Band Structure and Positron Annihilation in Metals: Be and Mg†

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The angular correlation of positron annihilation radiation from oriented beryllium and magnesium crystals has been measured. The derivatives of the angular distributions from beryllium show fine structure and marked anisotropy compared to the observed nearly isotropic behavior of magnesium. A qualitative theoretical interpretation of the data is given in terms of the Bloch functions of the conduction band. It is emphasized that the correlation curves are sensitive to the details of these wave functions and do not yield directly cross-sectional areas of the Fermi distribution.

THE possibility of measuring electron momentum anisotropies in solids by annihilation radiation correlation has been demonstrated by us on oriented graphite.[1] The extent to which core vs conduction electrons contribute to angular correlation measurements in metals has been the subject of a paper on aluminum and copper.[2] In this note we present new data on oriented beryllium and magnesium[3] crystals and interpret the results in light of the theoretical discussion of reference 2.

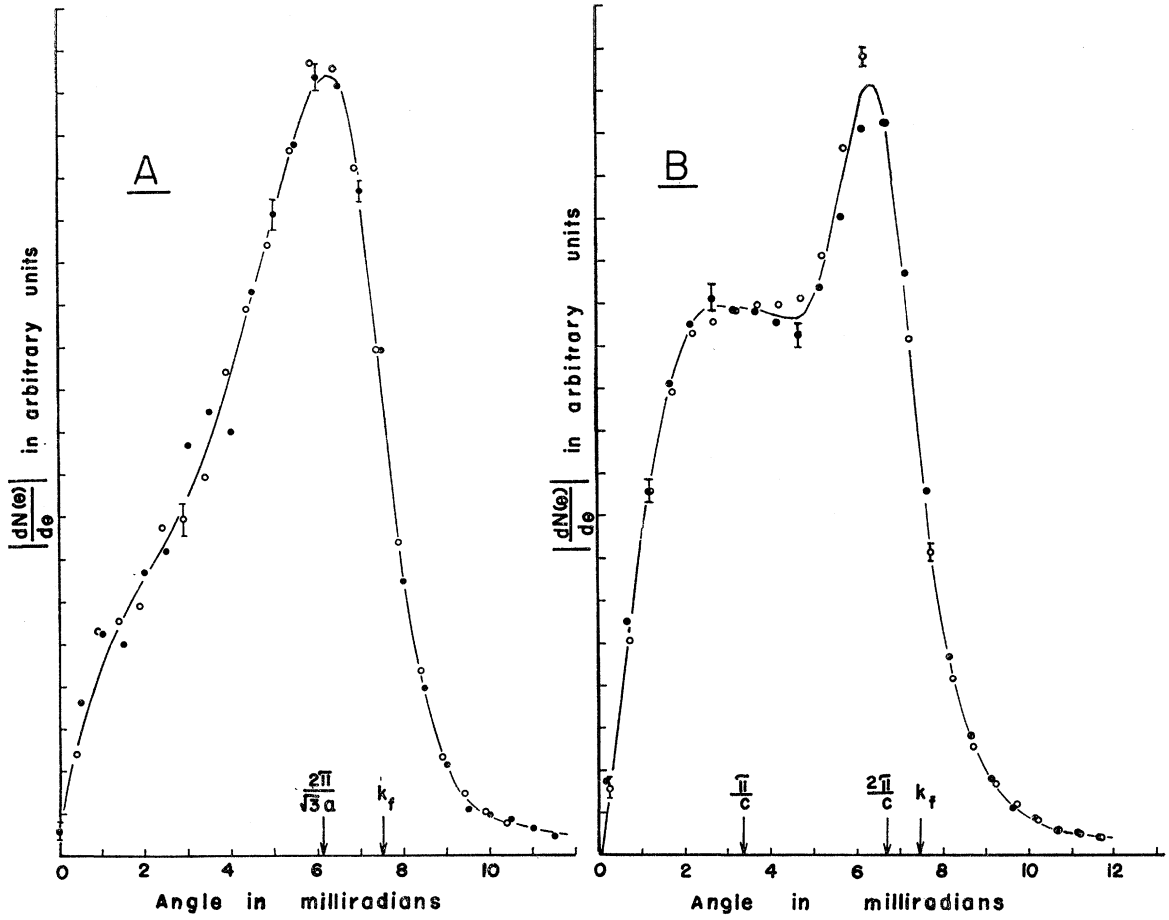

FIG. 1. The absolute magnitude of the derivative of the angular correlation curve for beryllium. The open circles are the data for negative angles folded about 0°. k_f represents the angle corresponding to the free-electron value of the Fermi radius. The solid curves are visual fits to the data. (*A*) p_z perpendicular to the $(10\bar{1}0)$ plane, (*B*) p_z perpendicular to the (0001) plane.

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[1] S. Berko, R. E. Kelley, and J. S. Plaskett, Phys. Rev. **106**, 824 (1957).
[2] S. Berko and J. S. Plaskett, Phys. Rev. **112**, 1877 (1958).
[3] Preliminary results were presented at the April 1962 Meeting of the New England Section of the Am. Phys. Soc.; independent measurements on Be have recently been reported by A. T. Stewart, J. J. Donaghy, J. H. Kusmiss, and J. B. Shand, Bull. Am. Phys. Soc. **7**, 343 (1962); and to be published in Phys. Rev.

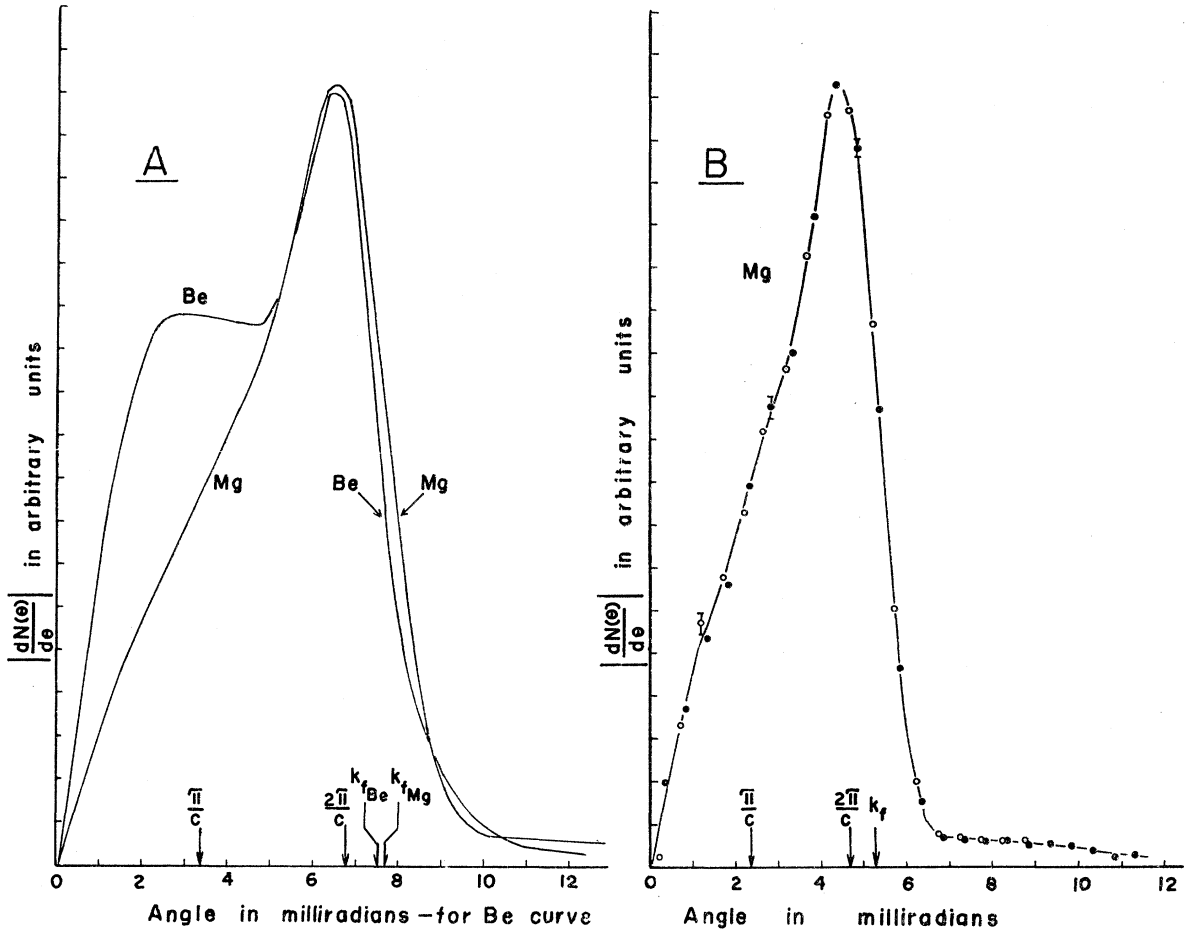

FIG. 2. (*A*) comparison between beryllium and magnesium with p_z perpendicular to the (0001) plane. The angular scale has been adjusted for the magnesium curve, in order to make θ, corresponding to $(2\pi/c)$ for magnesium, equal to that of beryllium. k_f represents the angle corresponding to the free-electron value of the Fermi radius. (*B*) The absolute magnitude of the derivative of the angular correlation curve for magnesium, with p_z perpendicular to the (0001) plane. The open circles are the data for negative angles folded about 0°. The solid curves are visual fits to the data. k_f represents the angle corresponding to the free-electron value of the Fermi radius.

If we neglect the positron-electron interaction compared to the positron-lattice and electron-lattice interactions, the probability of two photons being emitted with momentum $\mathbf{p}$ is proportional to[4]

$$\Gamma(\mathbf{p}) \propto \left| \int_{\text{crystal}} e^{-i\mathbf{p}\cdot\mathbf{r}} \psi_+(\mathbf{r})\psi_-(\mathbf{r}) d\mathbf{r} \right|^2,$$

where $\psi_+(\mathbf{r})$ and $\psi_-(\mathbf{r})$ are the positron and electron wave functions in the periodic lattice potential. The standard long-slit correlation apparatus[4] measures a counting rate

$$N(\theta) \propto \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \sum_{\text{electrons}} \Gamma(p_x p_y p_z) dp_x dp_y,$$

where the correlation angle $\theta=(p_z/m)$ $(\hbar=c=1)$. If, and only if, ψ_+ is a constant and $\psi_-(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})$ can the measurement at an angle θ be considered as being proportional to the cross-sectional area of the Fermi distribution at the point $k_z=p_z=\theta m$. In that case, the expected distribution should be a parabola with a cut off at $\theta_f=p_{\text{Fermi}}/m$. If, however, one considers Bloch waves so that $\mathbf{p}$ and $\mathbf{k}$ space are not equivalent anymore, a Bloch electron, $\psi_-(\mathbf{r})=u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$, contributes a δ function to the angular correlation not only at $\mathbf{p}=\mathbf{k}$, but at all points $\mathbf{p}_i=\mathbf{k}+\lambda_i$, where λ_i are the reciprocal lattice vectors of the crystal $(\lambda_i\cdot\mathbf{R}_j=2\pi\delta_{ij})$; the weight of the contribution at $\mathbf{p}_i$ is proportional to $|A_{\lambda_i}|^2$, where

$$A_{\lambda i}=\int_{\text{cell}} \exp(-i\lambda_i\cdot\mathbf{r})u_{\mathbf{k}}(\mathbf{r})\psi_+(\mathbf{r})d\mathbf{r}.$$

In view of the above, it is felt that it is premature to attribute a deviation from parabolic distribution to the positron-electron interaction, as was done for Na,[5]

[4] For a review of the subject, see P. R. Wallace, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1960), Vol. 10. For more recent work on metal crystals see I. Ya. Dekhtyar and V. S. Mikhalenkov, Doklady Akad., Nauk S.S.S.R. **140**, 1293 (1961).

[5] A. T. Stewart, Phys. Rev. **123**, 1587 (1961).

without having realistic wave functions for $\psi_+(\mathbf{r})$ and $\psi_-(\mathbf{r})$.

In reference 2 it is shown that large deviations are expected from parabolic distributions as one approaches the Brillouin zone faces. Using nearly free electron theory it is shown that in the case of the overlap of the Fermi distribution into the second zone one expects to observe distinct "humps" in the angular distribution at the zone faces and that the distribution could "cut off" beyond the angle corresponding to the Fermi surface. The size of this effect depends on the energy gap and on the distance of the Fermi surface from the zone face. In order to check these predictions we have selected the hcp metals Be and Mg, known to have zone-overlapping Fermi distributions. The experimental apparatus was similar to that described previously[2] except that the detectors consisted of 2-in. diam by 7-in. long NaI crystals with 7-in. long lead collimators subtending an angle of 0.6 mrad. The use of these high-efficiency detectors resulted in a greatly reduced background accidental rate. The experiments were carried out at room temperature. In order to demonstrate small deviations from parabolic distributions, we have plotted in Figs. 1 and 2 the absolute magnitude of the derivative of the angular correlation curve. The derivatives were obtained by taking the difference of the experimental points at second nearest neighbors without any further smoothing. Figures 1(A) and 1(B) demonstrate the large anisotropy found in Be and also the deviations from the parabolic distribution (linear derivative), particularly along the c axis. The height and exact shape of the second peak of Fig. 1(B) is, of course, very sensitive to the resolution and alignment of the setup, and will be further studied with better angular resolution. We also obtained anisotropy along different directions of the basal plane, and will discuss the details in a subsequent publication. We interpret the large initial slope of Fig. 1(B) as due to the contributions of the "humps" about the six rectangular faces of the Brillouin zone, as one cuts perpendicular to these faces with p_z parallel to the c axis. The hexagonal face at π/c should not contribute because of the expected vanishing energy gap in first order at that face. The "cutoff" is somewhat outside of the angle corresponding to p_{Fermi} for free electrons. Figure 2(B) shows the experimental curve along the c axis for magnesium, with a much less pronounced structure. We found practically no anisotropy in magnesium. In Fig. 2(A) we compare beryllium with magnesium by normalizing to the same c.

It is obvious that a detailed model computation is needed in order to interpret the quantitative features of these curves. Such a computation will need the knowledge of $\psi_+(\mathbf{r})$ in the respective metals, as was done for aluminum and copper in reference 2. Short of such a computation we can conclude qualitatively that the energy gaps in the band structure of Be are larger than those of Mg, and that the deviation from free-electron wave functions is larger in Be, giving rise to a more anisotropic Fermi surface. The Fermi surface in Mg should, by inference, be nearly spherical (in the extended zone scheme). These conclusions are born out by the existing band computations in Be[6] and Mg.[7] We conclude that precision positron annihilation experiments can yield information about conduction electrons in metals; however, the angular correlations are sensitive to details of the wave functions, and therefore cannot be used to study the topology of the Fermi surface in a direct way.

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[6] C. Herring and A. G. Hill, Phys. Rev. **58**, 132 (1940).
[7] L. M. Falicov (to be published).