Using Swiss light to dispel the shadows

Arguably one of top intellectual challenges facing solid state science is the question of the mechanism of high-T_c superconductivity. Both their unusually high T_c's and their maybe even more unusual normal state properties have conspired to make the cuprate high-T_c superconductors among the most intensively studied solids in existence. Photoemission spectroscopy has played a very important role in their investigation over the last twenty years, as it offers a direct window on the character and dynamics of the low-lying electronic states responsible for superconductivity. Milestones along the photoemission path [1] have included determination of their Fermi surface topology and form, the anisotropic energy gaps related to their d-wave superconducting order parameter and the existence of a pseudo-gap in their normal state.

The drosophila for high-T_c photoemission investigations is the bilayer system $Bi_2Sr_2CaCu_2O_{8+\delta}$, or Bi-2212 for short. This system is such a favourite because it delivers excellent cleavage surfaces and has a high T_c (maximally 95K). Considering the fact that the topology and shape of the Fermi surface is a basic characteristic of every metal, it was a highly remarkable situation that until now the origin of one of the two primal Fermi surface features of Bi-2212, namely its **shadow Fermi surface** (SFS), was still not understood. Here, we briefly relate how the circle has been closed, from the Swiss discovery of the SFS in 1994 [2], to how the strengths of the Swiss Light Source could be harnessed to finally dispel the shadows surrounding this phenomenon.

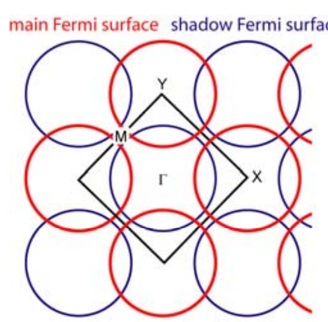

Figure 1: *Schematic of the main (red) and shadow (blue) Fermi surface in Bi2212 high-T_c superconductors.*

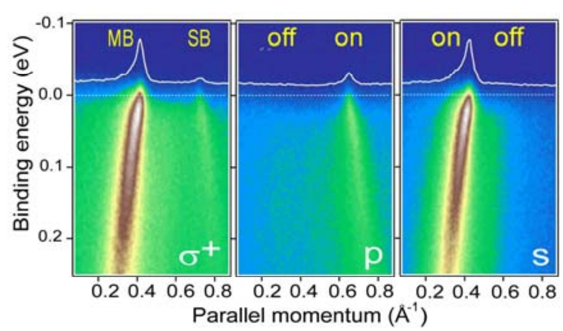

Figure 2: *Polarisation dependent ARPES data along the nodal (ΓY) k-space direction in Bi2212.*

Figure 1 shows a simplified schematic of the Fermi surface of a modulation-free sample of Bi-2212. The black box shows the commonly used (tetragonal) Brillouin zone, and the red (blue) circles represent the main (shadow) Fermi surfaces. The ΓM direction is parallel to the Cu-O bonds in the CuO_2 planes of the superconductor, whereas ΓY and ΓX have the nickname 'nodal' directions, as at these points on the Fermi surface the superconducting energy gap has its node. The data that gave us the first clue as to the microscopic origin of the SFS is shown in Fig. 2. Plotted is the photoemission intensity (colour scale) with binding

energy on the y-scale (zero is the Fermi energy) and crystal momentum (or wave vector) on the x-scale, in this case along the ΓY nodal direction. This data exploits one of the advantages of synchrotron radiation from the Swiss Light Source: its variable polarisation. The left-hand panel is recorded with circular polarised light (σ^+), the centre panel with p-polarised light and the right panel with s-polarisation. The σ^+ data show first the main band (labeled MB) and then, weaker, the shadow band (labeled SB). The big surprise was that s(p)-polarisation only shows the main(shadow) bands, never both together. This is clear evidence that the main and shadow states have different, in fact *opposing*, mirror symmetry with respect to the ΓY line in k-space. Intriguingly, along the ΓX nodal direction, both s (on-on) and p-polarisation (off-off) give the same behaviour for both main and shadow states.
How can a supposedly tetragonal crystal support states with different symmetries along the two Brillouin zone diagonals?

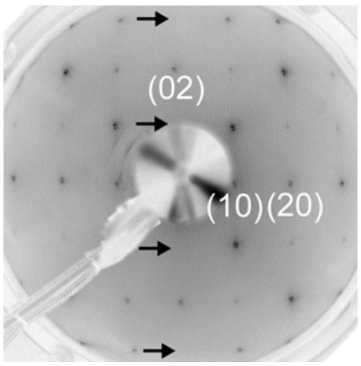

Figure 3: *LEED image taken from the (Pb,Bi)O termination layer of a twin-free (Pb,Bi)-2212 high-T_c superconductor.*

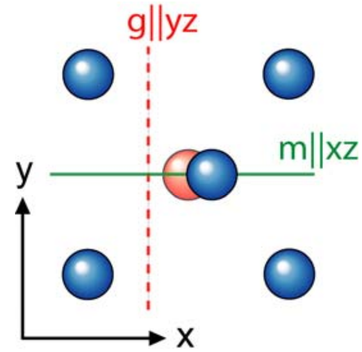

Figure 4: *Sketch of the true orthorhombic atomic positions (blue balls). If the system were tetragonal the central atom would be at the red position. The mirror (green) and glide-mirror (red) planes are marked.*

The answer came from electron diffraction data from modulation- and twin-free Pb-doped Bi-2212 crystals grown in the Amsterdam mirror furnaces. These display characteristic extinctions (missing spots) in the LEED patterns. These missing spots (marked with arrows in Fig. 3) can be attributed to (0,*k*) reflections (*k* being odd) within an *orthorhombic* unit cell. These systematic absences in the LEED pattern do not come about simply because the lattice constants *a* and *b* are not equal, but arise from a significant shift of an atom from its tetragonal position, such as the displacement of the central atom shown in Fig. 4. The red ball represents the undistorted, tetragonal position and the offset, blue ball the displaced orthorhombic position.
The orthorhombic symmetry and the atom displacements are also found in high-quality single-crystal x-ray and neutron diffraction data [3]. These orthorhombic displacements mean that the only remaining mirror plane is the ***xz*** plane (relevant for nodal ΓX data); the diagonals are no longer crystalline mirror planes at all and there is now a glide plane running parallel to ***yz*** (relevant for nodal ΓY data). It is this glide plane that is responsible for the parity flip seen in the photoemission data [4].
Thus, the shadow Fermi surface chapter in the Bi-based high-T_c superconductors can finally be closed. We prove that the shadow Fermi surface has nothing to do with short-range antiferromagnetic spin correlations, but is rather due to orthorhombic displacements of atoms from the ideal tetragonal positions (both in the Bi-O planes and to a lesser extent in the CuO_2 planes). This causes a back-folding of bands within the new, smaller orthorhombic Brillouin zone, and gives the bands different mirror symmetry in the ΓY and ΓX Brillouin zone

quadrants. The fact that these distortions are felt strongly by the Cu-O derived electronic bands, and even influence the mirror symmetry of these states illustrates that the canonical Brillouin zone and Fermi surface for the Bi-based high-T_c needs to be revised. The only experimental challenge remaining would be to detect the hybridisation gaps opening up where the 'main' (red) and 'shadow' (blue) Fermi surfaces shown in Fig. 1 intersect.

References

[1] A. Damascelli, Z. Hussain and Z.-X. Shen, Rev. Mod. Phys. 75, 473 (2003)
[2] P. Aebi *et al.*, Phys. Rev. Lett. **72**, 2757 (1994)
[3] C. C. Toradi *et al.*, Phys. Rev. B**39**, 227 (1988); N. Jakubowicz *et al*., Phys. Rev. B**63**, 214511 (2001); P. A. Miles *et al.*, Physica C **294**, 275 (1998)
[4] V. Arpiainen and M. Lindroos, Phys. Rev. Lett. 97, 037601 (2006)

Publications

- **Experimental proof of a structural origin for the shadow Fermi surface of $Bi_2Sr_2CaCu_2O_{8+\delta}$**
  *A. Mans, I. Santoso, Y. Huang, W. K. Siu, S. Tavaddod, V. Arpiainen, M. Lindroos, H. Berger, V. N. Strocov, M. Shi, L. Patthey, and M. S. Golden**
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