Fermi surface of the organic superconductor

$\kappa_L$-(DMEDO-TSeF)$_2$[Au(CN)$_4$](THF) with domain structures

The energy band calculation is a good method to predict the shape of the Fermi surface for organic conductors, but the resulting Fermi surface is sometimes sensitive to the adopted parameters of S and Se atoms. The quantum oscillation measurement is a powerful tool to investigate the Fermi surface. Kawamoto et al. reports the energy band calculation and the quantum oscillation of the title compound.

The $\kappa$-type conductors are reduced to a triangular lattice of dimers with anisotropic transfers $t$ and $t'$. This model gives a square lattice in the $t'/t = 0$ limit, but a one-dimensional chain in the opposite limit ($t'/t = \infty$). For the $\kappa$-(BEDT-TTF)$_2X$ superconductors, $t'/t$ is between 0.58 and 1.1, and falls in between the square and triangular lattices. The title compound with $t'/t = 1.71$ is located in the highly anisotropic triangular lattice region. The large anisotropy makes the $\beta$ orbit an elongated ellipse with $k_Fc/kFa = 1.54$. As a result, the cross-sectional area of the overlapping $\alpha$ orbit, $S_\alpha$, is 26% of the first Brillouin zone ($S_{BZ}$), and is considerably larger than the typical value, $S_\alpha \sim 16\%$ seen experimentally, in the isotropic $\kappa$-(BEDT-TTF)$_2X$ compounds. The $\beta$ orbit, $S_\beta$, is exactly the same as $S_{BZ}$. The degeneracy of the energy band on the zone boundary occurs when the crystal has glide planes or screw axes having translational symmetry perpendicular to the boundary. For the title compound, this symmetry is lowered by a structural phase transition at 209 K where domains form. As a result, the Fermi surface splits at the zone boundary, and the $\beta$ orbit becomes a magnetic breakdown orbit. The value of the energy gap should be quite small, because the low temperature structure is similar to the high temperature one.

The Shubnikov-de Haas (SdH) oscillations show two closed orbits as shown in Fig.1. The observed $S_\alpha$ is 24(2)% of $S_{BZ}$, and that of the $\beta$ orbit is 103(2)%. The observed large $S_\alpha$ verifies the elongated elliptical $\beta$ orbit predicted from the above band calculation using the parameter set with 4d orbitals of Se. The magnetic breakdown orbit is observed in the SdH oscillations under the low field region, consistent with the small energy gap at the zone boundary. The observation of the SdH effect shows that the title compound has a clean electronic system despite of the domain structures.

For details, see an article, “Fermi surface and in-plane anisotropy of the layered organic superconductor $\kappa_L$-(DMEDO-TSeF)$_2$[Au(CN)$_4$](THF) with domain structure”, Phys. Rev. B to be published by T. Kawamoto (A02), T. Mori (A01), Y. Takahide (A03), S. Uji (A03), D. Graf, J. S. Brooks, T. Shirahata (A05), M. Kibune, H. Yoshino, and T. Imakubo (A05).