where the angle φ is measured from the [111] axis in the $(1\bar{1}0)$ plane. This expression is plotted in Fig. 2 (solid line), and good agreement with the data is obtained when $m_t/m_l = 0.40 \pm 0.05$. From the measured values of $P[111]$, $P[110]$, and $m[110]$ we calculate $m_t = (0.26 \pm 0.02) \times m_0$ and $m_l = 0.65 \pm 0.10$. The calculated value of m_t is in good agreement with the experimental value of $(0.26 \pm 0.04) m_0$.

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[4]The provisional estimate for the size of the neck in nickel from the galvanomagnetic measurements is that it subtends an angle $6.5° \pm 1.0°$ at the center of the Brillouin zone. The value determined from the angular widths of the peaks in the magnetoresistance associated with open orbits is $6° \pm 1.5°$. The independent estimate obtained from the difference in the Hall coefficient when measured for a general magnetic field direction and with the field along the symmetry axis is $7° \pm 1.5°$. The latter estimate depends upon the assumption that the multiply connected sheet of the Fermi surface contains electrons of only one sign of spin; if the spin degeneracy were not resolved the Hall effect data would correspond to an angle 3.5°. E. Fawcett and W. A. Reed (private communication).

[5]We are indebted to J. C. Phillips for pointing out the applicability of this equation.

MANY-ELECTRON EFFECTS AND EXCHANGE SPLITTINGS IN NICKEL

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Magnetoresistance measurements have shown[1] that one sheet of the Fermi surface of Ni has the same topology as that of Cu, Ag, and Au.[2] It consists of one spheroid in each Brillouin zone connected by narrow necks passing through the L centers of the (111) zone faces. The diameter of the necks are about three times smaller than those of Cu. In the preceding Letter, measurement of the effective masses of the neck is reported. We show here that the exchange splittings[3]

$$\Delta E_d = E(L_3\downarrow) - E(L_3\uparrow),$$

$$\Delta E_c = E(L_{2'}\downarrow) - E(L_{2'}\uparrow) \quad (1)$$

can be estimated from this and other data.

If we assume that the $d\downarrow$ bands of Ni are full, the high-field Hall data[4] give

$$n(s\downarrow) + n(s\uparrow) + n(d\uparrow) = 1.0 \quad (2)$$

and from saturation magnetization data and gyromagnetic ratios[5]

$$1.0 + n(s\downarrow) - n(s\uparrow) - n(d\uparrow) = 0.54 \quad (3)$$

where, e.g., $n(s\downarrow)$ is the number of electrons per atom contained in the $s\downarrow$ Fermi surface. Combining (2) and (3), we have

$$n(s\downarrow) = 0.27. \quad (4)$$

Three models of the band structure of Ni have been proposed to explain the multiply connected Fermi surface. These are shown in Fig. 1. Model (a) uses[6] the Cu band structure for spin $\downarrow$, with $E_F \simeq 9$ eV reduced by $\delta E_F = 0.7$ eV relative to Cu[7] to yield the reduced neck diameter. The calculated density of states[8] near $L_{2'}$ is 1.6 times the free electron value. This gives a precise value in (a) for

$$n(s\downarrow) = 0.50(1 - 1.6 \times \tfrac{3}{2} \delta E_F / E_F) \quad (5)$$

and

$$n(s\downarrow) = 0.41 \quad (6)$$

in comparison to the rough value of 0.33 obtained previously.[6]

The discrepancy between (4) and (6) suggested[9] models (b) and (c). In (b), $n(s\downarrow)$ is reduced compared to (a) because of increased s-d repulsion. Calculation shows[9] that (4) is satisfied for

$$E_g = E(L_{2'}\downarrow) - E(L_3\downarrow) \leq 0.8 \text{ eV} \quad (7)$$

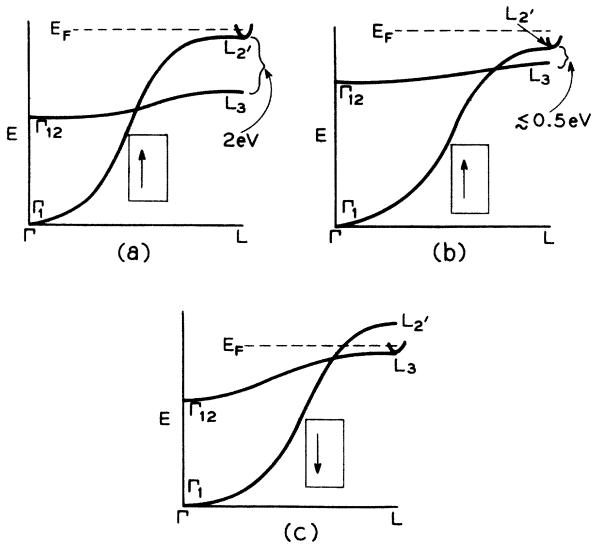

FIG. 1. Alternative models for the band structure of ferromagnetic Ni, with special reference to the neck found in galvanomagnetic experiments. For the sake of clarity only the s-p band $\Gamma_1 L_{2'}$ and one twofold degenerate d band $\Gamma_{12} L_3$ are sketched. The neck is denoted by the U in each figure. The boxed arrows indicate spin direction; the unpaired electron spins are $\downarrow$.

which is two times smaller than that proposed in model (a). On the other hand, the neck may actually occur in the $d\downarrow$ band, model (c), with E_F just above $L_3\downarrow$. The masses quoted in the preceding Letter are an order of magnitude smaller than those found in the d band.[9] We discard (c) and focus our attention on (b).

Near $\vec{L}$, we expand $E(k)$ in powers of $\vec{k}-\vec{L}$. Because E_g is comparable to $E_f = E_F - E(L_{2'})$, the expansion takes the form

$$E(\vec{k}') - E(L_{2'}) + h^2 k_l^2/2m_l - \gamma(h^2 k_t^2/2m) = (E_g/2)\{[1 + (2/E_g)(1/m_t - \gamma/m)k_t^2]^{1/2} - 1\} \quad (8)$$

where k_l and k_t denote the components of $\vec{k}-\vec{L}$ parallel and perpendicular to $\vec{L}$. The factor $\gamma \simeq 1.7$ includes the effect of the lower L_3 state.[9]

Calculations of the curvature of the one-electron energy bands of Cu (see Figs. 4 and 8 of reference 7) and Ni[10] along Λ near $L_{2'}$ give $m_l/m = 0.23 \pm 0.03$ for both crystals. Precision measurements[11] of the angular variation of the neck mass in Cu (similar to those reported for the neck area of Ni in the preceding Letter) can be fitted with $m_l/m = 0.27 \pm 0.02$ in (8), in good agreement with the one-electron value. The large value $m_l/m = 0.66 \pm 0.1$ obtained in the preceding Letter is therefore noteworthy.

In normal metals such as Na or Cu m^*/m often exceeds the one-electron value by 10-20%. Many-electron corrections might thus be represented phenomenologically by a correction β to the one-electron masses:

$$m/m^+ = (1-\beta)\{1 + (\text{interband terms})\} \quad (9)$$

with $\beta \simeq 0.1 - 0.2$ in Cu.[7] The chief difference between Cu and Ni is the high density of states at E_F in Ni due to the partially filled d band. The value of β required to explain the observed value of m_l in Ni is

$$\beta_l \simeq 0.65 \pm 0.1. \quad (10)$$

The large increase in β from Cu to Ni is probably caused by correlation of $d\uparrow$ electrons with $\downarrow$ conduction band electrons near $L_{2'}$.

The one-electron transverse mass is given by

$$m/m_t(k_t) - \gamma = (\lambda/E_g)[1/\alpha(k_t)], \quad (11)$$

$$\lambda = (2/m)|\langle L_3|p_t|L_{2'}\rangle|^2. \quad (12)$$

The factor $\alpha(k_t)$ represents the nonparabolic corrections associated with fourth and higher order terms in k_t; $\alpha(0) = 1$.

We have found that the interband energy λ is quite small because it involves wave functions from different shells ($3d$ and $4p$). It is also sensitive to the radius of the d shell, which depends on E_g. Over the range of interest we find that λ depends linearly on E_g in three band calculations for Cu[7,10] and two for Ni[10]. The results are shown in Table I. From this table and (11), we find that in the one-electron approximation

$$E_g = 1.3 \text{ eV}. \quad (13)$$

This result is suspect, however, for many-electron effects on m_t should be comparable to those for m_l. Assuming $\beta_t = \beta_l$ as given by (10) we find

Table I. The interband energy numerator λ as a function of E_g for several "muffin-tin" potentials representing Cu and Ni.

Reference	Element	E_g (eV)	λ (eV)
7	Cu	1.8	1.6
7	Cu	1.6	1.7
10	Cu	1.2	2.7
10	Ni	0.29	5.0
10	Ni	0.15	5.0

that the one-electron value of m_t/m at E_F is 0.11. From (11) and Table I we obtain a many-electron estimate for E_g,

$$E_g = 0.5 \text{ eV}. \tag{14}$$

The agreement of (7) and (14) confirms our approximation $\beta_t = \beta_l$.

We can use the neck diameter and transverse mass reported in the preceding Letter to obtain

$$E_f = E_F - E(L_{2'}\downarrow) = 0.13 \text{ eV}. \tag{15}$$

From the calculated density of states near the top of the d band[12,13] it is known that

$$E_F = E(L_3\downarrow) - 0.05 \text{ eV}. \tag{16}$$

From (14) through (16) we obtain

$$\Delta E_d = 0.7 \text{ eV}. \tag{17}$$

To estimate the exchange splitting ΔE_c of the conduction band, we note that the interband optical edge[6] and Faraday resonance[14] at 0.3 eV must be associated[9] with the conical interband energy surface in the $\downarrow$ bands with apex at L defined by

$$E_c(\vec{k}) - E_d(\vec{k}) = E(L_{2'}\downarrow) - E(L_3\downarrow) = 0.3 \text{ eV}. \tag{18}$$

From (15), (16), and (18) we find

$$\Delta E_c = 0.5 \text{ eV}. \tag{19}$$

The magnitude of band exchange splittings has been a matter of controversy since Slater's original paper[12] on Ni. From free-atom spectroscopic data he estimated an intra-atomic exchange integral $J_{mm'} = 0.85$ eV between d states of different azimuthal quantum number m. The exchange splitting is then

$$\Delta E_d = 0.6 J_{mm'} = 0.5 \text{ eV}. \tag{20}$$

which agrees quite well with our value (17). This was to be expected, since Slater showed that (20) yields approximately the correct ferromagnetic ordering energy as inferred from the Curie temperature.

Van Vleck has criticized[15] Slater's estimate of ΔE_d on the ground that the quenching of orbital angular momentum in the crystal means that J should be a weighted average of $J_{mm'}$ and J_{mm}, the latter being a Coulomb energy, which Van Vleck estimates to be 7.6 eV. This "strong intra-atomic interaction" picture has recently been taken up by Hubbard[16] and Kanamori[17] who propose a renormalized exchange interaction of order half to one d band widths (2-4 eV in Ni).

The energy bands of Ni have been calculated[10] using a Thomas-Fermi-Slater exchange potential associated with 4.8 $d\downarrow$ electrons and 4.2 $d\uparrow$ electrons. The results are $\Delta E_d = 1.0$ eV, $\Delta E_c = 0.3$ eV. The local exchange potential overestimates the former and underestimates the latter, as expected.

In conclusion the exchange splittings estimated here support the one-electron band model and reject the strong intra-atomic interaction model.[15-17] On the other hand, the large correlation effect on m_l shows that an adequate description of the magnetic transition must include many-electron effects.

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