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POSITRON ANNIHILATION IN MAGNETIZED IRON

P. E. MIJNARENDS and M. H. H. HÖFELT (*)
Reactor Centrum Nederland, Petten (N. H.), the Netherlands

Abstract. — Results are reported of 2 γ angular correlation measurements in magnetized iron single crystals. The spin density distribution, customarily ascribed to a negative conduction electron polarization, is inverted to display Δρ(p). In this way it is expected that the results will be more amenable to theoretical interpretation. In the present paper preliminary results are given and an attempt is made to relate these to the band structure of iron.

From the analysis given by Berko [1] it follows that the difference and sum angular correlations are not directly proportional to the difference and sum momentum densities Δρ(p) and ρ_{tot}(p), respectively. Instead, they are given by

\[ \Delta N(p_2) = \int \Delta R(p) \, dp_x \, dp_y \]
\[ N_{tot}(p_2) = \int R_{tot}(p) \, dp_x \, dp_y, \]

where \[ \Delta R(p) = C \rho_{tot}(p) \Delta \rho(p) + P_{eff} \rho_{tot}(p) \]
\[ R_{tot}(p) = C \rho_{tot}(p) + P_{eff} \Delta \rho(p) \approx C \rho_{tot}(p). \]

Here \( P_{eff} \) denotes the polarization of the positron beam and \( P_{tot} \) is the effective total electron polarization as seen by the positron. Since \( P_{eff} \) and \( P_{tot} \) are not known separately one considers the ratio

\[ Q(p) = \frac{\Delta R(p)}{R_{tot}(p)} = \frac{P_{eff} (\Delta \rho(p)/\rho_{tot}(p)) + P_{tot}}{P_{tot}}. \]

Apart from the scaling factor \( P_{eff} \), this only differs from the corresponding ratio \( Q(p) \) of the \( \rho \)'s by the (small) additive constant \( P_{tot} \). The uncertainty in \( P_{eff} \), therefore, means an uncertainty in the zero level of \( Q(p) \), but does not affect its shape. Moreover, an estimate of \( P_{tot} \) may be obtained from a measurement of the relative change in three-photon yield with field up and down. Measurements by Berko and Mills [6] yielded \( \frac{4}{3} P_{eff} \approx (53 \pm 9) \times 10^{-4} \), from which it follows that the zero level of \( Q(p) \) will not be more than 0.6 – 1% below that of \( Q(p) \).

Positrons emitted by a 50 mCi \( ^{22} \text{Na} \) source were focussed upon oriented single crystals of iron by a 17 kG magnetic field, which at the same time served to magnetize the crystals. The angular correlations were measured with a conventional long slit instru-

(*) Present address : Philips Research Laboratories, N. V. Philips' Gloeilampenfabrieken, Eindhoven, the Netherlands.
ment [7] having an angular resolution of $1.1 \times 85$ mrad. The crystal orientations are shown in figure 1. The fact that the [111] direction is not represented is expected to have a less serious effect in b.c.c. Fe than in an f.c.c. metal as Cu.

![Stereographic plot of the sample orientations.](image)

Figure 1. — Stereographic plot of the sample orientations.

Figure 2 shows a contour plot of $Q(p)$ in the (001) and (110) planes. Its most remarkable features are a thin positive shell surrounding the origin, containing peaks at $\sim 3$ mrad along the [100] axes, a wide negative region between 4 and $\sim 10$ mrad with deep minima along the [100] axes, and a positive region with very high peaks ($\sim 18\%$) at 14.5 mrad, also along the same axes. The sum distribution $R_{\text{tot}}(p)$, on the other hand, is only slightly anisotropic with bulges in the [110] directions, small peaks on the [100] axes at $\sim 2.5$ mrad, and a shallow local minimum at the origin.

An attempt to relate these observations to Wakoh and Yamashita's (WY) [8] computation of the band structure of iron will be limited to the [100] directions, since along these most detail is observed. As the directional dependence of $\mathcal{A}(k, p)$ on $p$ is the same as that of $\psi(r)$ on $r$, only states with $\mathcal{A}_1$ symmetry will contribute in these directions. Furthermore, in the vicinity of $\Gamma$ only $s$ states can contribute, since $\mathcal{A}(3d, k, p)$ vanishes as $p^2$. The conduction band hybridizes with the 3 d band of $\mathcal{A}_1$ symmetry. Consideration of WY's band structure diagram shows that along $\Gamma H$ the latter band intersects the Fermi level at a point $\sim 4$ mrad from $\Gamma$ for the majority spin direction, while the corresponding minority spin band lies entirely above the Fermi level. As a result there will be a small region with a net majority $d$ and $s$-spin density at angles just below 4 mrad (say 3 mrad). This may explain the positive peaks found in that position.

The length of the (002) reciprocal lattice vector is 17 mrad. Subtracting this from the position of the peak at $\sim 3$ mrad, one arrives at the large peak found at 14.5 mrad. Thus, the latter is connected to the small peak by an Umklapp-process in which both 3 d and conduction electrons may take part. The large height of the secondary peak is explained by the small value at large momenta of $R_{\text{tot}}$ in the denominator of $Q(p)$.

The third feature of interest is the deep minimum around $\sim 6.5$ mrad. A similar minimum, although at slightly lower angles, was observed in a polycrystal by Berko et al. [2], and interpreted by them in terms of a negative conduction electron polarization. However, the strongly negative region observed in the present experiment extends all the way up to $H$, i.e. far outside the $s$-like part of the Fermi surface. It seems unlikely therefore that any conduction electron spin density could account for it. Moreover, since in that part of $k$-space the $3d$ states of $\mathcal{A}_1$ symmetry of both spin orientations are full, the negative region can only be explained by assuming that $\mathcal{A}_+ \neq \mathcal{A}_-$ owing to the exchange polarization of the 3 d wave functions. Computations of $\mathcal{A}_+$ and $\mathcal{A}_-$ in order to investigate this point are in progress.

![Contour diagram of the ratio $Q(p) = \Delta R(p)/R_{\text{tot}}(p)$ in the (001) and (110) planes. Indicated values in percents.](image)
References