Higher-momentum components of the e^+ and e^- wave functions in Li and K

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Two-dimensional angular correlations of positron-annihilation radiation in Li and K have been measured with high angular resolution. The results are compared with two-photon momentum densities calculated by the Korringa-Kohn-Rostoker method. The comparison shows good agreement for the (110) and (200) higher-momentum components and thus implies that many-body enhancement effects are comparable with those in the (000) zone.

The measurements of momentum density by two-dimensional angular correlation of positron-annihilation radiation are very sensitive to the wave functions of the conduction electrons in metals, as well as to the positron wave function.[1] In the independent-particle model the two-photon momentum density, $\rho^{2\gamma}(\vec{p})$, for positron annihilation in a solid is

$$\rho^{2\gamma}(\vec{p})=\sum_{\vec{k},l} n_l(\vec{k})\left|\int d^3r\, e^{-i\vec{p}\cdot\vec{r}}\,\psi_+(\vec{r})\psi_{\vec{k},l}(\vec{r})\right|^2 ,$$

where $\psi_{\vec{k},l}(\vec{r})$ and $\psi_+(\vec{r})$ are the electron and positron Bloch wave functions and $n_l(\vec{k})$ is the occupation number of the state $\vec{k}$ in the band l. For a periodic potential at zero temperature we have[2]

$$\rho^{2\gamma}(\vec{p})=\sum_{\vec{k},l}\sum_{\vec{G}} n_l(\vec{k})\,|A_{\vec{k},l}(\vec{G})|^2\delta(\vec{p}-\vec{k}-\vec{G}) ,$$

where $A_{\vec{k},l}(\vec{G})$ are the Fourier coefficients of the positron-electron wave function product and $\vec{G}$ a vector of the reciprocal lattice. The coefficient $A_{\vec{k},l}(\vec{G}=\vec{0})$ gives a large contribution to $\rho^{2\gamma}(\vec{p})$ centered at $p_x=p_y=0$. The remaining $A_{\vec{k},l}(\vec{G})$ give rise to the higher-momentum components (HMC) of the electron and positron wave function product centered at each surrounding reciprocal lattice point $\vec{G}$. The $\vec{G}=\vec{0}$ component reveals best the shape of the Fermi surface while the HMC reflect more details of the wave functions of the electron and the positron. This paper reports a study of these higher-momentum components in Li and K. We compare theoretical predictions with two-dimensional angular correlations which are projections of the two-photon momentum density

$$N(p_x,p_y)\propto\int\rho^{2\gamma}(\vec{p})\,dp_z .$$

For Li preliminary results have already been reported.[3] The anisotropy of the Fermi surface was discussed in that work. For K, precise long-slit data were measured[4] to determine the effective mass of the positron. The analysis showed that the HMC must be taken into account. In that paper a model of the higher-momentum components was assumed, since no other information was available. That lack was a partial motivation for the present study.

The single crystals of Li and K were grown by a modified Bridgman technique. The angular correlation of annihilation photons was measured in two dimensions[5] using high-density proportional chambers. The experiment for Li was done at 100 K (i.e., just above its martensitic transition temperature), and the full width at half maximum (FWHM) of the angular resolution function was 0.6×0.6 mrad^2. The measurement of the single crystal of K was done at helium temperature and the experimental resolution function was 0.45×0.45 mrad^2 FWHM. In both experiments the orientation was chosen such that the projection of the momentum distribution onto the $(1\bar{1}0)$ plane was observed. In this orientation, the relevant HMC do not overlap in Li and K. Indeed, in between the projected HMC the intensity observed is due only to the core annihilation, which can thus be determined. This situation cannot be achieved in higher-valence metals such as Al in which HMC have been studied previously.[6] We have taken advantage of the symmetry of rotation of the core contribution to subtract the latter from the data[7] in order to obtain the higher-momentum components.

The band structure $E(\vec{k})$ and the two-photon momentum density $\rho^{2\gamma}(\vec{p})$ have been calculated using the Korringa-Kohn-Rostoker (KKR) method[8] together with a multiple scattering expression for $\rho^{2\gamma}(\vec{p})$.[9] The potentials were constructed from overlapping free-atom charge densities. The positron potential was obtained by removal of the exchange term and reversal of the sign. No electron-positron correlation was included.

In Figs. 1 and 2 we show the measured and calculated higher-momentum components for Li and K. The smaller bump is mostly due to the (110) higher zone, while the larger bump comes from two zones, $(01\bar{1})$ and $(10\bar{1})$, which coincide in projection. The higher components are much weaker, the $(00\bar{2})$ being barely visible in the noise of

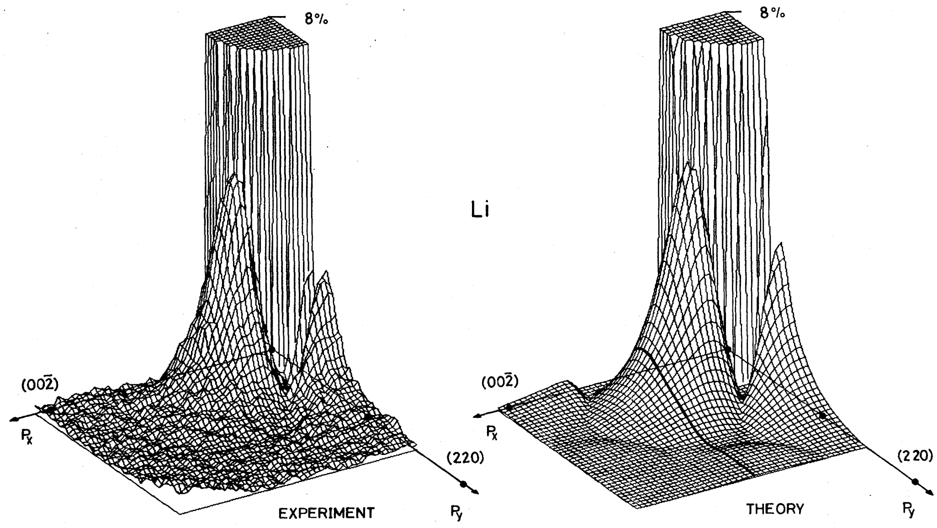

FIG. 1. Higher momentum components of the experimental angular correlation of annihilation photons from Li compared with the KKR calculation. The results are given as a fraction of the conduction-electron contribution at $p_x = p_y = 0$.

the experimental data, which is consistent with the small calculated value. The shapes of the measured HMC are quite different in these two metals. For Li, the HMC intensity is a sharp function of the momentum whereas in the case of K the HMC appear as nearly hemispherical contributions centered on the neighboring $\vec{G}$ points. In both measurements the (00$\bar{2}$) HMC are present with an intensity less than 0.3% of the central peak. In Fig. 3 we plot the intensity profile along a line parallel to [110] as indicated in the inset and by the heavy lines in Figs. 1 and 2. The shapes of the measured HMC are well reproduced by the calculation and the intensities are in reasonable agreement. From this we conclude that the many-body enhancement effect in the (110) zones is similar to that in the central zone for Li and K.

In conclusion, we have shown that the different shapes of the HMC and their intensities in Li and K are well reproduced by the KKR band structure calculation. The strongly different shapes reflect the difference in the wave functions of the two materials. In K the *s*, *p*, and *d* components of the electron momentum wave function are comparable in amplitude and interfere destructively over a surface which

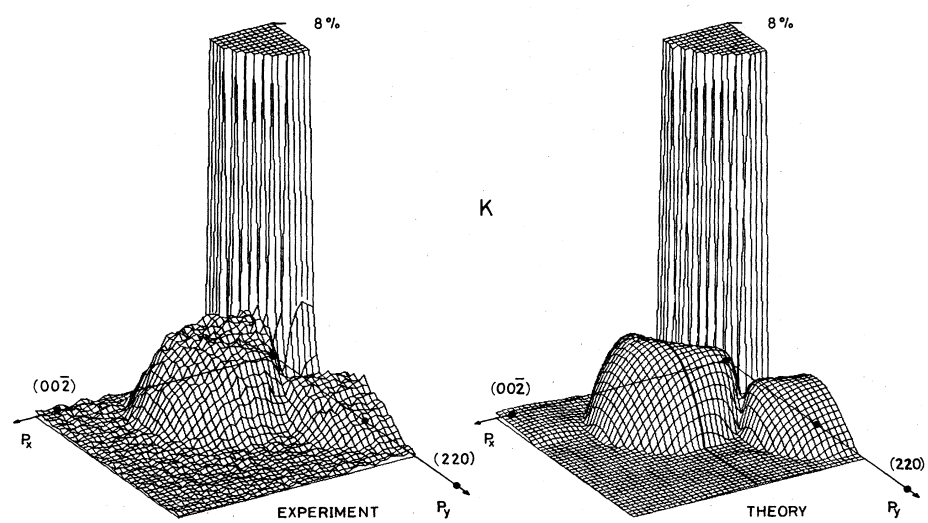

FIG. 2. Higher momentum components of the experimental angular correlation of annihilation photons from K compared with the KKR calculation. The vertical scale is as in Fig. 1.

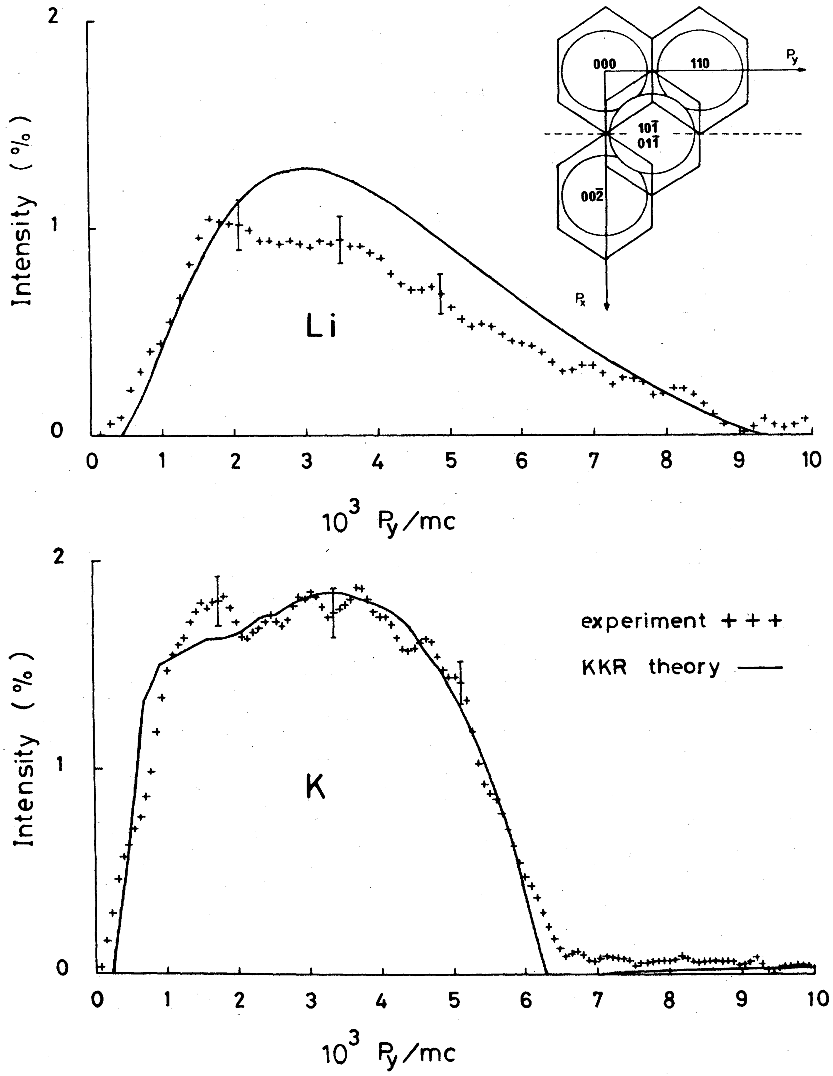

FIG. 3. Profile through the projection of (01$\bar{1}$) and (10$\bar{1}$) HMC's as shown in the inset and by the heavy lines in Figs. 1 and 2. Typical statistical errors are shown, but the scatter of points has been reduced by a smoothing procedure. The vertical scale is as in Fig. 1.

crosses the [110] direction near (0.65 0.65 0). Beyond this region the intensity increases and then falls off with increasing momentum. In Li such destructive interference does not take place and, hence, the momentum density simply decreases with increasing momentum. We plan to discuss these details more extensively in the future, together with the temperature dependence of the higher-momentum components, Fermi surfaces, and other many-body effects.

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