Metal-Insulator Transitions in Complex Oxides Probed by High Resolution X-Ray Compton Scattering

The Coulomb repulsion in transition metal oxides (TMO) tends to localize individual d electrons on metal atoms while the hybridization with the oxygen *p* electron states de-localizes these same electrons. These competing effects explain the metal insulating transition (MIT) in a TMO. Several theories have been put forward to explain the MIT, some generalize the concept of the Fermi liquid, while others attempt to describe highly correlated behavior by using Hubbard models. In this context, the comparison of the measured electron momentum density with the predictions of theories gives an indication of their correctness. Detecting the energy of photons scattered at a fixed angle in back-scattering geometry from a mono-energetic beam incident on the sample gives access to the Compton profile (CP), which is a projection onto one dimension of the electron momentum density.

Recently, the combination of X-ray Compton scattering experiments and reliable density functional theory (DFT) calculations has revealed unique information about the MIT in the bi-layer manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$ [1]. This TMO undergoes a characteristic MIT when a magnetic field is applied, which is known as the colossal magneto-resistance (CMR) effect. Presently, intensive research is being carried out in developing spintronics technology based on this property. Until now, the CMR effect has been understood with models in which only the *d* electronic states of Mn are involved. The X-ray Compton scattering results have helped to gain a deeper understanding of the phase transition under consideration and have demonstrated the need to consider the *p* electronic states of oxygen as well. CP differences between the metallic and insulating state have shown that Compton scattering is an incisive probe of the electronic behaviour across the MIT.

Figure 1 shows results of the Compton scattering experiment compared to the DFT. The $La_{2-2x}Sr_{1+2x}Mn_2O_7$ single crystal with x = 0.35 has been studied as a function of temperature and magnetic field. Quantitative agreement has been found between DFT calculations and experiment with respect to the CP anisotropy in the two metallic phases (i.e. the low temperature ferromagnetic and the CMR phase under a magnetic field of 7 T). Robust signatures of the metal-insulator transition (MIT) have been identified in the momentum density for the paramagnetic phase above the Curie temperature. In particular, a strong deviation for low electron momentum has been noticed by comparing the CP anisotropies of the paramagnetic (insulating) and ferromagnetic/CMR (metallic) phases as shown in Fig. 1.

In Fig. 2, the power spectra of the CP anisotropies reveal that the experimental data for the metallic phases and the theory are in agreement and that

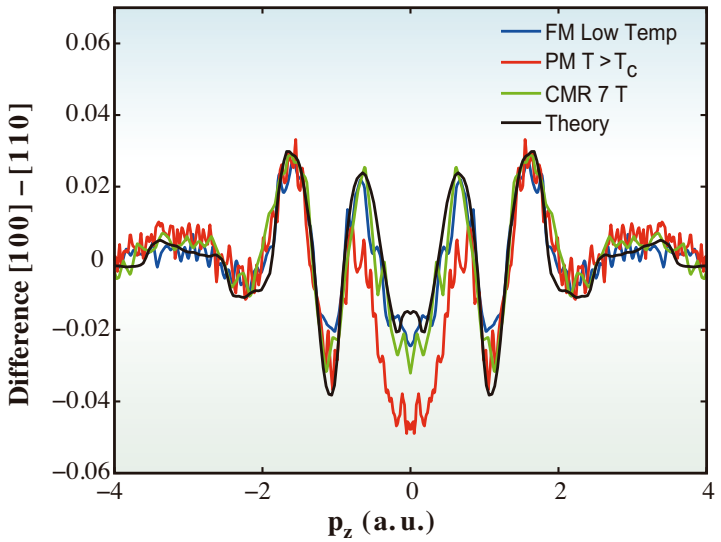

Fig. 1. Anisotropy of the CP [100]-[110]. In the legend, Low Temp FM is for the ferromagnetic phase at 20 K, PM $T>T_c$ is for the paramagnetic phase at 131 K, CMR 7 T is for the colossal magnetoresistance phase in an external field of 7 T at 131 K and Theory is for the DFT calculations. The data are in units of the CP amplitude at the origin.

the wave functions are of a delocalized nature. However, the experiment for the insulator shows a clear tendency to shift spectral weight towards short distances. Thus, the localization trend for the insulator wave functions becomes clear.

The anisotropy of the 2-dimensional momentum density in Fig. 3 shows important contributions of oxygen *p* electrons to the Fermi surface (FS). In the insulator, some of these *p* electron contributions at low momentum must redistribute since the FS vanishes. Thus, an important outcome of this work is the determination of the number n_e of displaced electrons across the metal-to-insulator transition. The value of n_e (about 0.7 electron per Mn atom) can in fact be extracted from the area enclosed by the anisotropy difference of Fig. 1. Therefore, by measuring the number of displaced electrons across the MIT, X-ray Compton scattering opens new opportunities for studying quantitatively the phase diagrams of other complex materials such as magnetite [2].

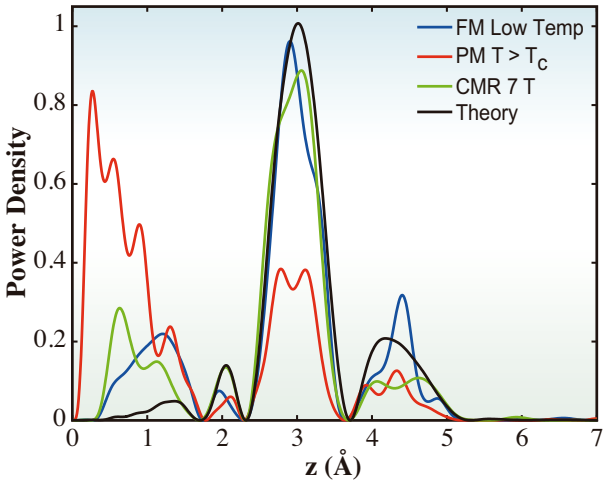

Fig. 2. Comparison in real space of the power spectra of the CP anisotropies. All the curves are normalized to a unit area. The notations in the legend are as in Fig. 1.

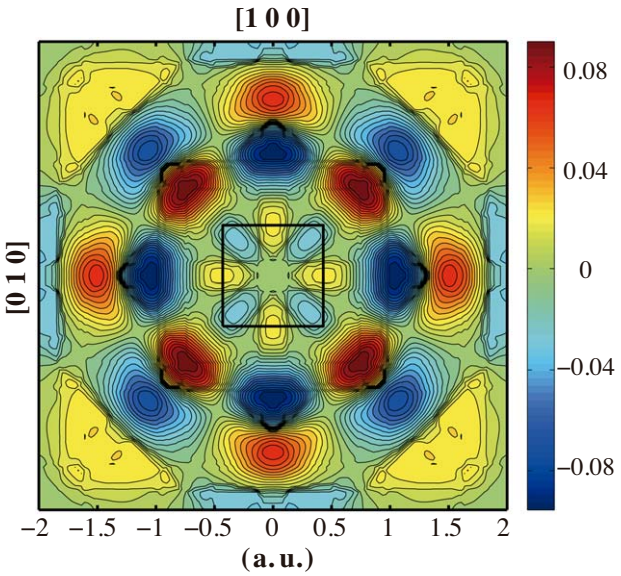

Fig. 3. Anisotropy of 2D projection of the theoretical electron momentum density onto the (001) plane. The first Brillouin zone is shown by a square. The anisotropy integration along the [0 1 0] axis yields the theory curve of Fig. 1. The data are in units of the momentum density amplitude at the origin.

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References

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[2] H. Kobayashi *et al.*: Phys. Rev. B **80** (2009) 104423.