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[8]In Fig. 1 the upper two curves present the results for samples which are under just enough stress to insure good electrical contact. We estimate the resultant strain to be of the order of 10^{-5} to 10^{-6}.

[9]A similar conclusion has been inferred for OH^- by Lombardo and Pohl from their electrocaloric measurements of Li-doped alkali halides. G. Lombardo and R. O. Pohl, Phys. Rev. Letters 15, 291 (1965).

[10]Although the center of mass undergoes a simple translation, the ion executes a combined rotational-translational motion. For brevity, we will refer to this motion as "translational."

[11]See Ref. 4, p. 252.

[12]It is clear from Fig. 3(c) that the width, with respect to E_z, of the H. E_z band appears broadened by the hyperbolic approach of the lower A_1 states toward each other. The concentration dependence of the band widths and the peak displacement to lower E_z can be accounted for, to within a factor of 2, in terms of random electric fields produced by nearly OH^- ions.

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POSITRON ANNIHILATION AND THE ELECTRONIC STRUCTURE OF RARE-EARTH METALS*

R. W. Williams, T. L. Loucks, and A. R. Mackintosh†

Institute for Atomic Research and Department of Physics, Iowa State University, Ames, Iowa

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We have measured the angular correlation of the photons from two-quantum positron annihilation in single-crystal disks of the rare-earth metals holmium and erbium, and in yttrium, which has a similar crystal and electronic structure. The coincidence distributions in the three metals are similar and highly anistropic, and the qualitative features of the c-axis (0001) results are reproduced by a calculation based on the independent-particle model. In the antiferromagnetic phase, the distribution for the c-axis holmium crystal is modified, and this change is ascribed to the appearance of magnetic superzone energy gaps.

The experiments were carried out with a conventional parallel-slit geometry,[1] using a magnetically focused Co^{58} positron source. The angular resolution of the apparatus was approximately 0.25 mrad. The results for holmium in the paramagnetic phase at room temperature are shown in Fig. 1(a). The b-axis $(10\bar{1}0)$ data do not depart greatly from the parabola corresponding to three free electrons per atom, but the c-axis curve drops sharply at low angles and has a pronounced hump at about 3 mrad. The large anisotropy in the coincidence curves is in accord with the results of recent band-structure calculations on hexagonal close-packed rare-earth metals.[2,3] This anisotropy is clearly manifested by the Fermi surface of holmium calculated using the augmented-plane-wave (APW) method. Sections of this surface are shown in the reduced zone in Fig. 2 and a noteworthy feature is the large, approximately flat electron and hole regions normal to the c axis. These surfaces run parallel to each other over a large region when spin-orbit coupling is taken into account in a relativistic APW calculation,[4] and we propose that their separation primarily determines the Q vector of the periodic magnetically ordered phases. The mixing of states due to the magnetic periodicity would destroy large areas of these surfaces, thus causing the large observed reduction in electrical conductivity in the ordered state.[5]

The structure in the angular distributions for the c-axis crystals indicates that these metals can provide a sensitive test of the independent-particle theory of positron annihilation. We have therefore calculated the angular distribution of photons in yttrium, using the independent-particle model,[6] according to which the number of coincidences at an angle θ is

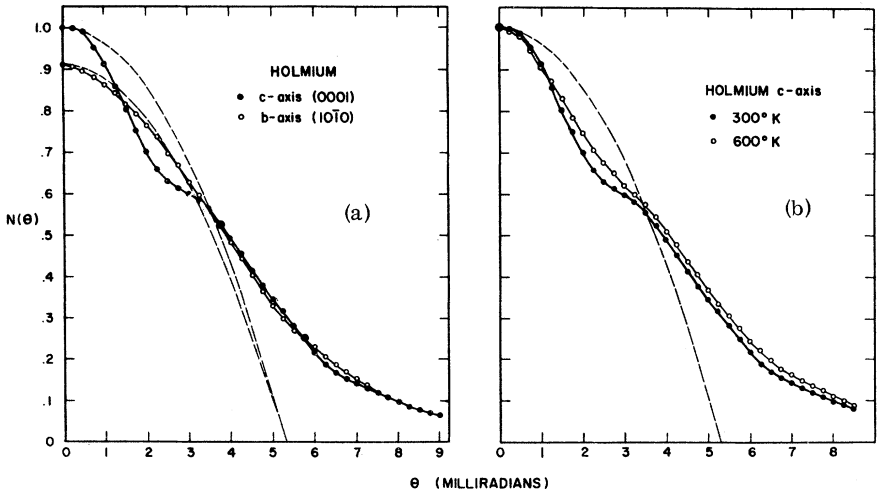

FIG. 1. (a) Photon coincidences as a function of angle in holmium at 300°K. The number of coincidences at the peak is approximately 10^5 for each crystal and the curves are normalized to equal areas. The dashed curves correspond to three free electrons per atom and are fitted at the peaks. (b) The temperature dependence of the coincidence distribution in the c-axis crystal. The peak number of coincidences is again approximately 10^5.

proportional to

$$N(\theta)=N\left(\frac{\hbar p_z}{mc}\right)=\int\int_{-\infty}^{\infty} dp_x dp_y \sum_{\vec{k}} F(\vec{p},\vec{k}), \qquad (1)$$

where the sum is over all occupied states and

$$F(\vec{p},\vec{k})=\left|\int \psi_{\vec{k}}(r)\psi_+(\vec{r})\, e^{-i\vec{p}\cdot\vec{r}} d^3r\right|^2. \qquad (2)$$

The energy eigenvalues for the electrons and the Fermi surface were calculated by the APW method, using a muffin-tin potential with exchange, while the eigenfunctions $\psi_{\vec{k}}(\vec{r})$ were expanded as a linear combination of 22 APW's. The ground-state positron wave function $\psi_+(\vec{r})$ was obtained from a numerical solution of the Schrödinger equation for the same potential,

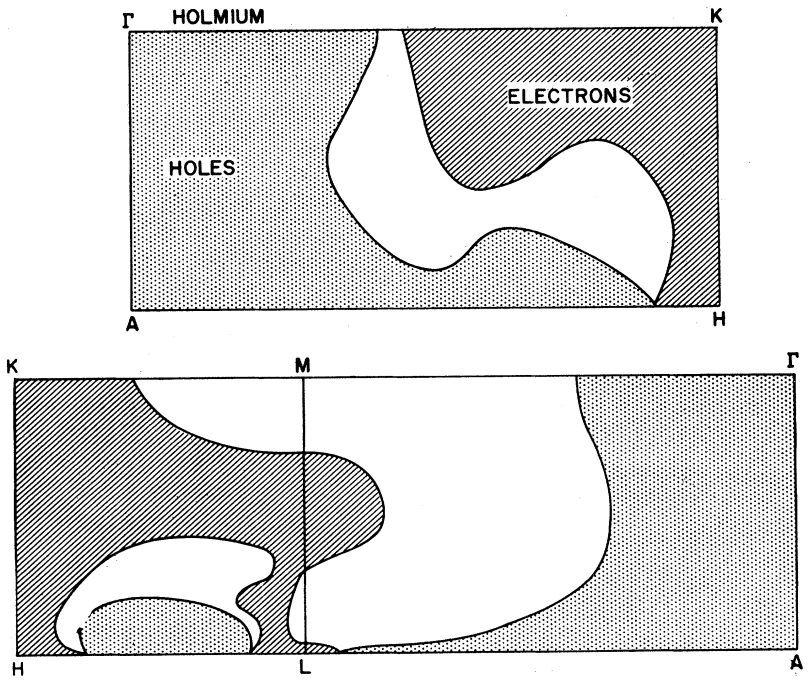

FIG. 2. Intersections of the calculated holmium Fermi surface with the faces of 1/24th of the Brillouin zone.

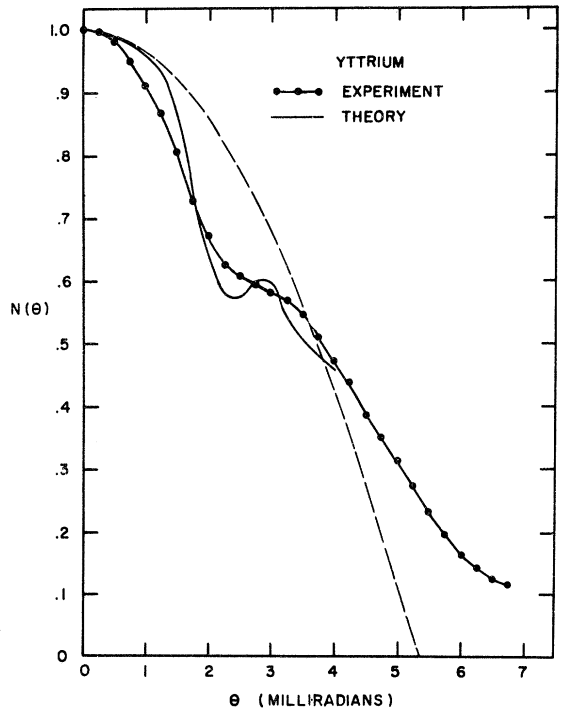

FIG. 3. The calculated and observed coincidence distributions in a c-axis yttrium crystal. The free-electron parabola is also shown. The experimental peak height is approximately 6×10^4 counts. No correction has been made for core annihilation in the experimental curve, but the calculations have been corrected for the experimental resolution.

without exchange. The theory (Fig. 3) reproduces the rapid drop at low angles and the hump, which is a manifestation of the flat d-like bands. The theoretical hump is much more pronounced than that in the experimental results, and we believe this discrepancy to be primarily due to Coulomb correlation in the electron-positron system.

Measurements were also made on the c-axis holmium crystal at 60°K and the results, shown in Fig. 1(b), are significantly different from those at room temperature. The magnetic moments at this temperature form a spiral, and we therefore attribute the change in the results to the modification of the electron distribution by the periodic magnetic order.

The results of this study, therefore, show clearly that the electronic distribution in holmium is highly anisotropic and is substantially modified by the helical ordering of the localized moments. The qualitative agreement between theory and experiment for the c-axis yttrium crystal indicates that the theoretical band structures for these metals are at least qualitatively correct. The Coulomb correlation does not completely eliminate the structure in the photon distribution curves, so that the method is useful for studying the electronic structure of anisotropic metals and alloys. The independent-particle model appears to be a good first approximation but correlation effects probably suppress some of the detailed structure which it predicts. The angular distribution in erbium is very similar to that in holmium, and we are planning further experiments to determine whether the electronic structures of the hcp rare-earth metals are all similar, as commonly supposed, and to examine further the effects of magnetic ordering and Coulomb correlation on the photon distribution.

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