"Enhancement Factor" for Positrons in Sodium*

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Experimental data from positron annihilation in sodium single crystals show (a) that the Fermi surface is spherical and (b) that the momentum dependence of the "enhancement factor" of the polarization of the electron sea by the positron agrees with calculations.

INTRODUCTION

THIS paper describes a series of measurements of the angular correlation of photons resulting from the annihilation of positrons in single crystals of sodium. The sodium samples were in the form of thin disks, the plane faces of which were cut normal to the [100], [110], and [111] directions of the crystal. The measurements are closely related to the areas of slices through the Fermi surface perpendicular to these three directions. Two important results are established:

(1) The Fermi surface of sodium is spherical within the experimental error of 1.5%.

(2) The annihilation probability is velocity-dependent in agreement with the predictions of Ferrell and Kahana.[1,2]

The first of these results has been previously established by the more powerful de Haas–van Alphen[3] and cyclotron-resonance experiments.[4] However, since the interpretation of both of these experiments is complicated by the martensitic transformation which occurs in sodium at about 35°K,[5] the experiments described in this paper constitute a valuable, independent confirmation of these results.

The velocity dependence of the annihilation probability has not previously been observed. Very general arguments based on the exclusion principle predict an increased annihilation rate for electrons near the Fermi surface. The magnitude of this effect, as measured in these experiments, is in good agreement with the calculations of Ferrell and Kahana.[1,2]

EXPERIMENTAL

The measurements were made using the familiar long-slit apparatus.[6,7] A substantial increase in the angular resolution over that of previously reported experiments was achieved by increasing the sample-to-detector distance to 250 in. with detector slits at 0.050 in. The samples were maintained at a temperature of about 100°K during an experiment, thereby reducing the "smearing" effect[8] of the thermal motion of the positrons. A complete discussion of the experimental technique may be found in a recent review by one of the authors.[6]

DISCUSSION OF DATA

The data obtained in these experiments are shown in Fig. 1. Corrections have been made for the decay of the positron source and the areas under smooth curves drawn through the data points have been normalized to the same number of counts. The dashed line shown in the lower curve is the angular correlation curve—appropriately normalized—for MgO, and is expected to have very nearly the same form as the photon distribution arising from annihilations with the core electrons of sodium.[9] It is convenient to subtract this "background" of core annihilations and to plot all the points on one side of the 0° line. The result is shown in Fig. 2.

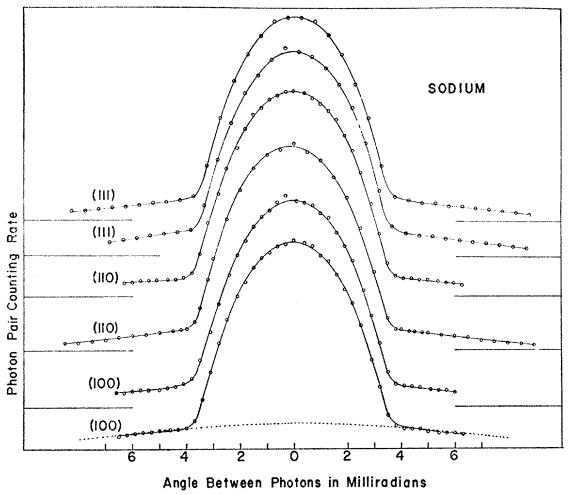

FIG. 1. Angular correlation of photons from positrons annihilating in single crystals of sodium of various orientations.

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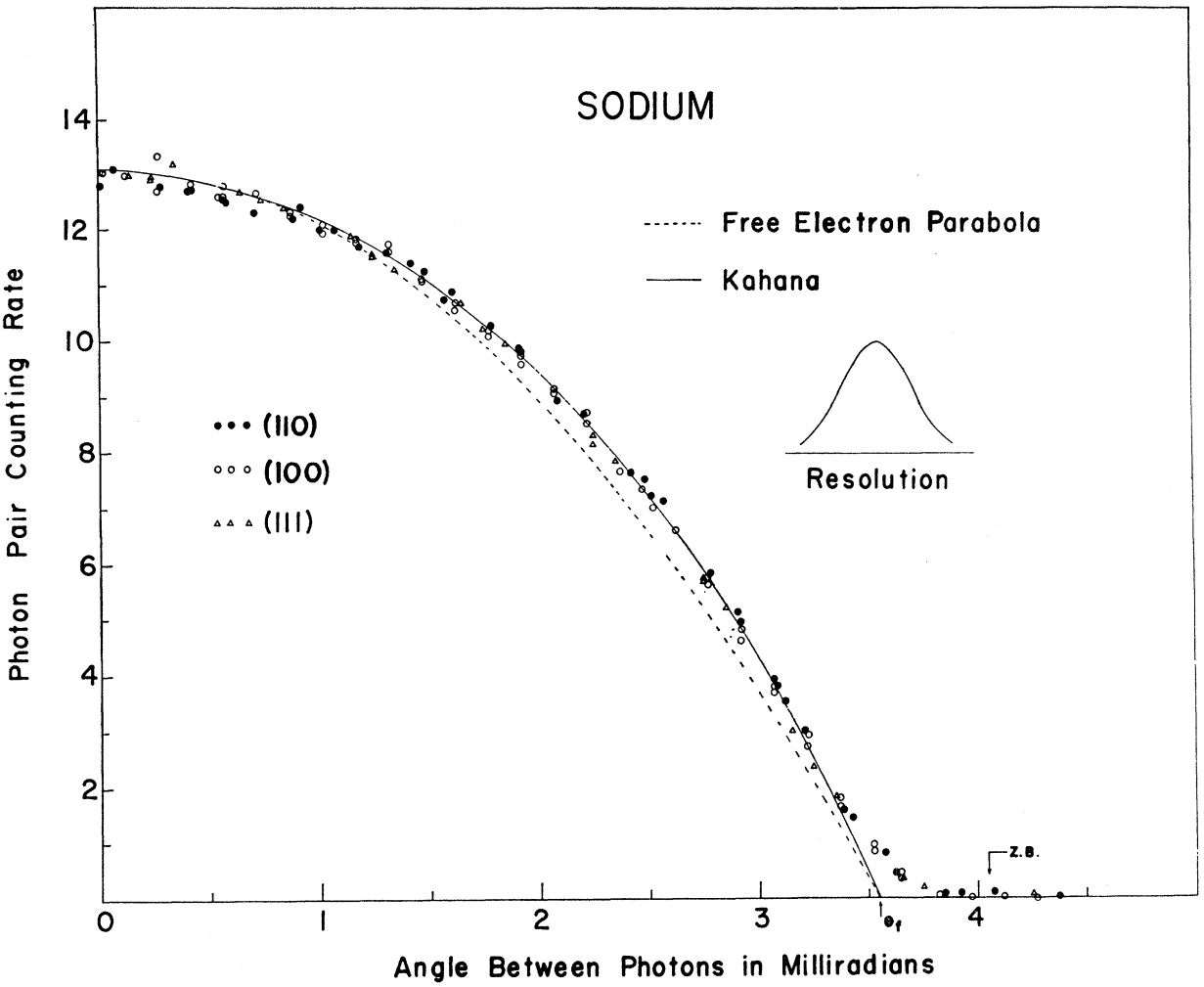

FIG. 2. The data of Fig. 1 with broad part subtracted, and folded about the center. The dashed line is parabola. The solid line is the distribution expected when "enhancement" is taken into account.

The measured distributions for the three principal directions are the same within the expected, statistical fluctuations of the experiment. The smooth curve drawn through the points has the form predicted by Kahana,[2] and is given by

$$I(k_z) = \int_{\gamma_z}^{\infty} \gamma \epsilon(\gamma) d\gamma,$$

where $\gamma_z = k_z/k_f$. The enhancement factor is given by Kahana as

$$\epsilon(\gamma) = a + b\gamma^2 + c\gamma^4.$$

Kahana has calculated values of a, b, and c for several values of r_s, the radius of a sphere which contains one electron. The best fit to our results was obtained by using values of b/a and c/a of 0.30 and 0.27, respectively, which are in good agreement with the values 0.26 and 0.22 obtained from Kahana's paper. If the annihilation probability were independent of velocity, the distribution would be expected to have the parabolic form shown by the dashed line in Fig. 2.

An enhanced annihilation rate was also observed in a similar series of experiments with lithium single crystals.[10] Since the Fermi surface of Li is appreciably anisotropic, the angular correlation curves for the three principal directions were different. Therefore, Kahana's calculation, which assumed a spherical Fermi surface, could not be compared directly with experiment. Using the values of c/a and b/a obtained from Kahana's paper for the atomic radius of lithium [3.23 atomic units (a.u.)], the calculated values of $I(\gamma)$ agreed very well with the "average" counting rate for the three directions.[11,12] The values of c/a and

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[11] This result has also been observed by J. Melngailis and S. DeBenedetti, Phys. Rev. **145**, 400 (1966).

[12] It should be noted that in the previous paper on Li Fermi surface, the enhancement factor for the higher-momentum components (HMC) was taken to be the same as the average for "free-electron" Li. Since the HMC are small for Li, the enhancement-factor problem is not vital. For future experiments this question will be more important and we hope it will be solved soon.

b/a were obtained from Kahana's paper by a smooth extrapolation of his published values of a, b, and c for atomic radii of 2, 3, and 4 a.u. This process yielded values of c/a and b/a of 0.17 and 0.22, respectively, for lithium.

To estimate the accuracy with which the lengths of the radius vectors in the three principal directions could be determined by this experiment, a series of calculations was made using a phenomenological model of the Fermi surface. The model consisted of a sphere of radius r with 12 "bumps" superimposed toward the nearest zone boundaries. The size and shape of the bumps were varied by changing the values of the principal radii. For each set of principal radii, the areas of slices through the model Fermi surface normal to the principal directions were calculated. The distortion of the model was increased until the differences of the calculated areas exceeded the experimental error of the differences in the measured counting rates. In this manner it was concluded that a difference of 1.5% in the radii k_{110} and k_{100} would result in observable differences in the measured counting rates.

No attempt was made to place upper limits on the amplitude of the higher-momentum components and the size of the energy gap in sodium. Based on our experience with lithium, such estimates could be reliably obtained from the almost-free-electron approximation.

CONCLUSIONS

The principal conclusions from this experiment can now be restated as follows:

(1) The principal radii of the Fermi surface of sodium are equal within an estimated accuracy of 1.5%.

(2) The annihilation rate for electrons near the Fermi surface is about 20% greater than the rate for electrons near the origin, in substantial agreement with Kahana's calculation.

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Lattice-Vibration Effects in the Spectra of ZnO:Ni and ZnO:Co

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The optical absorption spectra of $ZnO:Ni^{2+}$ and $ZnO:Co^{2+}$ have been studied in the visible region, at temperatures from 7°K up. From correlation with lattice phonon energies, evidence has been found for the assignment of much of the band structure to vibronic sidebands. For both crystals, some weak lines on the low-energy side of the bands have been shown by their concentration dependence to be due to transition-ion pairs. In ZnO:Ni, a level whose polarization shows it to be an A_1 appears 8 cm^{-1} above the strong E–$T_2(^3P)$ transition. It is suggested that the A_1 level is produced by the Jahn-Teller interaction.

1. INTRODUCTION

THE optical absorption spectra of transition-ion impurities in crystals often show more structure than expected from the static crystal-field model. Electron-lattice interaction[1,2] gives rise to absorption due to vibronic sidebands, with energy transfer to the host lattice as well as to the transition ion.[3] This sideband structure may be analyzed if the host lattice vibrations are known.

Previous work on the spectra of ZnO:Ni and ZnO:Co[4–6] has shown that satisfactory assignments can be made for the strong-field levels of cubic symmetry, but identification of spin-orbit components and the splittings produced by the small trigonal field is difficult. The present study of the spectra was undertaken to clarify the importance of the effects of low-symmetry fields, spin-orbit coupling, and vibronic interactions. Most of the spectra were taken at low resolution for convenience, but for sharp lines a higher-resolution instrument was used to supplement this. Results were taken at various temperatures from 7°K up, and polarization dependence and concentration dependence of the spectra were studied. No extensive theoretical analysis was attempted.

Section 2 describes the experimental procedures used. Section 3 gives the results obtained for the visible spectra of ZnO:Ni and ZnO:Co, and for some Zeeman measurements on the sharp lines of ZnO:Ni. In Sec. 4 an analysis of the ZnO:Ni results is presented, showing that the visible band has pronounced phonon structure.

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