Atomic Structures Studied by Aberration-corrected Transmission Electron Microscopy

August 26, 2008 (HP14). In the issue of *Science* dated July 25, 2008, Professor Knut Urban published a concise, but important invited review of the study of atomic structures by the recently introduced aberration-corrected transmission electron microscopy (TEM), which he and his group pioneered in the 1990s [1]. The new generation of aberration-corrected instruments suitable for TEM and scanning TEM (STEM) enables studies in condensed matter physics and materials to be performed at atomic-scale resolution. This meets the growing demand of nanosciences and nanotechnology for the atomic-scale characterization of materials, nanosynthesized products and devices, and the validation of expected correlations. Equipped with electron-energy filters and electron-energy loss spectrometers (EELS), the new microscopes allow studies not only of structure, but also of elemental composition and chemical bonding. The energy resolution is about 100 meV, with spatial resolution on the order of 100 picometers and an accuracy of a few picometers.

This new development is of direct interest and considerable importance to researchers in the field of superconductivity. For example, the Mannhart group of Augsburg, Germany, recently discovered superconductivity when studying the interface of two insulating perovskites $LaAlO_3$ and $SrTiO_3$ [2]. In their work and interpretation they were decisively aided by aberration-corrected STEM and EELS.

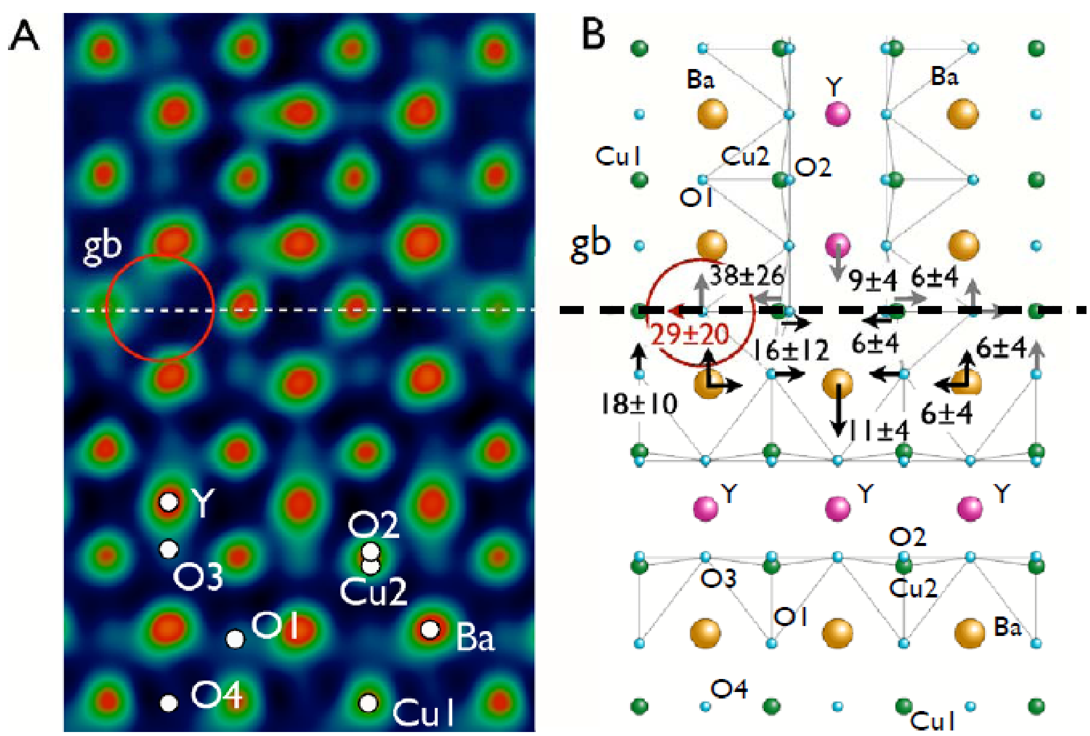

Fig. 1. A 90° tilt boundary in the superconductor YBa2Cu3O7. The structure was solved by employing the NCSI technique in combination with exit-plane wave function reconstruction. (**A**) Due to lateral mismatch of the lattice above and below the grain boundary (denoted "gb") the position of every third Cu-atom in the boundary is giving rise to diffuse intensity. The apex oxygen atom "O1" (red circle) relaxes towards this Cu-atom position. (**B**) Local atom relaxations across the boundary can be measured at an accuracy (95 % confidence level of a Gaussian regression analysis) of better than 5 pm.

As another example of superconductor research, the image and model of atomic bond relaxations at a 90^{o} tilt boundary in YBCO are shown in Figure 1 above [3]. The authors could measure the oxygen occupancy in the copper–oxygen chain and changes of the bond-lengths between copper and the apical oxygen, which are known to affect the local superconducting properties.

It is important to emphasize that the understanding of image results is generally not straightforward and possible only via extensive quantum-mechanical calculations. One cannot calculate the structure "backwards" from the exit-plane wave function. Rather, a "forward" calculation is necessary, in which the Dirac equation in small-angle approximation is solved numerically and iteratively improved to obtain the best fit between calculated and experimental exit-plane wave function.

[1] Knut W. Urban, "Studying Atomic Structures by Aberration-Corrected Transmission Electron Microscopy", *Science* **321**, 506-510 (2008).

[2] N. Reyren *et al*., "Superconducting Interfaces Between Insulating Oxides", *Science* **317**, 1196 (2007).

[3] L. Houben, A. Thust, K. Urban, "Atomic-precision determination of the reconstruction of a 90o tilt boundary in $YBa_2Cu_3O_{7-\delta}$ by aberration-corrected HRTEM", *Ultramicroscopy* **106**, 200 (2006).