The electronic structure of Cu measured with the new 2D-ACAR spectrometer

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The two-dimensional measurement of the angular correlation of the positron annihilation radiation (2D-ACAR) is a powerful tool to investigate the electronic structure of materials. Recently a 2D-ACAR spectrometer has been set up at the Maier-Leibnitz-Laboratorium [1]. With this spectrometer it is possible to explore the electronic structure of correlated materials and their behavior at temperature driven phase transitions. As a proof of principle we report on the reconstruction of the Fermi surface of Cu.

When a positron is implanted into a solid, it will thermalize within a few ps and annihilate with an electron. The resulting annihilation radiation carries the momentum information of the electron-positron pair. This information is contained in a Doppler shift from the mean value of 511 keV, and the angular deviation from exact antiparallel directions of the two γ quanta. With 2D-ACAR the latter is measured, which yields a specific projection of the two γ momentum density $\rho^{2\gamma}$. Since the positron is at thermal energies, the angular deviation is caused mainly by the electron momentum.

The low momenta that are measured with 2D-ACAR are due to occupied states near the Fermi surface in the case of a metal. Due to the fact, that electrons in a crystal are in delocalised Bloch states $\rho^{2\gamma}$ can be expressed as

$$\rho^{2\gamma}(\mathbf{p}) \propto \sum_{j,\mathbf{k}} \Theta(E_\mathrm{F} - E_{j,\mathbf{k}}) \sum_{\mathbf{G}} \left| C^j_{\mathbf{G}}(\mathbf{k}) \right|^2 \delta_{\mathbf{p}-\mathbf{k},\mathbf{G}} \quad (1)$$

where the sum goes over all the states $\mathbf{k}$ below the Fermi level in the jth band. $C^j_{\mathbf{G}}(\mathbf{k})$ is the Fourier coefficient at the reciprocal lattice vector $\mathbf{G}$. From this equation we see that filled bands give a continuous distribution and bands crossing the Fermi level yield breaks which are distributed through the reciprocal space.

The task of calculating the full three dimensional $\rho^{2\gamma}$ from measured projections can be expressed as a minimization problem using the following equation, where $R^\alpha_i(D)$ is the Radon transformation, i.e. the projection, of the density D at an angle of α:

$$\chi^2 = \sum_\alpha \sum_i \frac{\left(R^\alpha_i(D) - M^\alpha_i\right)^2}{\sigma_i^2} \quad (2)$$

The main purpose of the reconstruction is to get a three dimensional density D which agrees with the 2D-ACAR spectra M^α_i (where $i = 1...N^2$ runs over all pixels) for all measured angles α with the statistical error σ_i. If M is of size N^2, then D has a size of N^3. Consequently, the minimization problem is highly under-determined. This is the reason why an additional restriction is needed. It is applied by using the following regularisation: The resulting density D should be the lowest possible. For this aim, a Lagrange function with an entropy function $\sum_j D_j \ln(D_j)$ and χ^2 is constructed by the use of the Lagrange multiplier λ:

$$L(D) = \sum_j D_j \ln(D_j) - \lambda\chi^2 \quad (3)$$

L hast to be maximized in order to obtain D. It is possible to get a solution using an iterative gradient approach.

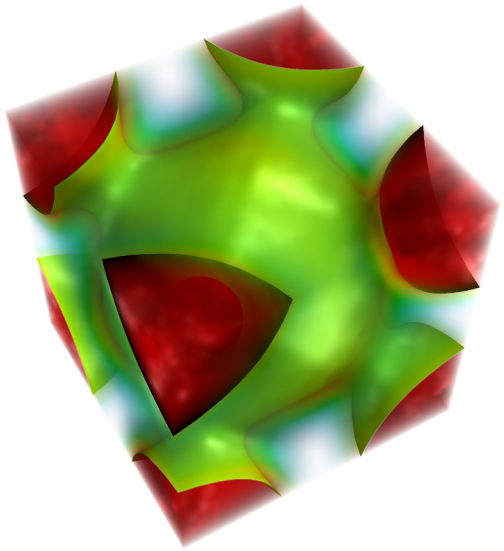

Figure 1: $\rho^{2\gamma}$ and Fermi-surface of copper calculated from 5 projections.

The main difference between this problem and a conventional problem of computerised tomography is the high symmetry: In case of $\rho^{2\gamma}$, which has the symmetry of the reciprocal lattice, the quality of the reconstruction can be greatly improved and the calculation time is reduced if the full symmetry is taken into account.

To calculate the three dimensional $\rho^{2\gamma}$ our algorithm was applied using five measured projections and all the equivalent directions. The data were then folded into the first Brillouin zone by the so called LCW procedure for three dimensions. The result is plotted in figure 1, which agrees well with previous measurements and calculations.

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REFERENCES

[1] H. Ceeh et al. *Rev. Sci. Instrum.*, **84**, 043905, 2013.