Local structure as a probe of stripes and its relation to $T^*$

S. J. L. Billinge, M. Gutmann and E. S. Božin

Department of Physics and Astronomy and Center for Fundamental Materials Research, Michigan State University, East Lansing, MI 48824-1116, USA

We describe atomic pair distribution function (PDF) analysis measurements of the local structure from a range of HTS materials. These are analyzed to search for the presence of, and characterize the nature of, fluctuating stripe phases in the bulk of superconducting HTS samples. We find evidence for the presence of local stripe phases in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$. At least in the 214 system of cuprates, we have evidence of a correlation between local charge inhomogeneities and $T^*$, the pseudo-gap closing temperature.

The existence, or otherwise, of fluctuating charge stripes in the high-temperature superconductors, and their importance to the superconductivity itself, remains one of the most important unsolved problems in High-Tc superconductivity [1]. Charge superlattice peaks are seen when the stripes are static and long range ordered [2]. Incommensurate, inelastic magnetic peaks have been used to infer their existence in a fluctuating, local sense [3]. Both observations are limited to a small number of the superconducting materials. The local atomic structure provides an independent probe for stripes. The Cu-O bond length changes as the charge-state of copper changes. Therefore, atomic scale charge inhomogeneities will result in enlarged Cu-O bond length distributions.

Using the atomic pair distribution function (PDF) analysis of powder neutron diffraction data we are attempting to determine whether or not the bulk of superconducting samples is generically in a fluctuating charge-stripe state. The Cu-O bond length changes as the charge-state of copper changes. Therefore, atomic scale charge inhomogeneities will result in enlarged Cu-O bond length distributions.

The PDF is a high resolution probe of the local atomic structure in a material. Neutron or x-ray powder diffraction data are reduced to the normalized sample-dependent total scattering factor, $S(Q)$, which is Fourier transformed to yield the atomic pair-correlation function [5,6]. This gives the real-space distribution of atomic pairs and directly probes the local atomic structure. The PDF can then be fit with PDFs calculated from models to extract structural information.

An enlarged Cu-O bond length distribution is seen in doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [7] consistent with the presence of stripes. Remarkably, the Cu-O PDF peak, measured at 10 K, broadens with increasing doping up to optimal doping where it abruptly sharpens again, regaining its unaltered (single valued) width in the overdoped state. This suggests that charge inhomogeneities (presumably stripes) are present in the copper-oxygen plane in the underdoped state but disappear in the overdoped regime. The disappearance of the local inhomogeneities coincides with the doping level where the pseudo-gap temperature, $T^*$, meets $T_c$ [8].

There is independent evidence in the PDF supporting the presence of an inhomogeneous charge distribution in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The presence of different Cu-O bond lengths gives rise to CuO$_6$ octahedral tilt disorder which is clearly observed in the PDF [7,9]. We also have single crystal neu-
tron data from La$_{1.875}$Sr$_{0.125}$CuO$_4$, collected on the single crystal total scattering diffractometer, SXD, at ISIS which shows structured diffuse scattering at low temperature which we believe to be from disordered tilts. Studies of diffuse scattering in single crystals are an important complement to PDF studies which are powder measurements.

There is also evidence for charge inhomogeneities in YBa$_2$Cu$_3$O$_{6+y}$ over a wide $x$-range, though it is not so direct as in the 214 materials. In this case a short Ba-O correlation overlaps the Cu-O nearest-neighbor peak making a direct observation of peak broadening difficult. However, we have carried out extensive local structural modeling using PDFFIT [10], a full-profile least-squares PDF refinement program, and find evidence for charge inhomogeneities [11]. At the same time, we suggest a resolution to the 10 year old controversy between the extended x-ray absorption fine structure (XAFS) and diffraction communities over a split position for the apical oxygen in this system: XAFS sees it, diffraction sees no evidence for it [12,13]. Our finding is that there is no evidence in the PDF for a split position for apical oxygen; however we can refine a split position for the planar copper along the $z$-direction. This may be what XAFS was seeing (since they are sensitive to pair correlations) and is evidence for charge inhomogeneities because changing the charge-state of copper in this structure causes it to displace along $z$. Unfortunately, the quality of our data is not good enough to systematically quantify the doping dependence. These studies are being extended to more superconducting systems.

We would like to acknowledge funding from NSF-DMR9700966. MG acknowledges support from the Swiss National Science Foundation.

REFERENCES