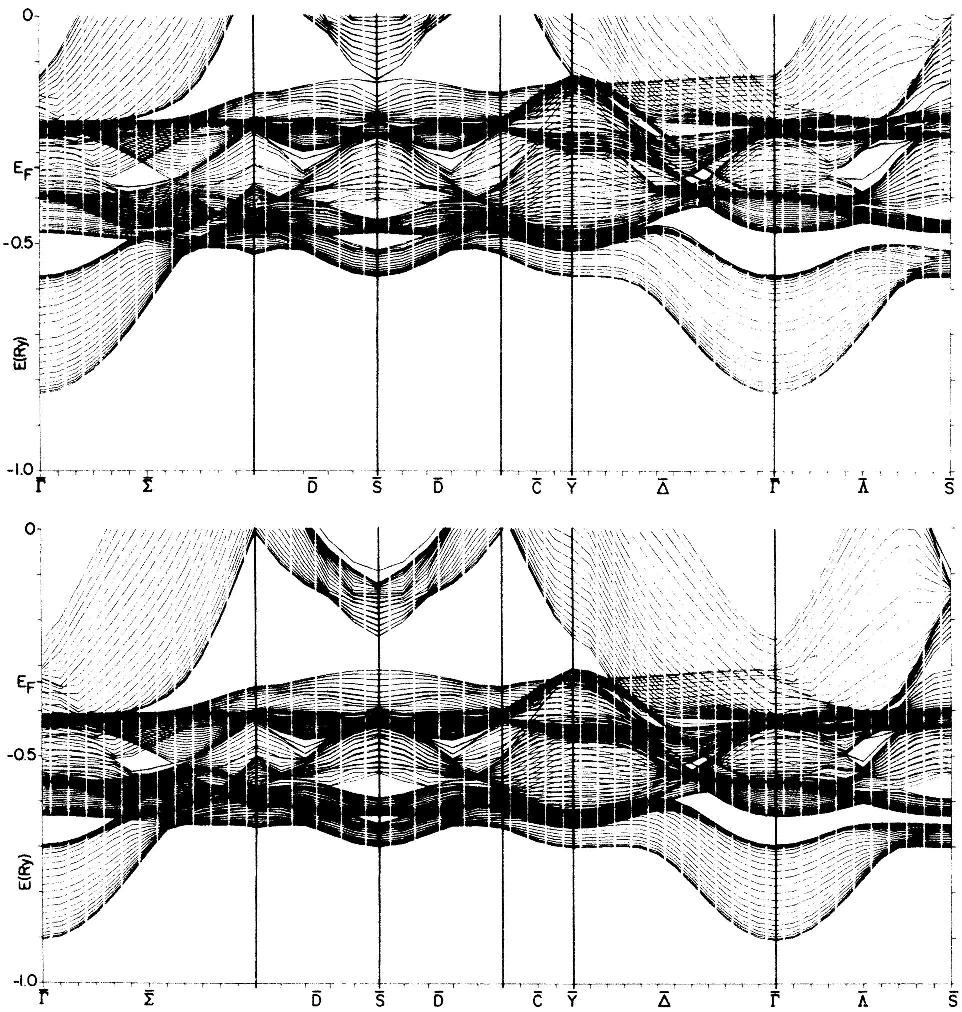

FIG. 2. Composite 2D energy bands for the minority (top) and majority (bottom) spin polarizations in a 29-layer (110) ferromagnetic iron film. Bulk states are indicated by dashed and surface states by solid lines.

mum *d* coefficients on the surface layer of 0.29 and 0.42, respectively, for a ratio of 1.4 to 1. The bulk bands at the gap bottom also show strong *s*-*d* hybridization, with the ratio of the surface *d* and *s* coefficients being just under 2 to 1 in the band just below the bottom of the gap. Thus, the lower surface state is a Shockley surface state[6] whose existence springs from the interaction between the *d* and *s*-*d* bands above and below the gap. Although its exact position would change with varying surface potentials, the surface state should be present with any reasonable surface potential assuming the calculation permits the effects of *s*-*d* hybridization. However, a calculation using only *d* basis functions, such as Desjonqueres and Cyrot-Lackmann,[4] would not produce these Shockley surface states and their resultant effects on the surface PDS.

In addition to these five large gaps in the majority spin bands, there are several smaller absolute gaps. At $\bar{S}$, a gap at -0.58 Ry extends $\frac{2}{5}$'s of the $\bar{D}$ line and persists along the $\bar{\Lambda}$ line $\frac{3}{10}$ the distance to $\bar{\Gamma}$ before pinching off. This gap does not contain any surface states. At $\bar{S}$ and -0.41 Ry there is a very narrow gap which pinches off and reopens about half way along the D line, pinching off again at the ends of the D line. Between $\bar{S}$ and the first pinch it contains a surface state which at $\bar{S}$ has $\bar{S}_2$ symmetry. This gap with its surface state extends along $\bar{\Lambda}$ $\frac{1}{3}$ of the distance from $\bar{S}$ to $\bar{\Gamma}$. Along $\bar{D}$, two crescent shaped gaps, symmetric about $\bar{S}$, at -0.48 Ry, each occupied by two surface states, extend from $\frac{2}{5}$'s the distance from $\bar{S}$ to the $\bar{\Sigma}$-$\bar{D}$ and $\bar{D}$-$\bar{C}$ intersections where they pinch off. All of these $\bar{D}$ gaps pinch off as we move perpendicularly away from the $\bar{D}$ line.

Aside from the over-all energy shift, the mi-

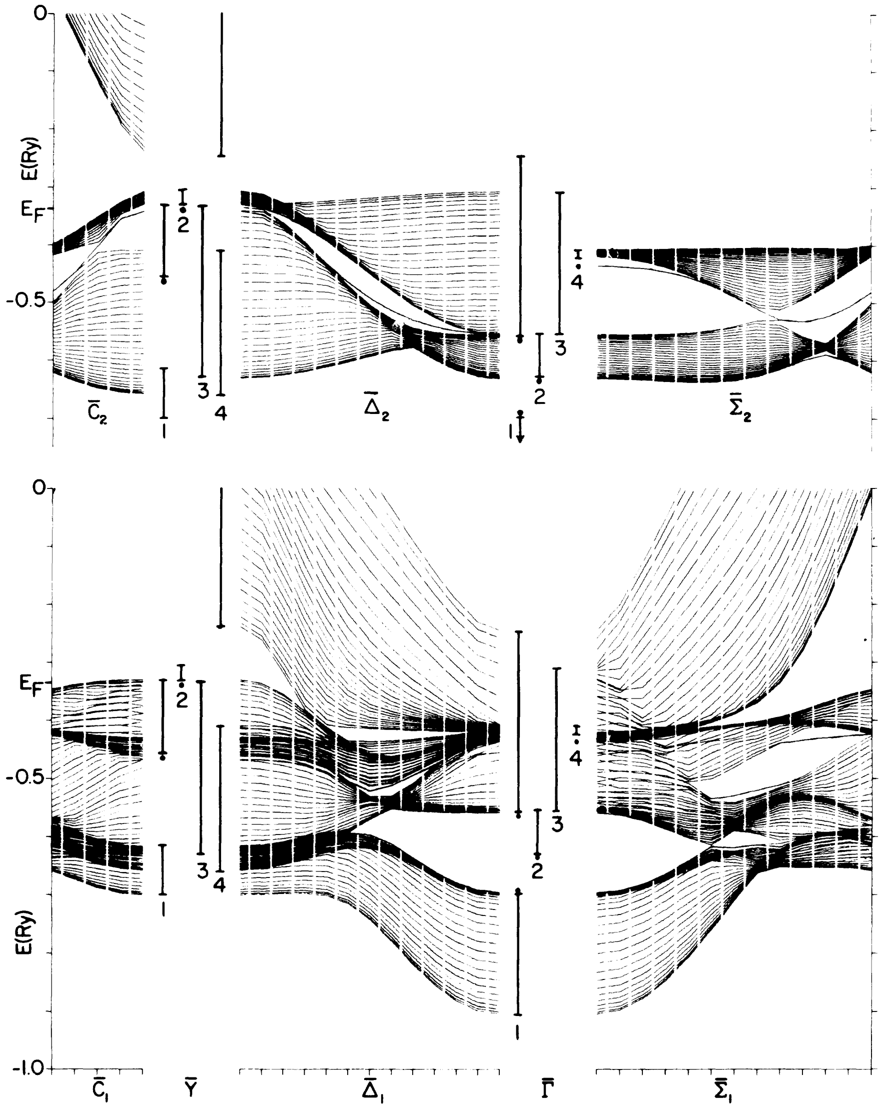

FIG. 3. Majority spin subbands at points (excluding $\overline{S}$) and lines of higher symmetry.

nority-spin energy bands differ from the majority-spin case at only a few points. The $\overline{\Gamma}_2$ surface state, at the top of the lower $\overline{\Gamma}$ gap in the majority bands is not present in the minority case. Also, in the center of $\overline{\Lambda}$ at an energy of -0.30 Ry, we find only two surface states in place of the three seen in the majority-spin case. The uppermost Tamm state has not dropped out of the continuum but the second Tamm state and the lower Shockley surface states are still present. However, on $\overline{S}$ at -0.15 Ry the gap seen in the majority bands has narrowed and two surface states have appeared around $\overline{S}$. The upper state has $\overline{S}_1$ symmetry at $\overline{S}$ and persists along $\overline{\Lambda}$ until the gap closes $\frac{1}{3}$ of the distance to $\overline{\Gamma}$. The second surface state has $\overline{S}_2$ symmetry at $\overline{S}$ and disappears into the bottom of the gap $\frac{1}{5}$ of the distance to $\overline{\Gamma}$. The uppermost $\overline{S}$ gap, which extended in the majority case down to -0.1 Ry, begins, in the minority case, at $+0.02$ Ry and does not contain a surface state below $+0.25$ Ry. The very narrow $\overline{D}$ gap at -0.24 in the minority-spin case differs by containing a surface state on both sides of the central pinch.

Figures 3 and 4 show, for the majority and minority spins, respectively, the subbands along the $\overline{C}$, $\overline{D}$, and $\overline{\Sigma}$ symmetry lines and at the $\overline{Y}$ and $\overline{\Gamma}$ symmetry points. Again the bulk states are shown as dashed lines while the surface states are drawn continuous. There are several interesting surface states in these subbands even though they vanish or become resonances when

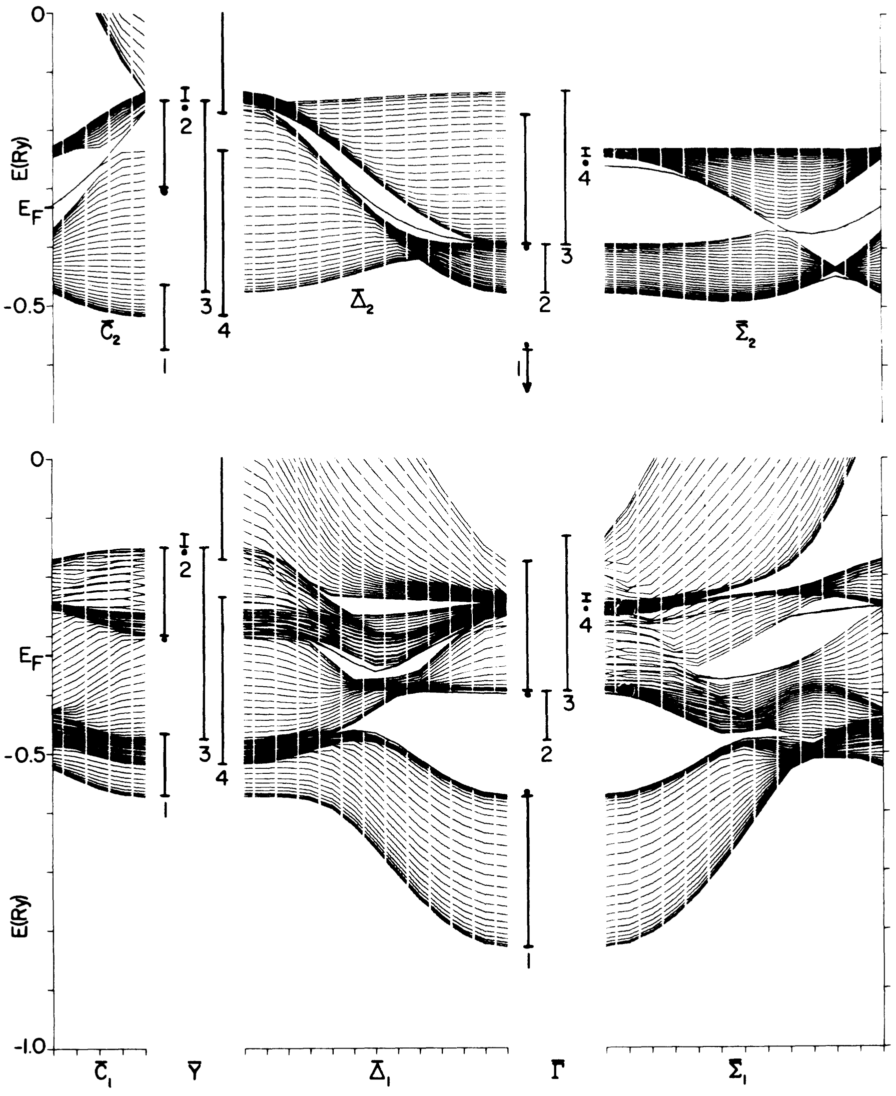

FIG. 4. Minority spin subbands at points (excluding $\bar{S}$) and lines of higher symmetry.

we move away from the symmetry line or point and the loss of symmetry causes their gap to disappear. For either spin there is a wide gap running the entire length of the $\bar{\Sigma}_2$ bands which is pinched off at a point about $\frac{2}{3}$ the distance from $\bar{\Gamma}$. The gap appears to narrow but not completely pinch off only because the pinch-off point lies between calculated points. Both sides of the gap contain surface states and provide an excellent example of Shockley and Tamm surface states in a 2DBZ. Beginning at $\bar{\Gamma}$, the upper bands are predominately *d*-like and are derived from bulk bands which include the pure *d* Δ_2 state. The lower bands, however, contain more *p* basis functions and come from bulk bands that include the *p*-*d* hybridized Δ_5 state.[7] Two-thirds of the way from $\bar{\Gamma}$, the Δ_2 and Δ_5 bulk energy bands cross causing the 2D bands to pinch off the gap and immediately reopen. This side of the gap contains a Shockley surface state created by the crossing of the *p*- and *d*-like bands. Notice this surface state pair[8] is formed by one band from the top and from the bottom of of the $\bar{\Sigma}_2$ gap. On the other side of the $\bar{\Sigma}_2$ gap, the attractive surface potential has pulled a surface state pair from $\bar{\Gamma}_4$ and the top bands of $\bar{\Sigma}_2$ into that gap. This induced surface state is a Tamm state and runs along the gap top until it vanishes into the top $\frac{5}{12}$ of the way along $\bar{\Sigma}$. Also in $\bar{\Sigma}_2$, and again for both spins a surface state exists along the bottom of the $\bar{\Sigma}_2$ bands from $\frac{8}{12}$ to $\frac{11}{12}$ of the way to the $\bar{\Sigma}$-$\bar{D}$ intersection. These surface states also vanish on leaving $\bar{\Sigma}$ because of the loss of symmetry.

For both spins, the lower gap in $\bar{C}_2$ constitutes a similar situation. Here the Shockley state is in the left-hand side of the gap. The gap pinches shut midway along $\bar{C}_2$. This pinching shut results from a mixed p-d D_3 state in the bulk bands dropping below a pure d D_4 state.[9] The right-hand side of the gap then has mainly d-like bands at its top and p-d hybridized bands along its bottom. For the majority spin, this gap contains a Tamm state going into a $\bar{Y}_2$ surface state at $\bar{Y}$. In the minority-spin case, the surface potential has not pulled the $\bar{Y}_2$ surface state below the $\bar{Y}_4$ continuum, and the right-band gap there does not contain a surface state. However, a more attractive surface potential, which might occur in a more accurate self-consistent calculation, could easily pull the surface state into this gap.

The $\bar{\Delta}_2$ band gap, for both spins, contains one surface state along the top third of the gap and a more prominent surface state in the bottom right center of the gap. In $\bar{\Delta}_1$, a surface state extends, from the upper $\bar{\Gamma}_1$ surface state, $\frac{1}{2}$ the distance to $\bar{Y}$ in the majority case and $\frac{1}{3}$ of the distance to $\bar{Y}$ in the minority-spin case. These states extend $\frac{1}{6}$ of the $\bar{\Sigma}$ distance in the $\bar{\Sigma}_1$ bands but, in no case, exist in an absolute gap. For the majority spin, there are also 3 other $\bar{\Sigma}_1$ surface states: at -0.42 Ry starting at the $\bar{\Sigma}$-$\bar{D}$ intersection, and -0.59 and -0.61 Ry in the lowest gap near the center of the $\bar{\Sigma}$ line. None of these states are in absolute gaps. For $\bar{\Sigma}_1$ in the minority spin bands, a similar surface state occurs at -0.25 Ry. At $\bar{Y}_1$ for both spins, we also find a $\bar{Y}_1$ surface state but this $\bar{Y}_1$ gap does not exist away from $\bar{Y}$ in any direction. The other surface states shown in Figs. 3 and 4 exist at least partly in absolute gaps and were discussed in Fig. 2.

In addition to the surface states, there are two bands of resonances, states which occur in the bulk bands and, while heavily localized at the surface planes, decay to some nonzero amplitude in the interior of the film. On the (100) face of ferromagnetic iron, we found two bands of resonances in each spin which encompassed the entire 2DBZ. Here there is only one broad band of resonances in each spin and it does not quite cover the entire 2DBZ. For the majority spin, the resonance band occurs at roughly -0.45 Ry and occupies an area in $\bar{k}$ space of nearly three-fourths of the 2DBZ. The area boundaries run, beginning at $\bar{\Gamma}$ to the middle of the $\bar{\Sigma}$ line, then up to $\bar{S}$, along $\bar{D}$ to $\bar{C}$, then to $\bar{Y}$, and back down to $\bar{\Gamma}$. The band varies in thickness up to nearly 0.15 Ry, although at any given $\bar{k}$ no more than four or five states will be resonances. The minority-spin resonance band has a similar extent but is roughly 0.2 Ry thick and occurs at a higher average energy, -0.25 Ry.

Examining the energy bands, in general, we fnid that the basis functions which predominate in an energy eigenstate in the bulk (i.e., center) of the film may not be the same ones that predominate at the film's surface. For example, along $\bar{\Lambda}$ $\frac{4}{10}$ of the distance from $\bar{\Gamma}$, consider the majority-spin states between -0.3 and -0.4 Ry. Of the eleven bulk states present (at this point there are no surface states or resonances), at least two have nearly constant total amplitude from the center to the film surface but the d functions which predominate in the center differ from those which predominate on the surface. In one, d_{xz}, d_{yz}, and $d_{3z^2-r^2}$ are most prominent and have amplitude in layer 2 of 0.24, 0.11, and 0.03, respectively. By the surface of the film, however, their amplitudes are 0.24, 0.003, and 0.12, respectively. The symmetry of the predominate d function has switched from d_{xz} and d_{yz} in the bulk to d_{xz} and $d_{3z^2-r^2}$ at the surface. In the second, d_{xz} is the fourth smallest d function in the central planes but increases by a factor of 12 on the surface plane to become the largest, while the other d function's amplitudes remain relatively constant. These changes would have considerable effects when considering reactions using orbital symmetry conservation,[10] and its application to catalysis in the transition metals,[11] since these techniques depend on the wave-function symmetries at the surface. If these techniques are to be used on a surface where the symmetry changes are common, the surface wave-function characteristics must be obtained from accurate surface calculations rather than assumptions based on the bulk symmetries.

We also observe antisurface states in these energy bands. These antisurface states, which are sometimes found at the edges of gaps containing surface states, result from the requirement that they must be orthogonal to the surface state. As an example, in the majority-spin bands midway along $\bar{\Lambda}$ at -0.44 Ry, we find an antisurface state at the top of the gap immediately above the top Tamm surface state. The total amplitude on each plane decreases from about 0.26 average on the center planes (0 and 1, -1) to about 0.04 average on the 13th and surface planes. Like the bulk states just discussed, this state also has d functions of different symmetries predominating in the center and surface layers of the film. However, because their surface amplitude is so small, these antisurface states will not play as significant a part in surface interactions as will the bulk states which have greater surface amplitude and are far more numerous.

III. DENSITIES OF STATES

Figures 5 and 6 are various planar (PDS) and total (TDS) densities of states for the majority and minority spins, respectively. In both spins, the TDS and PDS for the four intermost planes closely resemble the results for the (100) face[12] and the

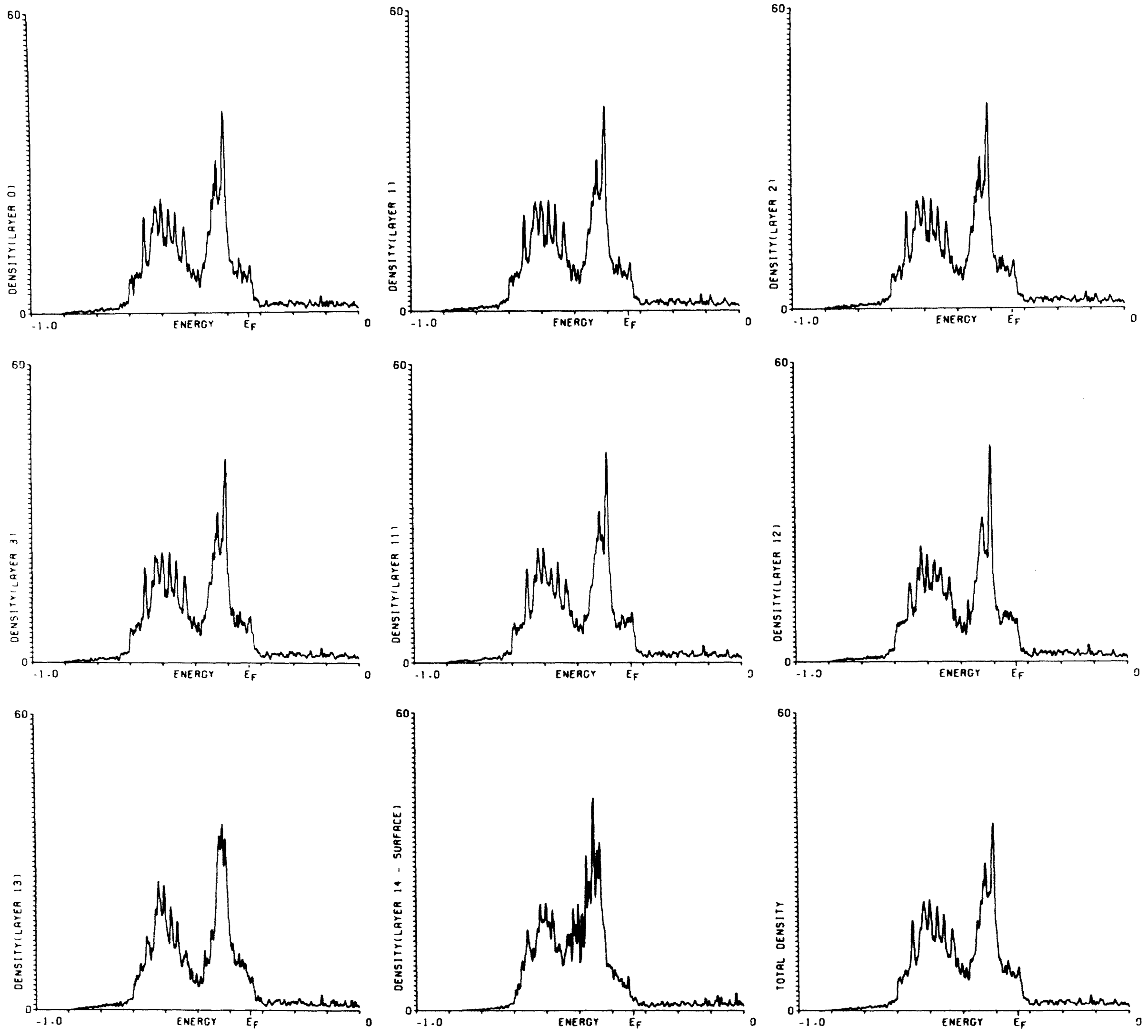

FIG. 5. Planar and total densities of states for the majority spins in units of electrons per atom per Ry. Layer 0 is the central plane and 14 is the surface plane.

bulk calculation of Tawil and Callaway.[2] In the results on (100) face, we found the even and odd numbered planes in the film interior showed small but noticeable differences in the PDS. Here, the PDS does differ slightly from plane to plane in the interior, but these changes do not repeat on even and odd planes (these changes are most noticeable in the first rise in the PDS). The changes in the PDS increased from plane to plane as we approach the surface although the structure is basically the same through layer 12, the second layer from the film surface. In both spins, the double peak (which lies above E_F in the minority spins) has practically coalesced into a single peak in layer 13 while the broad minimum (at E_F in the minority spins) remains. These changes are probably due to the surface states and resonances which seem to have a greater tendency to reach a peak amplitude on the layer 1 or 2 in from the surface than was seen on (100) face. The surface layer PDS shows the expected decrease in its first moment. Also, the broad minimum in the TDS and interior PDS has been filled with a large number of peaks in the surface PDS. These peaks can be correlated directly with surface states in the bands. For the surface majority-spin PDS consider the three peaks running from -0.53 to -0.50 Ry. These peaks coincide with the surface state which runs from the center of $\bar{\Sigma}$ across the 2DBZ through $\bar{\Lambda}$ to the center of $\bar{\Delta}$. For the minority-spin case, the tall peaks just below the Fermi level at -0.36 Ry

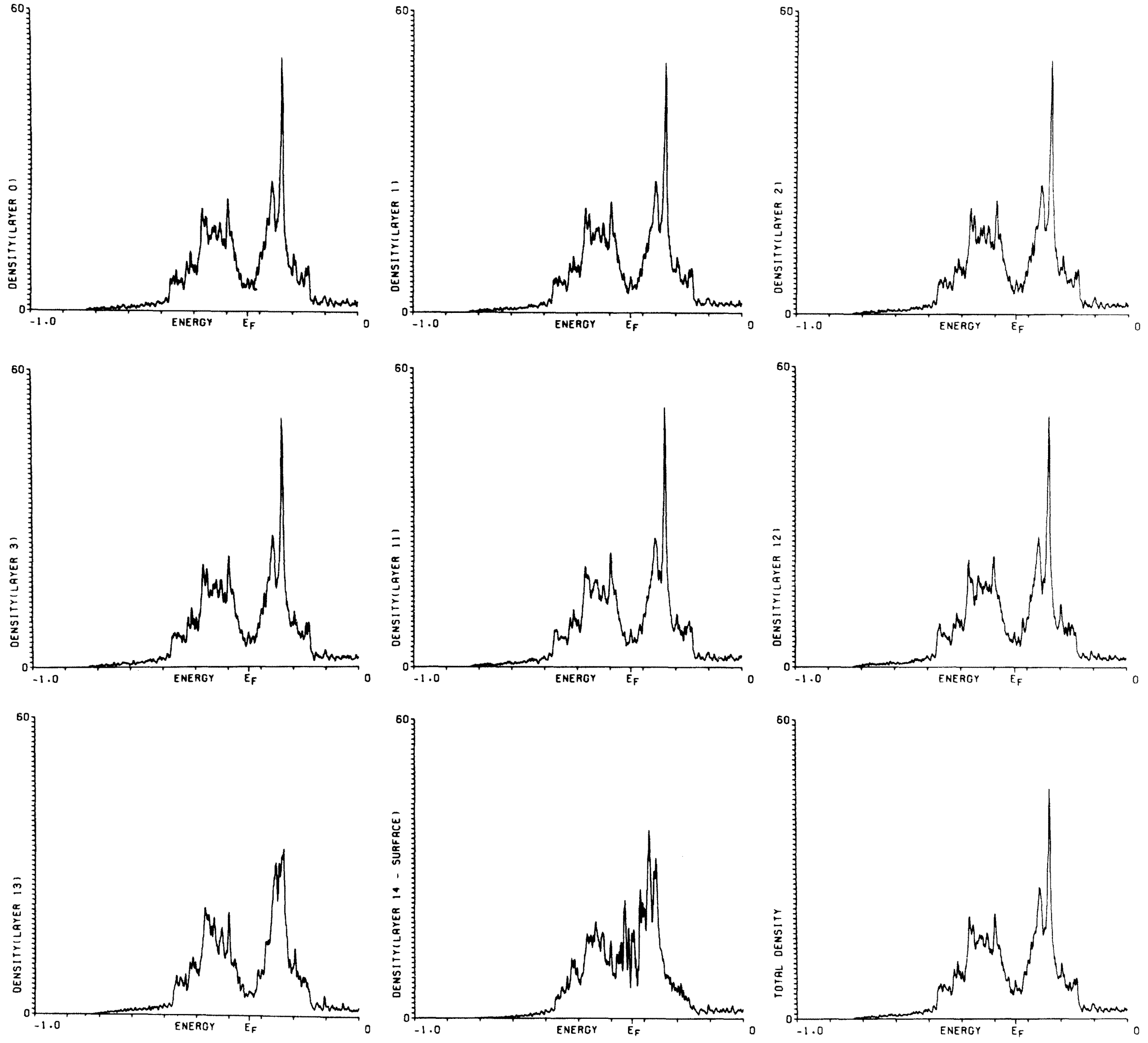

FIG. 6. Planar and total densities of states for the minority spins in units of electrons per atom per Ry. Layer 0 is the central plane and 14 is the surface plane.

can be attributed to the same surface state in the minority-spin bands. Much of the remaining structure in the surface PDS is also undoubtedly due to other surface states and resonances, but the individual contributions are smaller because these states fail to persist so extensively throughout the 2DBZ.

These results for the surface PDS contrast sharply with the results of Desjonqueres and Cyrot-Lackmann.[4] Since their results are not for a ferromagnetic sample, their TDS and PDS have an over-all energy shift compared to our results. However, while their TDS is similar to ours (the differences in sharp structure is due to different calculation techniques), their surface PDS has failed to fill in the center region and does not give any indication of the peaks seen in our results. We believe this difference can be traced to their failure to include 4*s* and 4*p* basis functions. From the band calculations, the surface states which caused the peaks just discussed were found to contain considerable *s*-*d* hybridization and to result not so much from the surface potential as from the hybridizing structure of the bands around these states. Since Desjonqueres and Cyrot-Lackmann's calculation uses only *d* basis functions, it does not adequately allow for *s*-*d* hybridization and fails to obtain these Shockley surface states.

After the surface parameter shift of −0.022 Ry, we obtained a total of 8.014 electrons per atom on the surface layer at the Fermi energy, −0.345 Ry, compared to 8.000 electrons per atom on the average and in the central layers. Like the (100) face results, the relative fractions of electrons belonging to each spin were practically unchanged ($5.161\uparrow/2.853\downarrow$ at the surface and $5.148\uparrow/2.852\downarrow$ in the center plane) between the surface and the bulk. There is an oscillation in the number of electrons per atom on the planes in from the surface (7.954 on 13, 8.031 on 12, and 8.010 on plane 11) which damps out as we go into the film. Whether this oscillation is a true Friedel oscillation or an artifact of our limited self-consistency in the correction for the surface potential will have to be decided by a more adequate self-consistent calculation.

For the (100) surface, we required a shift in the diagonal surface parameter of -0.0217 Ry to obtain surface charge neutrality. Here, on the (110) face, we require nearly the same shift, -0.022 Ry. In contrast, Desjonqueres and Cyrot-Lackmann[3] required shifts of $+0.018$ and $+0.009$ Ry, respectively. Although the fact that their bulk parameters and ours are obtained from different bulk calculations may account for some of this discrepancy, we believe the lack of s and p functions in their basis set and the corresponding differences in the surface PDS are the principal cause of this discrepancy.

IV. CONCLUSION

For the (110) surface of ferromagnetic bcc iron, as in the previous calculation on (100) surface, we find numerous gaps, containing anywhere from 0 to 3 separate surface states. Several of the surface states, such as the lowest one at $\bar{\Gamma}$ and the surface states in the large gap from $\bar{\Sigma}$ to $\bar{\Delta}$, persist throughout the 2DBZ and have noticeable individual effects on the surface PDS. Many of the surface states are caused not so much by the surface potential as by the hybridization in the 3-D bulk band structure. These surface states emphasize the need to include an adequate set of basis functions in any attempt to calculate the surface properties of transition metals. Calculations using only d basis functions such as Desjonqueres and Cyrot-Lackmann[4] will not obtain these hybridized surface states and will yield an inaccurate indication of the planar density of states.

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[7] The Δ symmetry point is included in the projected $\bar{\Sigma}$ energy bands because at $\bar{\Sigma}$ we have $\bar{k} = (0, 0, \alpha)$, while $\vec{k}_\perp$ in the surface normal direction is $(\beta, \beta, 0)$. Thus $\vec{k} = \bar{k} + \vec{k}_\perp$ lies on the Δ line when $\beta = 0$.

[8] The surface states always appear in pairs which are even and odd under reflection through the central plane. If the amplitude of the surface state has vanished at the center of the film the pair is degenerate and may be combined to form surface states on the left- and right-hand surfaces.

[9] At $\bar{C}$ we have $\bar{k} = (\frac{\bar{1}}{2}, \frac{\bar{1}}{2}, \alpha)$. Then $\vec{k}$ lies on the D line when $\vec{k}_\perp = 0$.

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[12] We used a slightly different smoothing procedure here than in Ref. 1. We took an energy mesh of 0.001 Ry and gave each energy level a width of 0.005 Ry so that each level contributed $\frac{1}{5}$ to each of four mesh intervals and the remaining $\frac{1}{5}$ was shared proportionally to its overlap with the two outside mesh intervals. This procedure smoothes out much of the noise from our discrete sampling techniques.

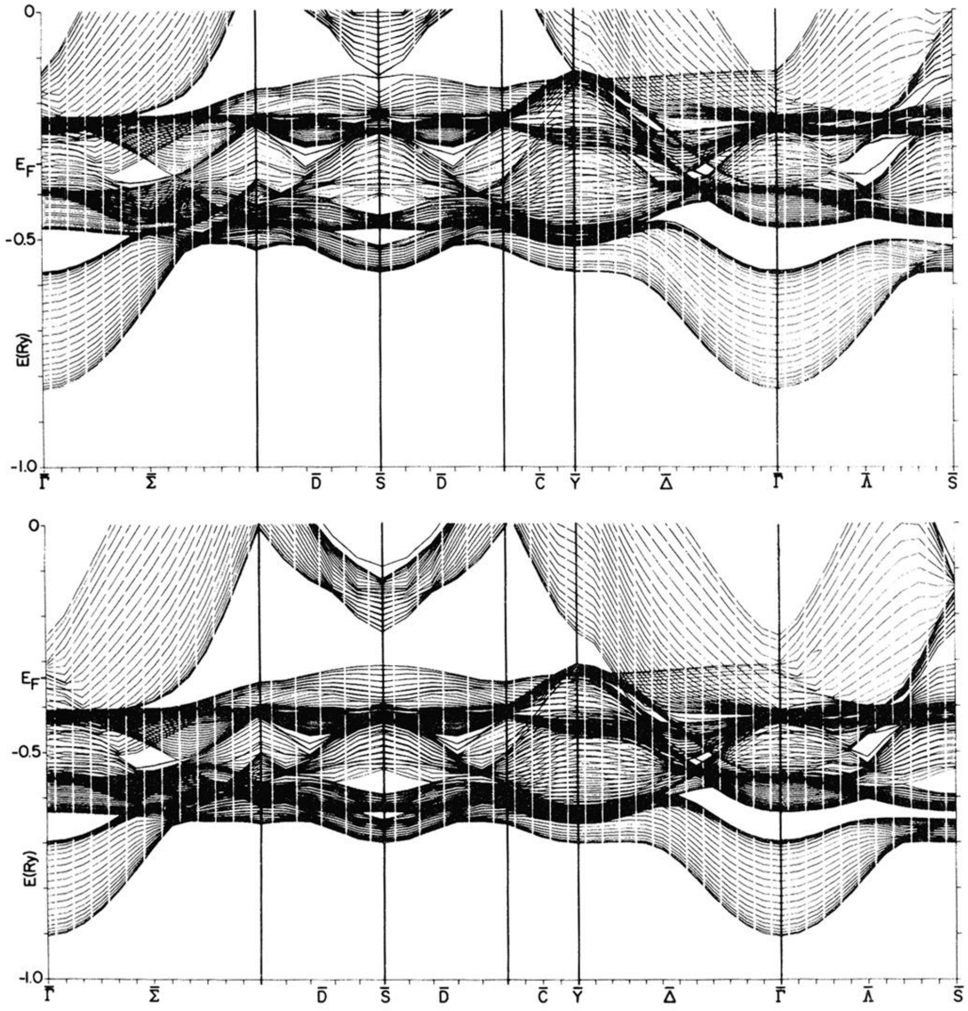

FIG. 2. Composite 2D energy bands for the minority (top) and majority (bottom) spin polarizations in a 29-layer (110) ferromagnetic iron film. Bulk states are indicated by dashed and surface states by solid lines.

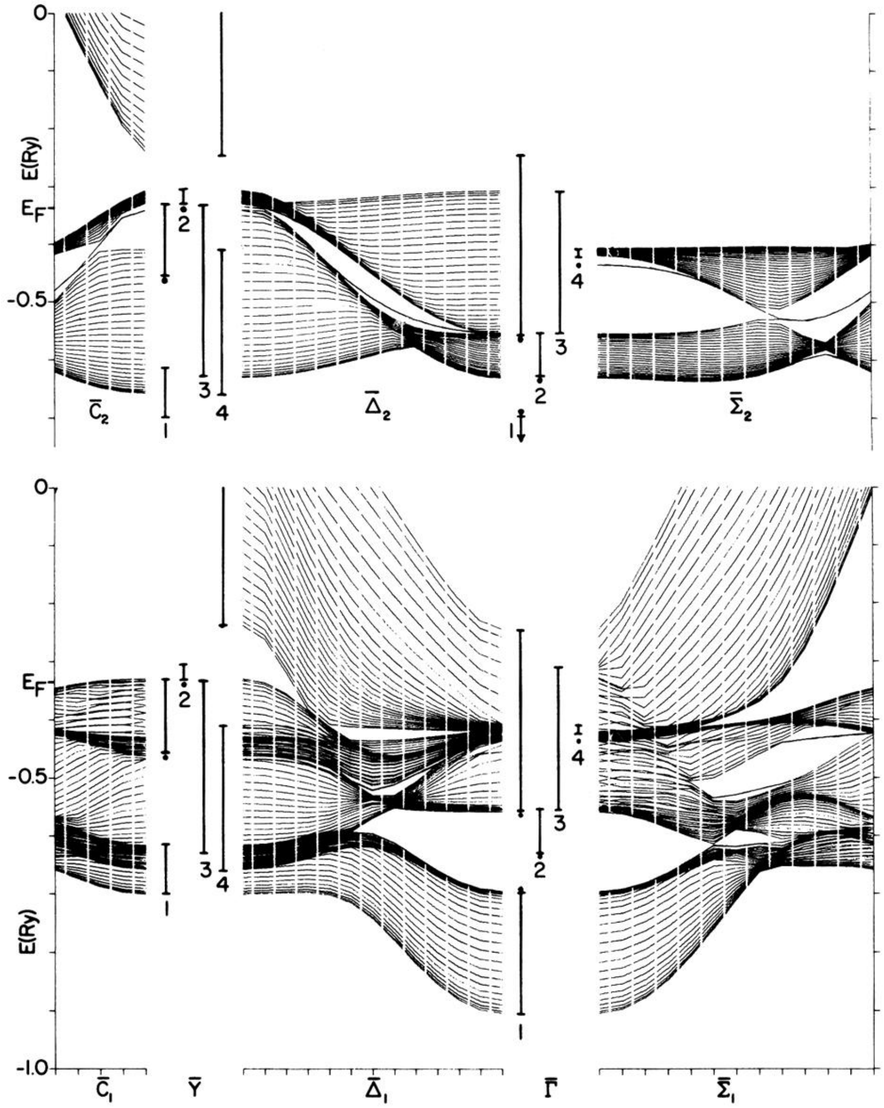

FIG. 3. Majority spin subbands at points (excluding $\bar{S}$) and lines of higher symmetry.

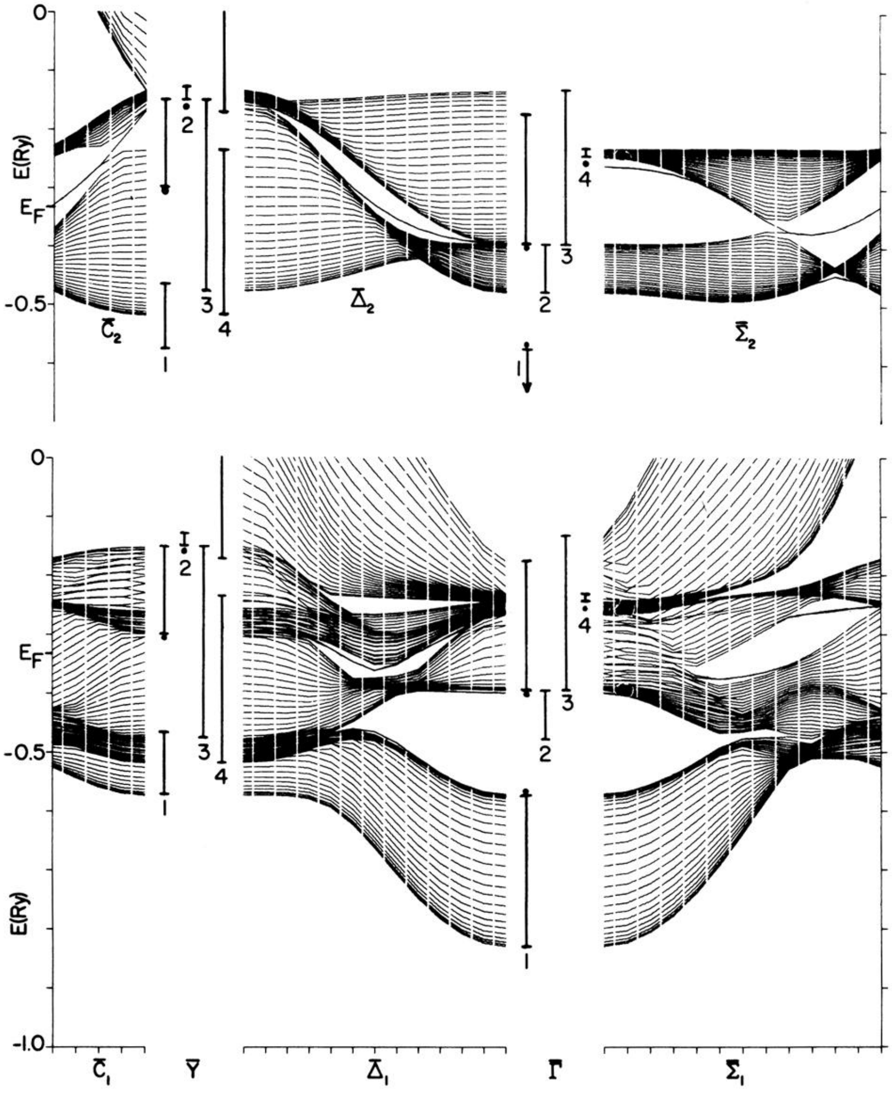

FIG. 4. Minority spin subbands at points (excluding $\bar{S}$) and lines of higher symmetry.