Appl. Phys. 13, 81—85 (1977)

Applied Physics

The Results of Study of the Anisotropy of Free-electrons Momenta Distribution in Mg, Zn, and Cd by Means of the Positron Annihilation Method*

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Received 9 May 1975/Accepted 19 October 1976

Abstract. The angular correlation of annihilation radiation was measured for single crystals of Mg, Zn, and Cd in seven crystallographic directions. The results of distribution of the z-component of the conduction electron momenta were compared with the cross-sectional-area distribution of the double Brillouin zone for two directions [0001] and [10$\bar{1}$0]. The results were analyzed also by the Mijnarend's method. The distributions of the electron momenta densities in the [0001] and [10$\bar{1}$0] directions are preliminarily discussed.

PACS Code: 71.20

The Fermi surface of Mg, Zn, and Cd have been examined several times by means of dHvA, RFSE and magnetoacustic methods as well as the annihilation method. The data concerning the nearly spherical shapes of those surface and their distribution in consecutive Brillouin zones which were obtained by the first methods mentioned above are relatively accurate and can be found in the Literature [1–4]. However, in the papers concerning the electronic structure of those metals examined by means of the annihilation method, the discussions were limited to the speculations about the minor differences between the angular correlation curves measured for various orientations of the crystals [5–7].

The only exception is the work of Kontrym-Sznajd and Stachowiak [8] on Zn. The situation can be explained by the fact that the Fermi surfaces of Mg, Zn, and Cd are nearly spherical. Subtle deviations from the ideal distribution are diffused for many reasons. Besides the influence of the limited resolution of spectrometer, diffusion is caused by the character of the annihilation method itself. This method gives the values proportional to the average number of the electron state in the cross section which is normal to the examined direction (long-slit geometry)—in the best it gives the averaging for the states along the normal to the given two directions (crossed-slit geometry).

In addition, in the topography of the Fermi surface, even those which are nearly spherical, annihilation with the core electrons and the positron-electron and electron-electron interactions cannot be neglected. Of particular importance is the so-called HMC effect, playing a leading role for momenta from the range for which a long slit "sees" annihilation acts with electrons having projections wave vector $k \approx G$ in a given direction [9], in the vicinity of the Fermi surface. It is difficult to take into account this effect due to complexity of the double Brillouin zone for the investigated metals and a number of crossings of the

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Fermi surface and surfaces restricting this zone. Therefore, we have decided to base the interpretation of our results on the free-electrons model with the HMC effect only partially taken into account. Under these simplifying assumptions the results of our measurements concerning the shapes and some dimensions of the Fermi surface, after some elaboration, were compared with the data obtained by means of other methods. Following there are the distributions of the momenta densities of electrons shown as they were calculated by means of the Mijnarend's method. They are discussed in this paper as well.

1. The Results and Discussion

The angular correlations were measured by means of the parallel-slit spectrometer with the resolution function of described by a method presented in [10] with a FWHM equal 0.46 mrad for single crystal samples oriented in the [0001], [10$\bar{1}$0], [11$\bar{2}$1], [10$\bar{1}$1], [11$\bar{2}$1], [10$\bar{1}$2], and [11$\bar{2}$2] directions separately for each of the examined metals. The statistical error at the maximum of the angular correlation curve ranged from 0.5 to 1% depending on the sample. The studied crystallographic directions are shown in Fig. 1 where the two Brillouin zones for hexagonal close-packed structure are presented. In Mg, Zn, and Cd the first zone states excluding small holes in the neighbourhood of the H points (caps) are occupied. In the second zone, the hole states are mainly in the vicinity of the HT line. Partially occupied electron states in the third zone are localized in Mg around the L points (butterflies or stars for Zn and Cd) along the KH lines (cigars) and directly above the horizontal plane (0002) (lens). In Zn there are small electron needles along the KH line and a lens like in Mg. In Cd the electron states of the third zone give the lens in the reduced zone scheme. Occupied electron states of the third zone show the number of electron states per atom of the order of 10^{-2}.

The measured angular distributions in [0001] and [10$\bar{1}$0] directions were divided into two groups: one corresponding to the annihilation with conduction electrons and the other—annihilation with the core electrons. The second was obtained by the approximation of the curve-tails with the best-fit Gaussian function. The difference obtained by the substraction of the Gaussian part from the measured correlation curves were taken as the curve responsible for the annihilation with the conduction electrons, and simultaneously for the z-component of the momenta of those electrons, in the crystallographic direction oriented along the z-axis.

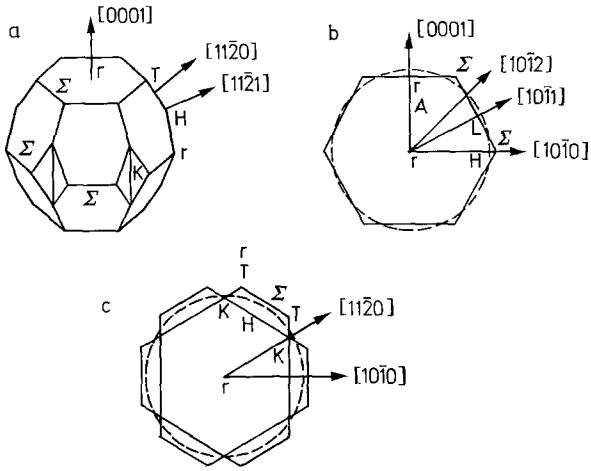

Fig. 1. a) The second Brillouin zone of hexagonal close packed structure showing the pertinent symmetry points; b) the intersection of the [1010] plane zone; c) the intersection of the ΓMK plane. Examined directions are shown

Distributions of the z-component for the [0001] and [10$\bar{1}$0] directions are shown in Fig. 2 as open circles. On the same figure the distributions cross sectional areas of the double Brillouin zones normal to the mentioned directions are shown by a solid line. This procedure was executed for each of the three examined metals.

The Brillouin zone dimensions have been calculated using lattice constants at room temperature. Comparison of the z-component of the conduction electron momenta with the cross sectional area distribution allows to draw a series of interesting conclusions concerning the shapes of the Fermi surfaces and the dimensions of different elements of these surface in the reduced zone scheme.

The analysis of the curves in the [0001] direction shows the contribution of the butterfly in the Mg exhibiting itself in such way that the open-circle curve in the region from 1.2 to 3.7×10^{-3} mc passes above the solid line curve. For Zn and Cd very important information is obtained concerning the controversial opinion on presence or absence of the stars. The curve in Fig. 2 suggests that in those metals the stars are not present, since in all range of momenta from 0 to $p = 2\Gamma$A the open-circle curve lies below the solid line curve. Large differences between these two curves near the low values of momenta confirm that the hole states in all three metals are located near the TΣ line.

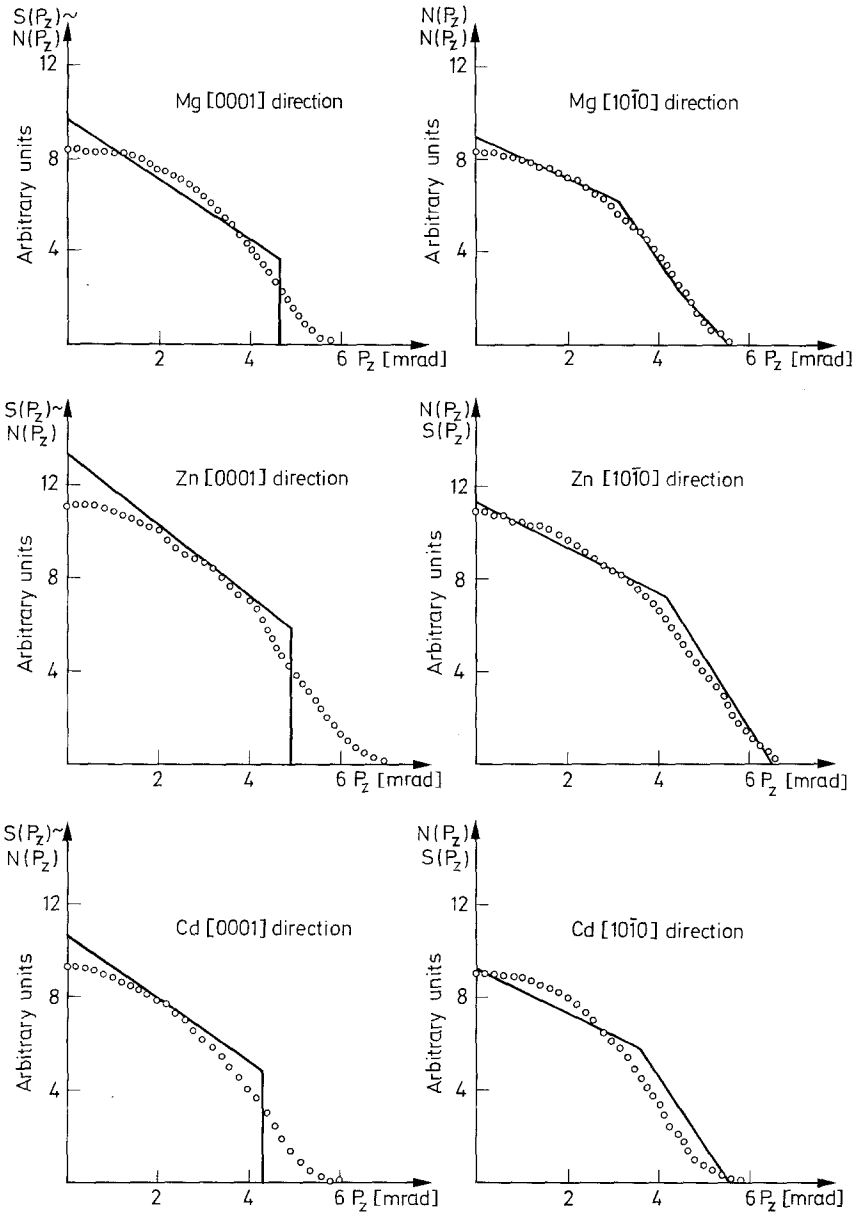

Fig. 2. Comparison of the distribution of z-component of the conduction electron momenta (open circles) with distributions of the crossectional areas of the double Brillouin zone (solid line) for Mg, Zn, and Cd

The angular correlation curves for $p \geqq 2\Gamma A$, for the discussed direction [0001], correspond to the cross section through the electron states of the lens. From the ratio of the area under this part of the curve to that under the whole curve we calculated the number of conduction electrons per atom in the lens for cadmium, which is 0.05 and is in good agreement with the calculation of Stark and Falicov [11] who proposed the value 0.0482. Disregarding the contribution of the needles and using the same method we obtained the number of conduction electron states per atom for inc as 0.07 which is a bit higher than 0.045 reported by the same authors.

The values of the ordinates of the correlation curves for $p=2\Gamma A$ for the [0001] direction are proportional to the crossectional area of the lens. Calculated linear dimensions of these are as follows 2.7 ± 0.23 for Mg, 3.6 ± 0.35 for Zn, and 3.0 ± 0.41 for Cd (all in 10^{-3} mc). These results calculated from the lenses are in good agreement with the dimensions determined by means of other methods: 2.28 [1, 2], 3.35 [3] and 3.01 [4] in the same units.

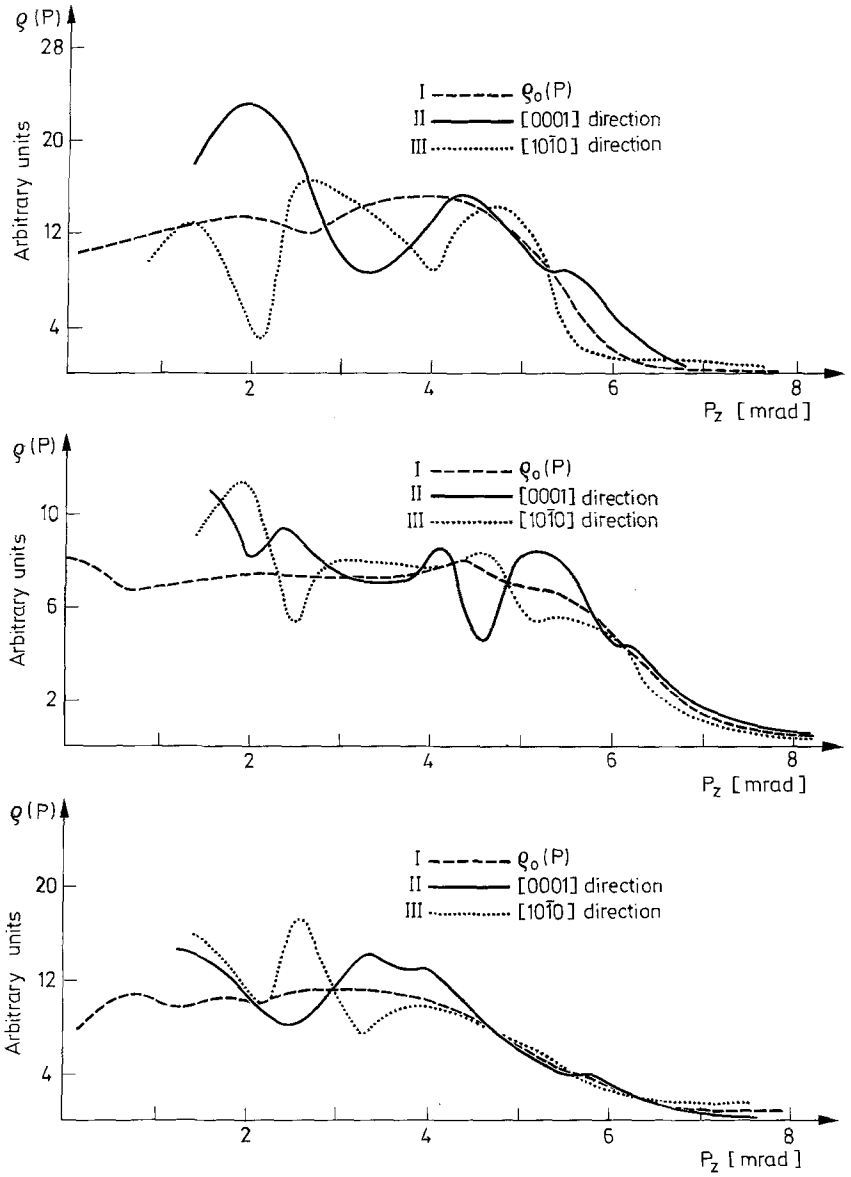

Fig. 3. Distributions of electron momenta density for Mg, Zn, and Cd in [0001] (curve II) and [1010] (curve III) directions. Dashed curve (I) represents the radial component $^{\varrho}{}_{0}(p)$

Similar comparison of distribution in [10$\bar{1}$0] direction confirms the informations listed for [0001] direction although they are less obvious because of the overlapping of the electron and the hole states. Because of the simplifications mentioned above, these figures bear an error greater than that calculated from the statistical error. Nevertheless, we believe that for sufficiently small statistical error and properly taking into account the HMC and other effects, the results obtained in this way may be as good as those derived from magnetic methods.

The calculations of the electron momenta density distribution were done numerically by means of Mijnarend's method [12, 13] for Mg, Zn, and Cd. To get those results the angular correlation curves have been used for seven orientations of the samples of each examined metal. Calculated distributions in [0001] and [10$\bar{1}$0] directions are proposed on the Fig. 3.

Curve I shows the radial component $\varrho_0(p)$. For each of the three metals reanging from 0 to Fermi momentum p_F the radial component does not exhibit visible fluctuations. From that we can conclude that it is adequate to use for calculations the experimental data of the seven correlation curves for obtaining relatively accurate distributions in certain crystallo-

graphic directions. The mentioned density distributions show, on the other hand, the strong fluctuations which are much above expected values. Besides the experimental errors of the calculations strongly affecting the range of low momenta and the approximations typical for this method of calculations, the fluctuations could be influenced by interactions between the particles, which in effect bring the local perturbations of momenta densities. As a result of those interactions there is a screaning effect of positron leading to enhancement of annihilation [14, 15] especially high for electrons near the Fermi surface. In a recent work [16] it is was suggested that the increase of the electron momentum density takes place in the region of intersection of Fermi surface with HMC Fermi surface localized in the nearest center of the reciprocal lattice. The effect associated with this was confirmed in [8]. Since for Mg, Zn, and Cd intersections of those spheres takes place in both direction [0001] and $[10\bar{1}0]$ the similar effect should be observed on the distribution curves in those directions. In [0001] direction the intersection of the spheres takes place for electron state of the lens; while for $[10\bar{1}0]$ direction interesting spheres projected on the Γ MK plane from the lens shapes with the center at M. The expected effect of increased momenta density is very evident for Mg in both discussed directions; for Zn the increased momenta density was found, as predicted in $[10\bar{1}0]$ direction, while in Cd the effect for distribution in [0001] direction is much less clearly marked. Detailed analysis of the results by means of Mijnarends method be presented in separate paper.

Conclusions

Comparison of the angular distribution curves with the distribution of the Brillouin zones allows to localize the characteristic elements of the Fermi surfaces of Mg, Zn, and Cd, and determine some of the dimensions of those elements. It is believed that a similar method can be utilized for other metalic structures. Particulary interesting is the confirmation of suggestion of Stark-Falicov stating that there are no stars in zinc and cadmium.

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