Fermi Surface of Beryllium by Positron Annihilation*

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(Received March 12, 1962; revised manuscript received June 18, 1962)

Measurements have been made of the angular correlation of photons from positron annihilation in single crystals of beryllium. The data yield areas of cross sections of the Fermi sea. The observed distributions of areas show an anisotropy which is in reasonable agreement with qualitative ideas of the Fermi surface of beryllium. Some evidence is seen of the higher momentum components of Bloch wave functions for electrons near a Brillouin zone boundary.

THE angular correlation of photons from positron annihilation has been used to provide information about the electron momentum distributions in solids.[1] In recent years measurements have been made to examine the shape of the Fermi surface of various metal single crystals.[2–4] This paper presents a short account of some experimental results which yield data directly related to the dimensions of the Fermi surface of beryllium. As one might expect, the data show a large anisotropy in the Fermi surface.

The apparatus used was similar to that described previously[5,6] but the slits in the detector shield were 12-in. long and 0.050-in. wide subtending at the source an angle of 0.0005 rad. The coincidence counting rate is directly proportional to the number of photon pairs with z component of momentum between p_z and p_z+dp_z, i.e., $N(p_z)$ is measured directly. The direction z is determined by the experimental arrangement. Since the positrons are probably thermalized before annihilation,[7] and since the annihilation cross section is only slightly velocity dependent,[8] the $N(p_z)$ observed is, to a good approximation, the distribution of the z components of momentum of annihilating electrons. These are the results shown in Fig. 1. The data are plotted as a function of $k_z=p_z/\hbar$. Because $N(k_z)$ is symmetric, all the data have been shown on one side of the line of symmetry, $k_z=0$. The three curves, which have been normalized to equal areas, represent $N(k_z)$ for z the (0001), (1$\bar{1}$00), and (11$\bar{2}$0) directions. The height of the curve at a given abscissa k_z is proportional to the cross-section area formed by the intersection of a plane with the Fermi sea, the plane being normal to k_z and passing through the end point of k_z. If the Fermi sea were spherical, $N(k_z)$ would be a parabola (as shown by the sodium results in the same figure). It is evident from these measurements that the Fermi surface in beryllium is very distorted. From these data we are attempting to construct a phenomenological Fermi surface for beryllium.

One might expect that in addition to areas the results should yield values for the maximum wave vector k_F in the z direction. The point at which the central parabolic portion of the curve meets the background identifies k_F. Consider the sodium data shown in Fig. 1. The almost horizontal line which is drawn to represent a background is an extrapolation of the data at large angles and also is approximately the appropriate momentum distribution for the electrons of the sodium ion core. Taking into account the estimated instrument resolution, a value of k_F is obtained in agreement with the free electron value, k_f, shown in Fig. 1.

If the same method of determining k_F is applied to the beryllium data, one obtains $k_F(0001)=2.05\pm0.06$/Å, $k_F(1\bar{1}00)=2.05\pm0.06$/Å, $k_F(11\bar{2}0)=2.10\pm0.06$/Å. These values are all larger than the free electron radius 1.94/Å and if real, imply large depressions in the Fermi surface for other directions. The large values cannot be accounted for by error in estimating the instrument resolution since the resolution for beryllium should be at least as good as it is for sodium. These apparently large radii are most likely caused by the higher momentum components of the electron wave functions and are thus not radii to the Fermi surface at all. In beryllium the Fermi surface is near a Brillouin zone boundary in many directions. For states near a zone boundary the electron wave function may be written in the almost free electron approximation as[9]

$$\psi_{\mathbf{k}}=\exp(i\mathbf{k}\cdot\mathbf{r})[A_0+A_n\exp(-i\mathbf{G}_n\cdot\mathbf{r})],$$

where $\mathbf{G}_n$ is a vector of the reciprocal lattice and $\frac{1}{2}\mathbf{G}_n$ is the vector from the origin of reciprocal space to the nearest point on the zone boundary concerned. The coefficients $A_0(\mathbf{k})$ and $A_n(\mathbf{k})$ are functions of the energy gap at the boundary as well as of $\mathbf{k}$. The electron

* Supported in part by the National Science Foundation.

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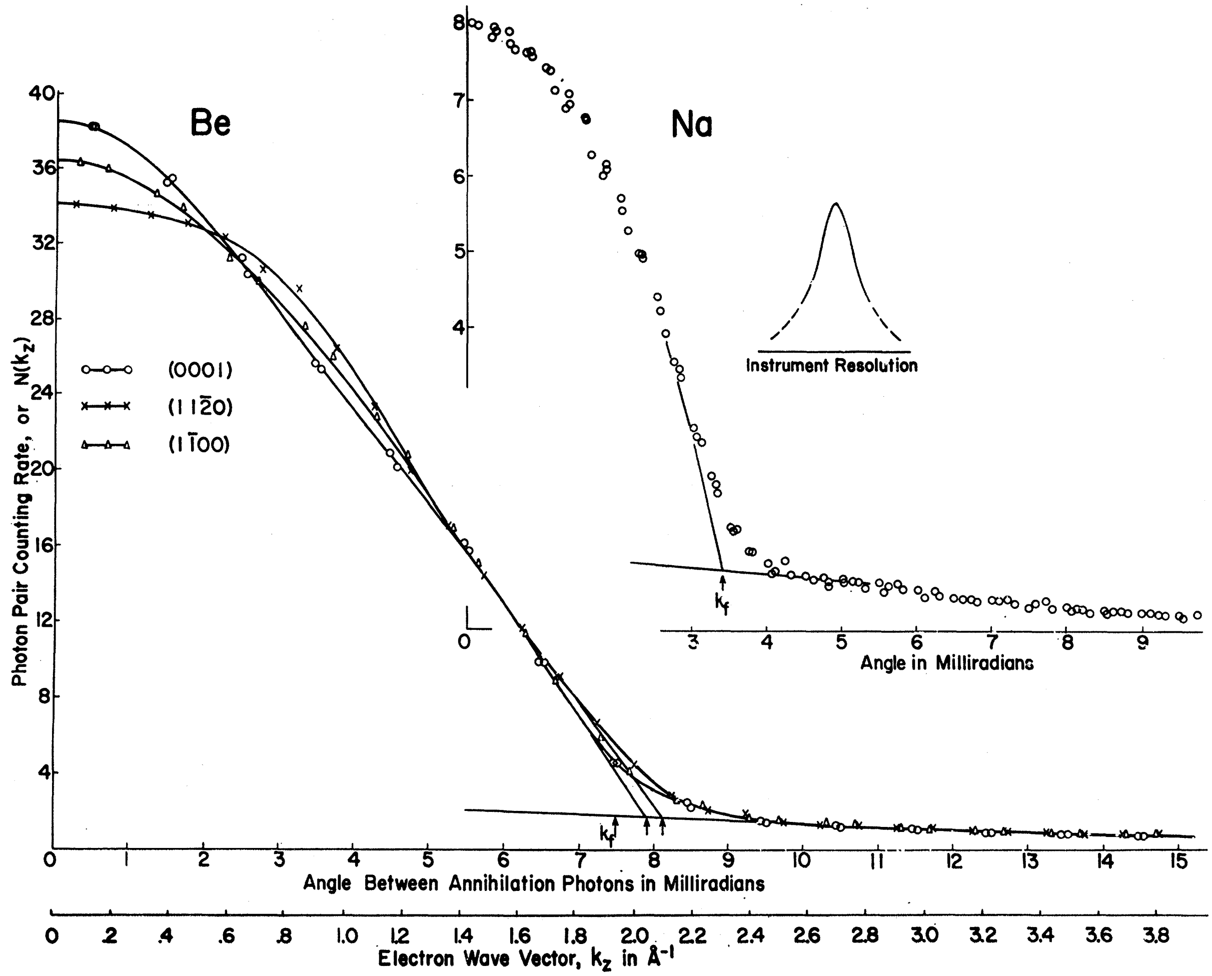

FIG. 1. The angular distribution of photons arising from annihilations with electrons in Be single crystals for three different crystallographic orientations. Shown also is the angular correlation curve for Na metal and the estimated instrument resolution.

described by this wave function has a momentum probability density, $P(\mathbf{K})$, proportional to

$$\left|\int \psi_{\mathbf{k}} e^{-i\mathbf{K}\cdot\mathbf{r}} d^3r\right|^2 \propto |A_0|^2\delta(\mathbf{K}-\mathbf{k})+|A_n|^2\delta(\mathbf{K}-\mathbf{k}+\mathbf{G}_n).$$

If the apparatus is set to detect annihilations with momentum $p_z=\hbar k_z$; and if $k_z>k_F$, the radius of the Fermi surface in the z direction, then the counting rate is proportional to the sum of the $|A_n(\mathbf{k}')|^2$ for all electrons $\mathbf{k}'$ such that some reciprocal lattice vector $\mathbf{G}_n$ can be found to make $(\mathbf{k}'-\mathbf{G}_n)_z=k_z$. If the Fermi surface is near a zone boundary there will always be one coefficient of appreciable magnitude,[10] and right at the zone boundary, $|A_n|^2=|A_0|^2=\frac{1}{2}$. Thus, the instrument set at $k_z>k_F$ measures the Bragg reflected intensity of the electrons nominally going in the opposite direction with wave vector $\mathbf{k}'$ given by $(\mathbf{k}'-\mathbf{G}_n)_z=k_z$. Further experiments at higher resolution should yield quantitative information about the higher momentum components of the electron wave function and hence possibly about the energy gap at various zone boundaries.

We have profited by many discussions with colleagues at the University of North Carolina, Chapel Hill, North Carolina.

[10] A more quantitative discussion is given in reference 3.