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Condensés

Electronic excitations in transition metal oxides with resonant inelastic X-ray scattering (RIXS)

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Introduction

Understanding the electronic structure of strongly correlated materials is a long-standing problem in condensed matter physics. Several properties of these materials like their anti-ferromagnetic insulating behavior in the undoped phase, the transition to the metallic state on doping and high T_C superconductivity are directly related to the electronic correlations. RIXS is a bulk-sensitive method for investigating electronic excitations of these materials complementary to methods which provide information on ground state electronic structure. The resonance is used to enhance the cross-section and choose a particular intermediate state. Here we measure excitations in the eV range which are on-site excitations of the crystal field. High resolution (300 meV FWHM) spectroscopy is a must for these measurements.

RIXS

Instrumentation

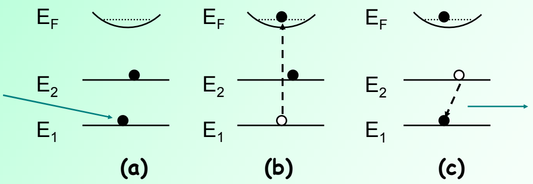


Fig. 1: RIXS principle
(a): An incident photon excites an electron of the inner shells.
(b): This electron goes to the Fermi level.
(c): Another electron fills the remaining core hole.
Final state of RIXS process with an hole in the core shells.

Fig. 2: Taiwanese beamline BL12XU at Spring-8.
single crystal pre-monochromator Si(111)
double channel-cut Si(400) crystal monochromator

Fig. 3: Analyzer (Cu K-edge)
- Si (553), Bragg angle 77.56°
- 2m spherically bent
- anodic bonding technique

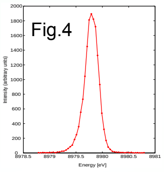


Fig.4 displays an overall experimental resolution of ~300 meV.

CoO and NiO

Fig.10: RIXS, Co quadrupolar peak
k // [100], E_i = 7709 eV

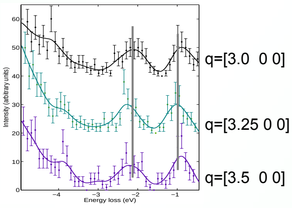


Fig.9: XAS, Co K-edge

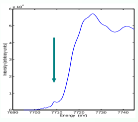


Fig.11: **k** // [100], q=[3.25 0 0]

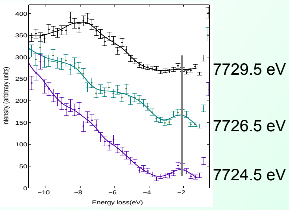


Fig.13: RIXS, Ni quadrupolar peak, **k** // [100], E_i = 8334 eV

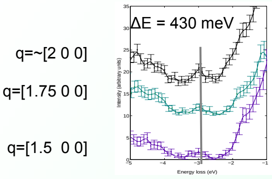
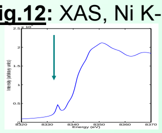


Fig.12: XAS, Ni K-edge



CuO

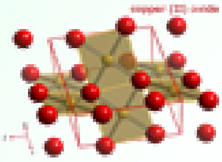


Fig.5: XAS, Cu K-edge

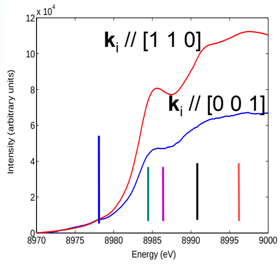


Fig.8: RIXS Cu K-edge, low resolution **k** // [001], **ε** out of plane
colors correspond to bars in fig.5.

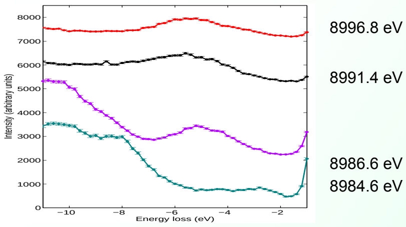
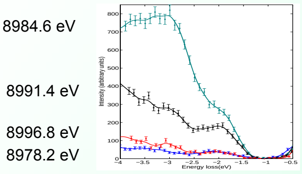


Fig.7: RIXS Cu K edge, **k** // [110], q = [2.26 2.26 0], **ε** in plane
colors correspond to bars in fig.5.



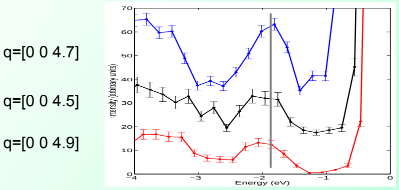


Fig.6: RIXS, **k** // [001], E_i = 8978 eV **ε** out of plane

A Constant Final State scan allows measurements through the edge preserving the transferred energy.

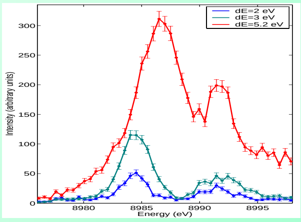


Fig.8: Constant final states, **k** // [110]
ε in plane

Ghiringhelli et al. [2] calculations assign the ~2eV feature at d-d excitations.

Conclusion

RIXS measurements in correlated materials provide new spectroscopic data and opportunity to understand more about the physics of the systems. Thanks to good experimental resolution, we see excitations in the eV range in transition metal oxides. In transition metal oxides, the excitations are localized with no dispersion. We interpret these as excitations of the crystal field. Higher energy excitations are related to charge- transfer.
High resolution RIXS is thus a powerful tool providing a way to measure excitations of the order of 1eV with bulk sensitivity in these compounds.

References:
[1] Zhang et al., *Phys. Rev. B*, **58**, 13520 (1998)
[2] Ghiringhelli et al., *Phys. Rev. Lett.*, **92**, 117406 (2004)

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