

90 YEARS



ON A POSSIBILITY
OF THE DETERMINATION OF A FERMI
SURFACE SHAPE BY THE ANGULAR DISTRIBUTION
OF γ -QUANTA GENERATED AT THE TRANSFORMATION
OF ELECTRON-POSITRON PAIRS INTO PHOTONS

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Recently, a number of methods has been proposed to determine the shape of the Fermi surface of electrons in metals [1–3]. These methods are based on studies of magnetic, galvanomagnetic, and resonance phenomena. A method based on the investigation of photons generated on the irradiation of a metal by positrons has been applied to determine the Fermi level (see, e.g., [4, 5]). The aim of the present letter is to draw attention to the basic possibility to apply this phenomenon not only to the determination of the Fermi level, but also for the investigation of the shape of the Fermi surface of electrons in a metal.

For this purpose, one should examine the angular distribution of γ -quanta generated on the irradiation of a small metallic sample with positrons by using coincidence counters. A sample should be a single crystal, rather than a polycrystal. As is well known [6], in the transformation of electron-positron pairs into photons in metals, the basic role is played by the conduction electrons, and not by the inner-shell electrons. The probability of the transformation of a conduction electron with wave vector \mathbf{k} and a positron with wave vector \mathbf{k}' into two photons with the total momentum \mathbf{p} (divided by $h/2\pi$, where h is Planck's constant) can be represented as [5]

$$w \sim \sum_{\mathbf{g}} \left| \int u_{\mathbf{k}}(\mathbf{r}) u_{\mathbf{k}'}^*(\mathbf{r}) \exp(-2\pi i \mathbf{g} \mathbf{r}) d\tau \right|^2 \times \delta(\mathbf{k} + \mathbf{k}' + 2\pi \mathbf{g} - \mathbf{p}). \quad (1)$$

Here, \mathbf{g} is a reciprocal lattice vector, $u_{\mathbf{k}}(\mathbf{r})$ and $u_{\mathbf{k}'}(\mathbf{r})$ are periodic parts of the wave functions of the electron and the positron in the crystal, the summation over \mathbf{g} is performed over all vectors of the reciprocal lattice, and the integration is performed over the volume of a lattice cell. As known [7], the positrons in a metal have time

to get thermal energies, so that the value of \mathbf{k}' can be approximately set equal to zero (in a typical case where the coordinate origin in the \mathbf{k} -space corresponds to the minimum of the positron energy). Therefore, it follows from (1) that the conservation law

$$\mathbf{k} + 2\pi \mathbf{g} = \mathbf{p} \quad (2)$$

should hold. The energy conservation law implies that, for the γ -quanta flying apart, the momenta p_1 and p_2 divided by h are significantly greater in modulus than the modulus of their sum \mathbf{p} .

First, let us consider the quantum transitions with $\mathbf{g} = 0$. For simplicity, we assume that the electrons of a metal are in the state of full degeneration. The vectors \mathbf{k} correspond to the electrons filling the \mathbf{k} -space inside the Fermi surface. Since $p_1 \approx p_2 \gg p$, a deviation of the angle between the first counter, the sample, and the second coincidence counter from 180° is determined only by the projection \mathbf{k}_\perp of the vector \mathbf{k} in the direction perpendicular to the line which joins, for example, the first counter and the sample (OX axis). Therefore, by determining the intensity distribution of γ -radiation in the plane perpendicular to the OX axis (YZ plane), one can use the contour of this distribution for the direct determination of a similar contour of the projection of the Fermi surface onto the $k_y k_z$ plane. Changing the orientation of the single crystal with respect to the counters, one can determine projections of the Fermi surface onto other planes in the same way, i.e. to reconstruct a shape of this surface. If the quantity $L_0 = \left| \int u_{\mathbf{k}}(\mathbf{r}) \cdot u_{\mathbf{0}}^*(\mathbf{r}) d\tau \right|^2$ can be considered approximately independent of k , the γ -radiation intensity corresponding to some value of $\mathbf{k}_\perp = \mathbf{p}_\perp$ is proportional to the number of electrons with wave vectors having the projection k_\perp , i.e. it is

proportional to the length of a segment, which is parallel to the axis k_x and passes through the end of the vector \mathbf{k}_\perp , inside the Fermi surface. Thus, if L_0 does not depend on k (or if this dependence is known and can be taken into account), the Fermi surface can be reconstructed, by using the γ -radiation distribution, even for a given orientation of the single crystal.

In the case where $\mathbf{g} \neq 0$, the probability of the transitions corresponding to this \mathbf{g} is proportional to $L_0 = \left| \int u_{\mathbf{k}}(\mathbf{r}) \cdot u_0^*(\mathbf{r}) \exp(-2\pi i \mathbf{g} \mathbf{r}) d\tau \right|^2$. If the quantity $L_{\mathbf{g}}$ is not very small, these transitions can also play an essential role. The transitions corresponding to a certain \mathbf{g} give rise to the appearance of an intensity distribution in the YZ plane which is restricted by the same contour as that in the case where $g = 0$, but it is shifted by a vector proportional to the vector $2\pi \mathbf{g}_\perp$ (where \mathbf{g}_\perp is a component of the vector \mathbf{g} which is perpendicular to the OX axis). As a result, the distributions corresponding to different g can superimpose one on another, and, in general, the intensity distribution pattern will be blurred. However, at some directions of the OX axis corresponding to small sums of indices (for example, the directions $[100]$, $[110]$, *etc.*), the distances between the ends of the vectors $2\pi \mathbf{g}_\perp$ are large enough. As a result, the images of the Fermi surface in the YZ plane corresponding to different \mathbf{g}_\perp are not superimposed (or are slightly superimposed). In this case, each spot will be a result of the superposition of coinciding contours, for which \mathbf{g}_\perp are identical (but \mathbf{g} are different). The intensity distribution in the YZ plane corresponding to the contour of the Fermi surface will be repeated many times, with the intensity decreasing with increase in the distance from the spot corresponding to $g = 0$. Thus, in this case, one can also examine the Fermi surface shape.

The above method would be applied to the investigation of the shape of a Fermi surface not only in pure metals, but also in alloys. In particular, it would allow one to investigate the deformation of the Fermi surface under phase transitions, for example, under the ordering.

It should be noted that the obtained intensity distribution pattern should be blurred due to finite sizes of the sample and the counters, the Coulomb interaction between the electron and the positron and between electrons of the metal, the possibility of transitions, at which phonons are emitted and absorbed, *etc.* The method proposed above can be obviously used if such a blurring is not too large. The study of an influence of the above-mentioned effects on the angular distribution of radiation should be the subject of a special investigation.

In conclusion, we take an opportunity to express our gratitude to I.Ya. Dekhtyar who has attracted our attention to the experimental works concerned with the measurement of the Fermi energy, by using the angular distribution of γ -radiation.

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Mikhail Aleksandrovich Krivoglaz is a prominent scientist in the area of solid state physics, Corresponding member of AS of UkrSSR, laureate of State's prizes of UkrSSR in science and technique. From 1951 to 1988, he had worked in G. V. Kurdyumov Institute for Metal Physics, NAS of the Ukraine. M.A. Krivoglaz made a fundamental contribution to the development of the theory of non-ideal crystals and laid the foundation of a number of trends in this field. In the theory of light absorption spectra by the impurity centers, he predicted (together with S.I. Pekar) the existence of narrow phononless lines in the electron-vibration spectra before the discovery of the Mössbauer effect. Together with A.A. Smirnov, he essentially developed the theory of properties of ordered alloys [M.A. Krivoglaz, A.A. Smirnov, *Theory of Order-Disorder in Alloys* (Elsevier, N.-Y., 1965)]. He is one of the founders of the theory of the scattering of X-rays and neutrons in non-ideal crystals, in which he developed the method of fluctuation waves, proposed a new systematics of impurities in crystals, and predicted some important effects (M.A. Krivoglaz, *X-Ray and Neutron Diffraction in Non-Ideal Crystals* (Springer, Berlin, 1996); M.A. Krivoglaz, *Diffuse Scattering of X-Rays and Neutrons by Fluctuations*, *ibid.*, 1996). In the theory of electron states in crystals, he developed a theory of fluctuations – autolocalized electron states of a new type that can appear in the systems with easily changing parameters (see the article in the present issue). The full bibliography of the works by M.A. Krivoglaz is presented in the book: M.A. Krivoglaz, *Life and Scientific Activity. Reminiscences. Selected Works* (Publ. House "Akadempriodyka", Kyiv, 2004) (in Russian).

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A.A. Smirnov was born in Novgorod. He graduated from the Leningrad State University in 1932. He began his scientific activity in Sverdlovsk (now Ekaterinburg, Russia), at the Ural Branch of the AS of the USSR (1932–1950); then worked at the AS of Ukraine (1950–1992) as Head of a department at the Laboratory of Metal Physics of the AS of the UkrSSR (1950–1955) and the Institute of Metal Physics of the AS of the UkrSSR (1955–1987). Academician-secretary of the Division of Physics of the AS of the UkrSSR (1963–1966), Vice-President of the AS of the UkrSSR (1970–1974). A.A. Smirnov was a founder of the international synchrotron trend. He pioneered in the development of the theory of interaction of electrons with

electromagnetic radiation and the theory of photon emission and absorption by electrons in the framework of nonlinear quantum electrodynamics. A.A. Smirnov elaborated the quantum theory of electron energy spectrum and electroresistance in ordered alloys, the theory of atomic distribution and mobility in the crystal lattice and the theory of phase transformations in substitution and interstitial alloys and subtractional solid solutions; the theory of charged particle channeling, the theory of neutron scattering in alloys, and the theory of diffusion in liquid metals. A.A. Smirnov, together with M.A. Krivoglaz, proposed a new method to study the shape of the Fermi surface in metals and alloys by analyzing the angular distribution of γ -quanta generated at annihilation of positrons and conduction electrons in single-crystalline samples. All those results were published by A.A. Smirnov in more than 220 scientific papers and summarized in seven monographies.