

spectroscopy with respect to the site of excitation, to the spin of the intermediate state and its Bloch-k- and symmetry-selectivity, which opens RIXS a broad field of applications for studies of electronic excitations. Especially shake-up processes in the intermediate state connected with excitations across the Hubbard gap of highly correlated systems have attracted much attention.

Keywords: inelastic X-ray scattering, electronic structure, resonant scattering

MS88.30.2

Acta Cryst. (2005). A61, C112

Theory and Calculations of Inelastic X-ray Scattering

Juha Aleksu Soinenin, Department of Physical Sciences, University of Helsinki, Finland. E-mail: aleksi.soininen@helsinki.fi

Non-resonant inelastic x-ray scattering (IXS) can be used to study the dynamics of the electronic excitations of the sample. Although in many cases the ground state of the sample is well described with the standard computational methods the excited states still pose a challenge. We will present computational results for IXS from core and valence electrons in solids. The behavior of the core excited states is dominated by the localization of the core-hole. In practice this means that the problem can be written as an effective single-particle problem for the final state electron. Since valence excited states are a combination of two delocalized states the problem cannot be reduced to an effective single-particle approach. One is forced to consider the whole complexity of the two-particle problem.

We will analyze recent experimental IXS results for core and valence excited states using band structure based approaches [1,2] and a real space multiple-scattering approach [3]. The role of the electron-hole interaction and quasiparticle effects in IXS will be reviewed. For the core-excited states an analysis of the momentum transfer dependence of the IXS cross-section respect to the final state local density of states will be presented. Calculated dispersions of valence-excitations will be compared to experimental results for selected cases.

[1] Soinenin J.A., Shirley E.L., *Phys. Rev. B*, 2001, **64**, 165112. [2] Soinenin J.A., Shirley E.L., *Phys. Rev. B*, 2000, **61**, 16423. [3] Soinenin J.A., Ankudinova A.L., Rehr J.J., to be submitted.

Keywords: inelastic X-ray scattering, electronic structure calculations, spectroscopy

MS88.30.3

Acta Cryst. (2005). A61, C112

Across the Mott Gap: Electronic Excitations in Transition Metal Oxides

John P Hill, Department of Physics, Brookhaven National Laboratory, USA. E-mail: hill@bnl.gov

Studies of the electronic excitations in strongly correlated systems are important because these excitations may play a key role in the materials' behavior and because such measurements provide stringent tests of the various theoretical approaches to the strongly correlated problem. Here, we report inelastic x-ray scattering studies of momentum-resolved excitations in cuprates and manganites.

In the 1D cuprate, SrCuO₂ results suggest that the excitation spectrum consists of a holon-anti-holon continuum together with a broad resonance, consistent with a parameter-free calculation of the dynamical response function [1]. In contrast, in the 2D cuprate system, La_{2-x}Sr_xCuO₄ [2] better-defined excitations were observed. At x=0, two broad peaks are found that are strongly momentum dependent. Higher-resolution measurements suggest that these are in fact comprised of a number of long-lived excitations. As carriers are doped into the system, excitations below 3eV are replaced by a momentum dependent continuum. Finally, the dependence of the excitations on the electronic ground state is revealed in 3D manganites in which the observed temperature dependence is correlated with changes in the magnetism and associated with intersite *d-d* excitations.

The author gratefully acknowledges his collaborators Y.-J. Kim and S. Grenier. Work supported by US DOE, DE-AC02-98CH10886.

[1] Kim Y.-J. et al., *Phys. Rev. Lett.*, 2004, **92**, 137402. [2] Kim Y.-J. et al.,

Phys. Rev. Lett., 2002, **89**, 177003. [3] Grenier S. et al., *Phys. Rev. Lett.*, 2005, **94**, 047203.

Keywords: inelastic X-ray scattering, electronic excitations, strongly correlated systems

MS88.30.4

Acta Cryst. (2005). A61, C112

Magnetic Inelastic X-ray Scattering as a Probe of Electronic Excitations in Correlated Electron Materials

Pedro A. Montano^a, Yinwan Li^{b,c}, J. F. Mitchell^c, B. Barbiellini^d, P. E. Mijnaerends^{d,e}, S. Kaprzyk^{d,f}, A. Bansil^d, ^aSUFD, U. S. Department of Energy, 1000 Independence Avenue, Washington DC 20585, USA. ^bDepartment of Physics, University of Illinois, Chicago IL 60680. ^cMaterials Science Division, Argonne National Laboratory, Argonne IL 60439. ^dPhysics Department, Northeastern University, Boston MA 02115. ^eDepartment of Radiation, Radionuclides & Reactors, Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands. ^fAcademy of Mining and Metallurgy AGH, 30059 Krakow, Poland. E-mail: pedro.montano@science.doe.gov

The magnetic x-ray scattering technique in the deeply inelastic (Compton) regime is emerging as a powerful new spectroscopic window for understanding the properties of magnetic electrons in complex materials. Here we consider results on three correlated electron systems of current interest: The double layer manganite La_{1.2}Sr_{1.8}Mn₂O₇, the perovskite manganite La_{0.7}Sr_{0.3}MnO₃ and the magnetite F₃O₄. First principles band theory computations using the conventional local density approximation (LDA) as well as computations going beyond the LDA framework for treating correlation effects are used to gain insight into recent magnetic Compton scattering measurements. We show how in the double layer manganite the [110] magnetic Compton profile (MCP) contains a distinct signature of the d-electrons of x²-y² symmetry, allowing us to monitor significant changes in the occupancy of these orbitals as a function of temperature over the range of 5-200K. An itinerant electron contribution is suggested at all temperatures in magnetite. In magnetite, we find that the magnetic moment associated with unpaired spins is non-integral and we adduce that the charge ordering model of the Verwey transition is not tenable.

Keywords: magnetic, compton, electronic

MS88.30.5

Acta Cryst. (2005). A61, C112

Correlations in Inelastic Scattering and Plasmon Filtered Imaging

Tobias A. Colson, A.F. Moodie, H.J. Whitfield, Department of Applied Physics, School of Applied Sciences, RMIT University, GPO Box 2476V, Melbourne, 3001, Australia. E-mail: tobias.colson@rmit.edu.au

It is often assumed that inelastic electron scattering from the plasmon is incoherent and confined to small angles. However it can be seen that this is not the case in elements and compounds that share the 'simple' metal form of electron correlation. A continuous electron density distribution results in a characteristic 'bare' plasmon spectrum. In this case it can be shown that through the filtering of electrons that have suffered multiple interactions with the plasmon region of a material, images can be formed from regions at thicknesses that would conventionally provide little to no contrast [1].

However, in order for this to occur, the primary interaction must be with conduction electrons, thereby generating a 'bare' plasmon form of low loss spectrum. When the primary interaction is no longer with the conduction electrons, then this 'bare' or simple form is lost.

Thus we endeavour to show that analysis and imaging from the low loss spectrum of EELS can provide information not only about the physical structure of the material e.g. dislocations, but also about electronic properties beyond the band gap.

[1] Moodie A.F. et al., *ultramic*, 2004, **101**, 247.

Keywords: plasmon, correlation, eels