unambiguous evidence for sizable high- (fifth-) rank superexchange terms as predicted theoretically by Levy, and Elliott and Thorpe. It is apparent that such terms are by no means unique to the Ce^{3+} ion and must be anticipated in most situations where the magnetic moment contains an appreciable orbital contribution.

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*National Research Council of Canada Postdoctoral Fellow. Present address: Bell Telephone Laboratories, Murray Hill, N. J.

†Present address: University of California, Los Angeles, Calif.

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NEW PHOTOEMISSION STUDIES OF THE *d* BANDS OF NICKEL AND COPPER

D. E. Eastman
IBM Watson Research Center, Yorktown Heights, New York

and

W. F. Krolikowski*
Stanford University, Stanford, California, and IBM Components Division, East Fishkill, New York

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New photoemission studies of the optical density of states of nickel and copper are reported. In contrast to other earlier measurements, both Ni and Cu have a sharp maximum at the top of the *d* band. The *d*-band optical density of states of Ni and Cu are consistent with a simple rigid-band model: The exchange splitting of Ni is estimated as $\delta E_{ex} \simeq 0.4 \pm 0.2$ eV.

Previous photoemission studies[1-3] of the optical density of states of Ni have found an anomalously strong peak at 4.5 eV below the Fermi level E_F. The observation of this strong peak is contrary to all one-electron band calculations (which are becoming increasingly successful in explaining numerous properties[4,5] of Ni). The conclusion was that a rigid-band model was not valid for the *d*-band optical density of states of Ni and Cu.

We report new photoemission results for Ni and Cu which differ from those previously published.[1,3,6,7] The most striking results of the new measurements are (1) the observation of a sharp maximum in the density of states at the top of the filled *d* band for both metals (for Ni at E_F and for Cu ~2 eV below E_F) and (2) a large reduction in the amplitude of the above-mentioned 4.5 eV peak in Ni. We find good agreement between our *d*-band optical density of states of Ni and Cu using a simple rigid band model with an exchange splitting of 0.4 ± 0.2 eV for Ni. In contrast to previous photoemission results, we find general agreement with one-electron band calculations. In particular, we observe good agreement between the optical density of states of Ni and the one-electron band calculations of Hodges, Ehrenreich, and Lang,[4] who determined an exchange splitting of 0.37 eV at E_F. The previously reported[1-3] anomalous peak 4.5

eV below E_F for Ni was found by us to be sensitive to surface conditions and, under clean surface conditions, to have a much lower amplitude.

Photoemission was measured in the 5- to 11.6-eV range using experimental techniques similar to those described by Spicer and co-workers.[2,8] An ac synchronous detection system with a cylindrical retarding collector was used. For Ni, a gold-plated spherical mesh collector was also used and gave somewhat improved energy resolution but otherwise identical results.

Ni films were prepared by evaporation onto smooth substrates using 99.999% pure Ni metal and an electron-beam gun in an ultrahigh-vacuum system. Ni, Au, and quartz substrates yielded identical results. The pressure rose from a base of $\sim 7\times10^{-11}$ Torr to $\sim 5\times10^{-9}$ during evaporation and then fell rapidly to $\sim 2\times10^{-10}$ immediately after evaporation. X-ray and electron diffraction measurements indicated polycrystalline fcc Ni with ~100- to 150-Å grain size. Cu films were prepared by evaporation onto smooth Cu substrates in an ultrahigh-vacuum system; pressures of $\sim 2\times10^{-9}$ were maintained during and after evaporation.[9] The effect of surface contamination was studied by varying the pressure during and after the film evaporation. For Cu, films prepared at $\sim 5\times10^{-8}$ initially resembled those prepared in better vacuum. Within an hour, however, a large peak of slow electrons appeared, the quantum yield increased, and a general smearing of structure occurred. The vacuum conditions were less critical for Ni. For example, an air leak of $\sim 1\times10^{-7}$ did not significantly distort the data at room temperature over a period of hours. However, short exposures to higher pressures strongly enhanced the above-mentioned distortion effects.

Measured energy distribution curves (EDC's) for Ni and Cu films are shown in Fig. 1(a) for a 10.2-eV photon energy. As the photon energy was varied in the 6- to 11.6-eV range, the structure in the curves remained stationary in initial-state energy E_i while smoothly changing amplitude. This observation indicates valence-band structure, a smooth density of states in the conduction band, and the dominance of nondirect transitions.[2,6] In this case the measured curves directly reflect structure in the optical density of states of the valence band.

Optical density-of-states curves for Ni and Cu, shown in Fig. 1(b), have been derived using the nondirect transition model,[2] in which transition probabilities are taken proportional to the product of the initial and final state densities. The occupied valence-band region below E_F follows directly from a set of energy distribution curves taken at various photon energies. Constant matrix elements are assumed. The dashed portions of the valence-band curves in Fig. 1(b) are less reliable than the solid portions because of scattering effects. The dashed portion of the valence band curve for Cu below −5.5 eV was deduced from cesiated Cu data[6] (which showed strong scattering effects). The empty conduction band shown for Ni consists of a 0.5-eV wide d-state region at E_F plus a simple parabolic band and is plausibly based on one-electron band considerations. The optical conductivity of Ni has been calculated using the nondirect transition model[2,6] and is in good agreement with the measured optical conductivity.[10]

The valence band of Ni [Fig. 1(b)] consists of a

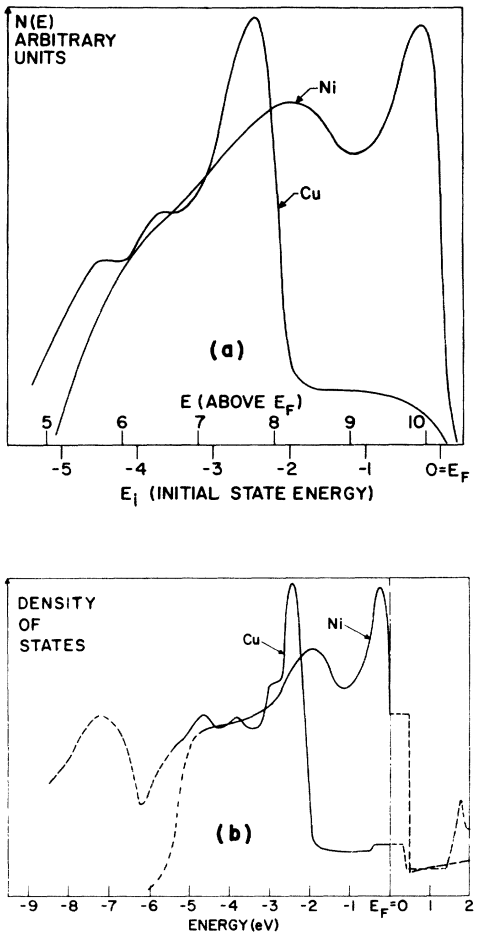

FIG. 1. (a) Energy distribution curves of Ni and Cu at $h\nu = 10.2$ eV. $E_i = E - h\nu$. (b) Optical density of states of Ni and Cu.

high-density d band extending from E_F to about −5.5 eV, with a sharp dominant peak at −0.2 eV, a second broader peak ~1.7 eV lower, and a third weaker peak ~4.5 eV below E_F. While the location of all structure previously reported is consistent in energy with that of Fig. 1(b), the amplitudes are extremely different. In the earlier work, the peak at −4.5 eV was dominant and the other two peaks were much less resolved. We have found the peak at −4.5 eV to be increased by air exposure as previously mentioned. EDC's very similar to those previously reported[1-3] could be produced by short exposures to low vacuum (~10^{-6} Torr). Also, a monolayer of yttrium, which lowered the work function from 5.2 to ~3 eV, strongly enhanced the −4.5-eV peak. From these studies we conclude that the large number of slow electrons in the −4.5-eV peak previously reported[1-3] probably resulted from surface effects. Surface conditions are important because the electron escape depths are very short. Energy distribution curves taken as a function of Ni film thickness for very thin Ni films (~3 to 100 Å) evaporated onto clean gold substrates indicate electron scattering lengths $L(E)$ ~ 5-15 Å for Ni for energies greater than ~7 eV above E_F.[11]

For Cu, it is seen from Fig. 1(b) that the d band extends from a dominant peak at the top of the d band ~2eV below E_F to ~8.0 eV below E_F. The low-density s-p derived band between E_F and −2 eV and the location of the top of the d band at ~−2 eV are in good agreement with the previous results.[6]

The Cu d-band density of states in Fig. 1(b) and a simple rigid-band model for the paramagnetic d bands of Ni and Cu have been used to predict a Ni density of states.[12] Results are shown in Fig. 2. The measured optical density of states of Ni and density of states derived from Cu show good agreement, especially within 3 eV of the Fermi level. The dashed portion of the Cu-derived curve, i.e., the peak at −5 eV, is less reliable because it was deduced from data on cesiated Cu.[6] The optical density of states for Ni derived from Cu data was determined by first placing 0.55 electron holes[4] in the minority-spin band (taken as a direct replica of the Cu d band), to agree with the magnetization. This places E_F ~0.4 eV below the top of the minority-spin d band. Then, the majority-spin d band was shifted downwards in energy by an exchange splitting $\delta E_{ex} = 0.4$ eV for best agreement with the measured Ni results. Estimated bounds on δE_{ex} are

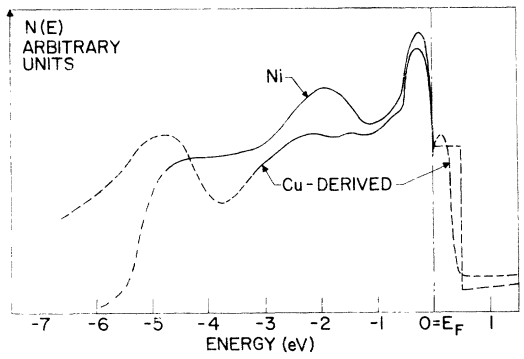

FIG. 2. Comparison of Ni optical density of states with Cu-derived optical density of states for Ni using rigid-band model with $\delta E_{ex} = 0.4$ eV.

$0.2 \lesssim E_{ex} \lesssim 0.6$ eV. The upper bound is well established because a doublet will appear just below E_F for larger splitting. For $\delta E_{ex} \lesssim 0.2$ eV, holes appear in the majority-spin band and the assumption of 0.55 spin-oriented holes becomes inconsistent, even considering smearing due to the experimental resolution (0.15 eV).

The experimentally derived splitting is in good agreement with the conclusion of Phillips (0.5 ± 0.1 eV) in a recent survey paper[13] and with the pseudopotential band calculation of Hodges, Ehrenreich, and Lang[4] ($\delta E_{ex} = 0.37$ eV at E_F, average splitting = 0.29 eV). The experimentally derived splitting is about $\frac{1}{2}$ the values determined by Wakoh and Yamashita (0.72 eV) using a Green's-function method[14] and Connolly (0.95 eV) in a self-consistent augmented-plane-wave band calculation.[5] We find good agreement between the optical density of states of Ni and the results of Hodges, Ehrenreich, and Lang[4] [see Fig. 3(a)]. We find disagreement between the measured results and the results of Wakoh and Yamashita[14] and Connolly.[5] As an example, we compare the optical density of states of Ni with the results of Connolly in Fig. 3(b). For both of the latter calculations, good agreement with the measured results can be obtained by reducing the exchange splitting to ~0.4 eV. To show this, we have taken the spin-up and spin-down density-of-states curves of Connolly,[5] and by treating the exchange splitting as an adjustable parameter,[15] have reduced the exchange splitting from 0.95 to 0.4 eV. The total density of states which results is shown in Fig. 3(b) (broken line) and is seen to be in good agreement with the measured optical density of states. The conclusion is that the modified free electron Slater exchange potential used by Connolly[5] overestimates the exchange

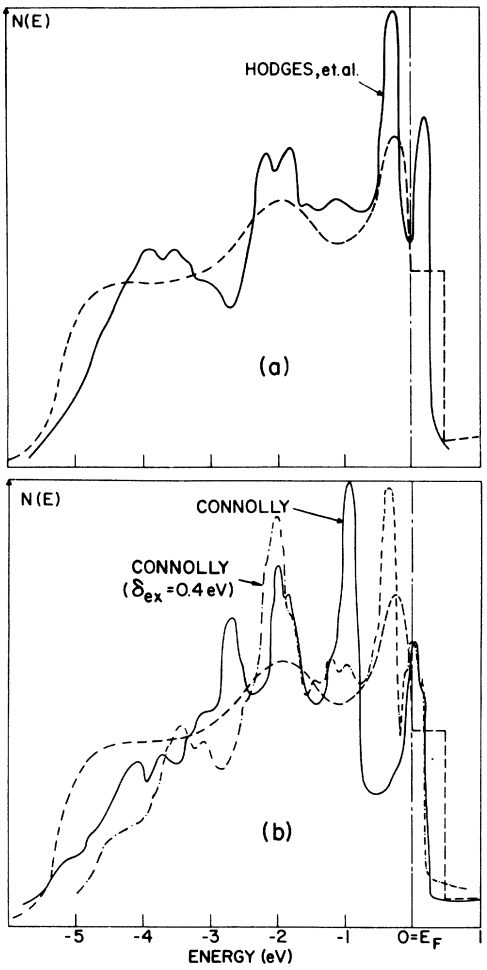

FIG. 3. Comparison of Ni optical density of states with band-calculation results of (a) Hodges, Ehrenreich, and Lang (Ref. 4) and of (b) Connolly (Ref. 5). In (b) the density of states resulting from Connolly's d bands with δE_{ex} reduced to 0.4 eV is also shown (broken line).

splitting in Ni. We note that the exchange splitting is not strictly rigid but is a function of energy in the band calculations of Hodges, Ehrenreich, and Lang[4] and Connolly.[5] However, the energy dependence of the splitting is small and is much less than the average splitting. Consequently, a rigid exchange splitting for the majority and minority spin bands of Ni is a good first-order approximation. This is shown by the majority and minority spin band density-of-states curves both in Fig. 12 in Ref. 4 and in Fig. 5 in Ref. 5.

Comparison of the Ni optical density of states in Fig. 1(b) with soft x-ray emission studies[16] and ion-neutralization studies[17] shows general agreement, although much sharper resolution is seen in the photoemission results.

In conclusion, we find that our optical density-of-states measurements for Ni and Cu are in general agreement with one-electron band calculations and can be related via a simple rigid-band model in a manner which is consistent with the itinerant electron band picture of ferromagnetic Ni.

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THREE-BODY CALCULATION OF DEUTERON-ALPHA SCATTERING AND POLARIZATION*

Paul E. Shanley
Department of Physics, University of California, Davis, California
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Three-body calculations using separable two-body interactions have been carried out for the deuteron-alpha system with the alpha particle assumed to be structureless. Phase shifts, angular distributions, and polarization have been calculated and found to be in substantial agreement with experiment.

Several recent studies[1] of the bound state and scattering properties of the three-nucleon system have shown that the major features of this system may be described by quite simple separable interactions if three-particle effects are treated exactly. There is considerable interest in applying these methods to problems involving complex nuclei, for example, the system neutron-proton-nucleus and, in fact, several model calculations employing s-wave two-body forces have been reported.[2-4] The aim of the present work is to apply these methods to the deuteron-alpha system,[5] considered as a three-body problem, and to compare the results with the wealth of experimental data that is available. In our approach the alpha particle must be treated as an elementary point particle with no internal structure. This assumption seems quite reasonable for this nucleus due to the compactness of the alpha particle and due to its large binding energy and lack of low-energy excited states.

We study the d-α system in terms of Amado's[6] formulation of the three-body problem generalized to include spin-dependent interactions. In this formulation two-body pair interactions are thought to proceed through a quasiparticle, or equivalently,[7] through a separable potential. In the neutron-proton system we introduce an s-wave interaction with parameters chosen[8] to fit the deuteron binding energy and the triplet scattering length. In the nucleon-alpha two-body subsystems we neglect Coulomb interactions and allow the neutron and proton to have the same interaction with the alpha particle. Studies[9] of neutron-alpha scattering below 10 MeV show that it is nonabsorptive and that only the partial waves $s_{1/2}$, $p_{3/2}$, and $p_{1/2}$ contribute significantly, with the scattering dominated by a $p_{3/2}$ resonance at 1.2 MeV. A separable interaction is introduced for each of these three partial waves with the parameters chosen to fit an effective-range analysis of low-energy n-α scattering carried out by Pearce and Swan.[10] The form factor in each partial wave is chosen to be

$$v(k)=k^{l}/(k^{2}+\beta^{2})^{l+1}, \tag{1}$$

which gives two parameters per interaction, a coupling constant and the range parameter β. The s-wave nucleon-alpha potential is made repulsive in an effort to simulate the effect of the exclusion principle in the interaction of a nucleon with a doubly closed-shell nucleus.

In order to study d-α scattering, one writes a set of coupled integral equations for the amplitudes describing the processes $d+\alpha \rightarrow$ correlated pair + third particle, where the correlated pair may be the deuteron or any of the three quasiparticles coupled to nucleon plus alpha. The final state, so described, is said to be a channel. We write the integral equations in an L-S representation and after partial-wave analysis they have the form

$$T_{\alpha\alpha'}^{(J)}(k,k';E)=B_{\alpha\alpha'}^{(J)}(k,k';E)+1/[(2\pi)^{3}]\sum_{\alpha''}\int_{0}^{\infty}n^{2}dn\,T_{\alpha\alpha''}^{(J)}(k,n;E)\tau_{\alpha''}(n;E)B_{\alpha''\alpha'}^{(J)}(n,k';E), \tag{2}$$