tion. Another consequence of the quadrupole ordering is that it significantly increases the magnetic-ordering temperatures of the pnictides. When we extend this model to DyP, DyAs, and HoP, we can explain the appearance of flopside spin structures.

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Spin Polarization of Photoelectrons from Nickel

Neville V. Smith and Morton M. Traum
Bell Laboratories, Murray Hill, New Jersey 07974
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The photoelectron spin polarization in Ni has been estimated numerically using an interpolated band structure and assuming direct optical transitions. In the experimental energy range of Bänninger *et al.*, agreement is obtained for the sign but not the magnitude of the polarization. Detailed predictions for the polarization as a function of both electron energy and photon energy are also presented and display striking variations.

A series of experiments by Bänninger, Busch, Campagna, and Siegmann[1] has revealed that the electron spin polarization (ESP) of photoelectrons emitted from Ni at photon energies just above threshold is positive in sign. A similar result has been obtained on Co and Fe.[2] This is somewhat surprising since the electrons have originated from close to the Fermi level where, on the basis of a Stoner-Wohlfarth-Slater band model, one expects the ESP to be negative (at least for Ni and Co). This interpretation, however, hinges upon the assumption that photoemission experiments sense the density of states (DOS). As noted in a paper by Anderson,[3] the conclusion may be reversed if one takes into account momentum conservation during the optical-excitation event. In such a direct transition approach, photo emission experiments sense not the DOS but rather the energy distribution of the joint density of states[4] (EDJDOS) defined by

$$D(\mathcal{E},\hbar\omega)=(2\pi)^{-3}\sum_{f,i}\int'_{\mathrm{BZ}} d^3k\,\delta(\mathcal{E}_f-\mathcal{E}_i-\hbar\omega)\times\delta(\mathcal{E}_i-\mathcal{E}), \quad (1)$$

where $\mathcal{E}_f$ and $\mathcal{E}_i$ are the electron energies in a final band f and an initial band i, and $\hbar\omega$ is the photon energy. The EDJDOS is essentially the density of states over an optical energy surface in k space, and therefore represents a much more restrictive sampling of the Brillouin zone than the ordinary DOS.

We have performed numerical calculations of the EDJDOS for the majority and minority spin bands of ferromagnetic Ni and have used the results to make various estimates of the photoelectron spin polarization (photo-ESP). We find that, in the photon energy range of Bänninger *et al.*,[1] a positive photo-ESP is predicted. Consequently, a positive sign for the experimental photo-ESP cannot, in itself, be construed as a breakdown of the Stoner-Wohlfarth-Slater band approach. (We hasten to add here that our calculations have been performed only for Ni. Anderson[3] points out that in the case of Ni, even a model based on the DOS could produce fortuitously a positive photo-ESP. Co, with its larger exchange splitting, seems to offer a more serious challenge.) Another per-

haps more important result of our calculations is the initial-state energy analysis of the photo-ESP over a wide range of $\mathcal{E}$ and $\hbar\omega$. The striking patterns of variation in the sign of the polarization which occur in the $\mathcal{E}$-$\hbar\omega$ plane, if detectable experimentally,[5] would provide a critical test of the simple band model for Ni.

The numerical calculations of the EDJDOS were performed using a histogram technique described elsewhere.[4] The band structure used was the interpolation scheme of Hodges, Ehrenreich, and Lang.[6] The parameters used in the scheme were the same as those used in earlier calculations by Pierce and Spicer,[7] namely, the b parameters listed by Ehrenreich and Hodges.[8] The quantities $D_\uparrow(\mathcal{E},\hbar\omega)$ and $D_\downarrow(\mathcal{E},\hbar\omega)$ are the respective EDJDOS functions for the majority- and minority-spin band structures, calculated in photon energy and initial-state energy intervals of 0.1 eV by sampling each band structure at a total of 375 000 points in the $\frac{1}{48}$ irreducible wedge of the Brillouin zone.

The various estimates of the photo-ESP were made by evaluating the function

$$p(\hbar\omega) = (J_\uparrow - J_\downarrow)/(J_\uparrow + J_\downarrow). \tag{2}$$

The partial yields $J_\uparrow$ and $J_\downarrow$ are defined by

$$J_{\uparrow,\downarrow} = \int_{\mathcal{E}_l}^{\mathcal{E}_u} T(\mathcal{E}) D_{\downarrow,\uparrow}(\mathcal{E},\hbar\omega)\, d\mathcal{E}, \tag{3}$$

where $T(\mathcal{E})$ is some sort of overall escape function.[9] The first estimates, illustrated in Fig. 1, are intended to simulate the actual conditions of the experiments of Bänninger *et al.*[1] The work function Φ was set equal to 4.7 eV. The upper limit $\mathcal{E}_u$ was set equal to the Fermi energy E_F, and the lower limit $\mathcal{E}_l$ was set equal to $E_F + \Phi - \hbar\omega$. Letting $T(\mathcal{E})$ equal a constant, we obtained curve a. Letting $T(\mathcal{E})$ equal the semiclassical threshold function[9] with an effective well depth of 13.5 eV, we obtained curve b. For $\hbar\omega$ just a few tenths of an eV above threshold we note that p tends to +100% for both curves a and b. This is of the correct sign but is far greater than the experimental value of +15%.

The inclusion of the semiclassical form for $T(\mathcal{E})$ does not change the qualitative shape of $p(\hbar\omega)$. Its main effect is to remove the negative excursion shown by curve a between $\hbar\omega = 6.1$ and 6.7 eV. For photon energies within about 0.1 eV of threshold $p(\hbar\omega)$ makes a dramatic reversal in sign. The existence of this feature is rather sensitive to the choice of Φ, E_F, and specific band model.

In the remainder of this note we discuss the sort of effects which might be observable if the experiments could be refined to the point where an energy analysis of the photoelectrons becomes possible. In Fig. 2 we show the variations of $p(\hbar\omega)$ for two arbitrarily chosen energy "windows" of width 0.5 eV. Curve a was obtained by setting $\mathcal{E}_u = E_F$ and $\mathcal{E}_l = E_F - 0.5$ eV. One envisages here an experiment where the slower electrons are rejected. It is assumed also that, where necessary, the work function can be lowered at will. Experimentally, one might achieve this by cesiation. Curve b shows the variation of $p(\hbar\omega)$ for another window obtained by setting $\mathcal{E}_u = E_F - 1.5$ eV and $\mathcal{E}_l = E_F - 2.0$ eV. $T(\mathcal{E})$ was taken to be constant in both curves. We merely comment here that if the assumptions of the simple band model

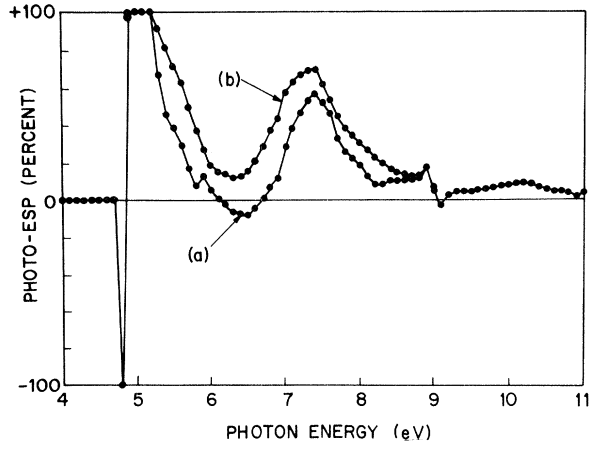

FIG. 1. Influence of threshold on the photo-ESP function $p(\hbar\omega)$ for $\Phi = 4.7$ eV, $\mathcal{E}_u = E_F$, and $\mathcal{E}_l = E_F + \Phi - \hbar\omega$: (a) with $T(\mathcal{E})$ a constant; (b) with $T(\mathcal{E})$ the semiclassical threshold function (Ref. 9).

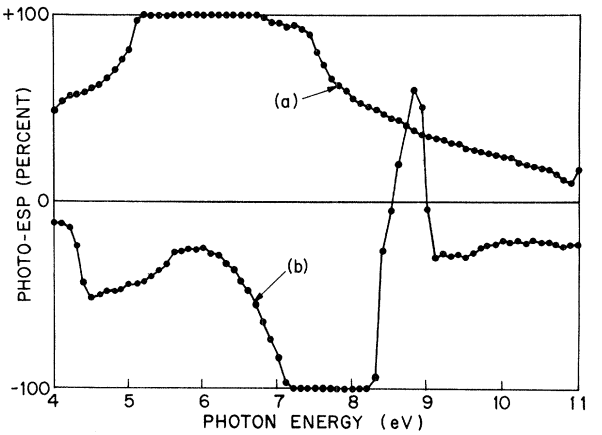

FIG. 2. Effect of energy discrimination on the photo-ESP function $p(\hbar\omega)$: (a) $\mathcal{E}_u = E_F$ and $\mathcal{E}_l = E_F - 0.5$ eV; (b) $\mathcal{E}_u = E_F - 1.5$ eV and $\mathcal{E}_l = E_F - 2.0$ eV.

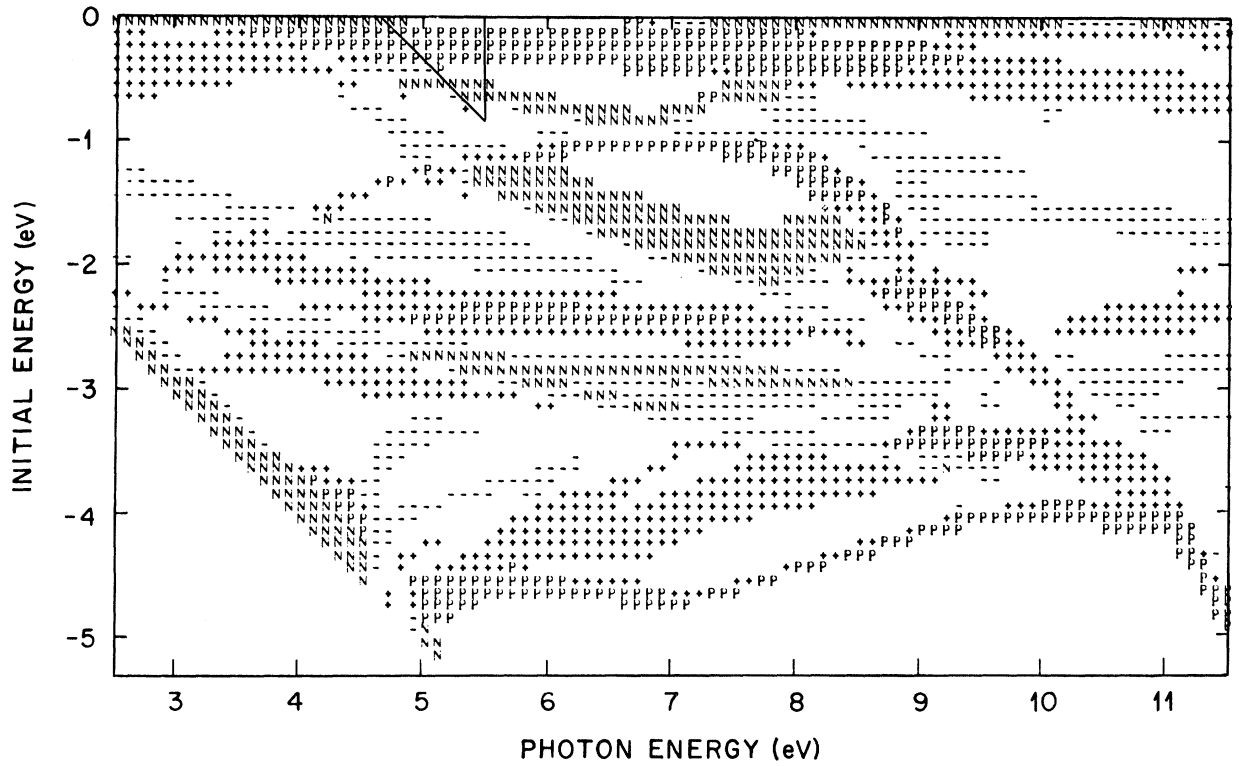

FIG. 3. Contour map of energy-discriminated photo-ESP function $p_0(\mathcal{E},\hbar\omega)$ evaluated in 0.1-eV initial-state and photon-energy intervals. The ranges $100\% > p_0 > 75\%$, $75\% > p_0 > 25\%$, $-25\% > p_0 > -75\%$, and $-75\% > p_0 > -100\%$ are denoted by P, $+$, $-$, and N, respectively. The triangle encloses the experimental energy range of Bänninger *et al.*, Ref. 1.

and direct transitions are correct, then the photo-ESP should show some spectacular variations with $\mathcal{E}$ and $\hbar\omega$. Also, there should be regions of the $\mathcal{E}$-$\hbar\omega$ plane where $p(\hbar\omega)$ reaches $+100\%$ or -100%.

Finally, we show in Fig. 3 a coarse contour map of the energy-discriminated photo-ESP function. The $\mathcal{E}$ and $\hbar\omega$ scales are divided into histogram intervals 0.1 eV wide, and the function

$$p_0(\mathcal{E},\hbar\omega) = (D_\uparrow - D_\downarrow)/(D_\uparrow + D_\downarrow)$$

is computed for each interval. The symbol P has been inserted into the interval if the function p_0 is large and positive; more specifically, if $75\% < p_0 < 100\%$. The plus symbol denotes $25\% < p_0 < 75\%$; the minus symbol denotes $-75\% < p_0 < -25\%$; and N denotes $-100\% < p_0 < -75\%$, i.e., large negative photo-ESP.

It is recognized that there are other experimental results which indicate that the simple band approach used here may be inapplicable. Pierce and Spicer[7] have reported an absence of any shifts in the photoemission spectra of Ni on varying the temperature, whereas such shifts are predicted by calculations very similar to those presented here. We note also the tunnelling ESP results of Tedrow and Meservey,[10] which indicate a positive ESP within only 1 meV of E_F. Finally, the many-body and renormalization effects indicated by Anderson[3] might be crucial for an understanding of photo-ESP measurements. It is recognized further that our calculations represent a gross oversimplification since we have neglected, among other things, the modifications to the bands due to the presence of a magnetic field and to spin-orbit coupling.[11] We feel however that the numerical results offered here present a useful starting prediction against which future experiments can be compared. Measurements at higher $\hbar\omega$ and as a function of $\mathcal{E}$ would be very desirable. If such experiments show no indication of the dramatic effects illustrated here, this might indeed be a serious blow for the Stoner-Wohlfarth-Slater band theory.

At the time of submission it has come to our attention that Wohlfarth[12] has also shown (using an interpretation based on the DOS) that the currently available photo-ESP data are not necessarily

incompatible with a simple band model.

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Projectile Polarization in the Coulomb Breakup of ^{6}Li

D. L. Disdier,* G. C. Ball, and O. Häusser
Atomic Energy of Canada Limited, Chalk River Nuclear Laboratories, Chalk River, Ontario, Canada

and

R. E. Warner†‡
Oberlin College, Oberlin, Ohio 44074

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The reaction ^{208}Pb(^{6}Li, αd)^{208}Pb was studied at $E_{^6\mathrm{Li}}$ = 24 and 27 MeV by observing d-α coincidences for particles emitted into the same solid angle. At $E_{^6\mathrm{Li}}$ = 24 MeV the reaction proceeds predominantly by a sequential process of Coulomb excitation of the 2.184-MeV, $J^\pi = 3^+$ state, followed by breakup into α and d. When the strong dipole polarization of the ^{6}Li projectile is taken into account, a $B(E2; 1^+ \rightarrow 3^+) = 24e^2$ fm^4 is found, in good agreement with a recent (e, e') experiment.

In a recent study[1] of the reaction ^{208}Pb(^{6}Li, αd)^{208}Pb, α particles were observed in singles spectra for incident energies between $E_{^6\mathrm{Li}}$ = 20 and 26 MeV. In an attempt to interpret the α spectra as arising from Coulomb excitation of the unbound $J^\pi = 3^+$ level at 2.184 in ^{6}Li, the following difficulties were encountered: (1) The shapes of the α-particle angular distributions were in disagreement with those calculated from first-order Coulomb excitation theory; (2) the derived $B(E2; 1^+ \rightarrow 3^+)$ disagreed by factors of between 2.4 (at $E_{^6\mathrm{Li}}$ = 20 MeV) and 5 (at $E_{^6\mathrm{Li}}$ = 26 MeV) with recent accurate measurements using the reactions ^{6}Li(e, e')[2] and ^{4}He(d, γ)[3] which yield[2] $B(E2; 1^+ \rightarrow 3^+) = (25.6 \pm 1.6)e^2$ fm^4. The authors of Ref. 1 concluded "that some assumptions underlying the present theory of Coulomb breakup may not be justified." Subsequently Wittern[4] suggested that the discrepancy may be explained by the inclusion of nuclear forces.

In the present work a novel α-d coincidence technique has been used to investigate the mechanism for the dissociation of ^{6}Li in the electric field of a heavy nucleus. The cross sections found are consistent with a two-step process for the dissociation of ^{6}Li and in disagreement with the conclusions of Ref. 1. Furthermore, conventional Coulomb excitation theory[5,6] gives an adequate description of the results provided nuclear polarizability[7] is taken into account.

A 0.9-mg/cm^2 thick target, enriched to 99.1% in ^{208}Pb, was bombarded with the ^{6}Li^{3+} beam from the Chalk River Laboratory's model MP tandem accelerator at $E_{^6\mathrm{Li}}$ = 24 and 27 MeV. Since ^{6}Li in its 2.184-MeV state is only 0.71 MeV above the α+d dissociation threshold, these particles emerge in a narrow cone ($\theta_{\mathrm{lab}} \leq 30°$). Coincidences between deuterons and α particles emitted into the same solid angle were detected in a ΔE_1-ΔE_2-E counter telescope. The ΔE_1 counters used were thick enough to stop all α particles emitted near 180° in the ^{6}Li rest frame, while the ΔE_2 and E counters provided particle identification for the longer range deuterons. Two such telescopes were used to obtain data at angles of 90°, 110°, 130°, and 150° for $E_{^6\mathrm{Li}}$ = 27 MeV and at 90°