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Names and affiliations of applicants (* indicates experimentalists): Marco GRIONI* IPN - Ecole Polytechnique Fédérale, CH-1015 Lausanne (Switzerland). Claudia DALLERA* Department of Physics, Politecnico di Milano, Piazza Leonardo da Vinci 32, I-20133 Milano (Italy) Atsushi FUJIMORI, Shin.Ichi UCHIDA Department of Physics, University of Tokyo (Japan)		

Report:

We exploited high-resolution x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS) to investigate the 4f configuration of metallic cerium across the isostructural α - γ transition, and the local electronic structure at the Cu sites of various cuprate samples.

Cuprates:



Fig. 1. Cu K edge XAS spectra of LSCO samples illustrate the Cu "d" character of in-plane holes induced by Sr doping.



Fig. 2. A Cu K α spectrum measured at pre-edge with light polarized at 45° from the c-axis is decomposed into "in plane" and "c-axis" contributions.

We exploited the chemical and symmetry sensitivity of high-resolution Cu K α PFY-XAS and Cu K α RIXS to study the local electronic structure of various cuprates, including single crystals of La_{2-x}Sr_xCuO₄ (LSCO, x=0.15, 0.30). Figure 1 illustrates the pre-edge rgion of the Cu K XAS spectrum from 1s \rightarrow 3d transitions. The structure, which reflects the "Cu d-symmetry" of the valence holes, grows with Sr doping, and disappears for light polarized along the "c" axis (dashed). The selectivity to polarization is even stronger in the corresponding RIXS spectra (1s² \rightarrow 1s3d^{N+1} \rightarrow 2p⁵3d^{N+1}) of Fig. 2. Here, a spectrum measured with linear polarization at 45° from the c-axis is decomposed into "in-plane" and "c-axis" contributions, separately determined from "pure" spectra measured with the polarization vector respectively perpendicular and parallel to the c-axis [1].

Cerium:



Fig. 3. Ce L₃ PFY-XAS of <u>Ce</u>Sc in the γ (300 K) and α (20 K) phases. The the relative weight of the various (spectator) 4f configurations changes across the transition.



Fig. 4. Ce L α RIXS spectra of the two phases measured in correspondence of the pre-edge (<u>cf</u>²) feature in the XAS spectrum. The "f²" weight is well visible, and larger in the α - phase.

Figure 3 shows Ce L₃ (2p \rightarrow 5d) XAS spectra of CeSc(7%), in the γ (300 K) and α (20 K) phases, measured in the high-resolution L α partial fluorescence yield (PFY) mode. The 4f electrons are "spectators" in the L₃ XAS process, but different Ce 4f configurations are separated by the 2p - 4f Coulomb interaction, and well visible in the difference curve (dashed line). We observe an increase of the 4f⁰ weight in the α -phase, reflecting the larger 4f-band hybridization and Kondo temperature (T_K(α)~1000 K vs. T_K(γ)~20 K). The new information from these data is the clear observation of a pre-edge feature ~5 eV below the main cf¹ peak, i.e. coinciding with the cf² final state in the 3d XPS spectrum (vertical bars). It was predicted [1], but never clearly observed due to the broad lineshape of conventional XAS spectra. Its intensity increases between 300 K and 20 K, indicating a larger weight of the 4f² configuration in the ground state of α -Ce. This is confirmed by RIXS data (2p⁶4f^N \rightarrow 2p⁵4f^N 5d \rightarrow 3p⁹4f^N 5d; Fig. 2) measured in correspondence with the pre-edge XAS feature. The cf² spectral feature (dashed) is here strongly enhanced relative to the main cf⁴ line, and a 50% increase of the 4f² weight in the ground state is established [2].



- [2] A. Kotani, T. Jo and J.-C. Parlebas, Adv. Phys. 37, 37 (1988).
- [3] C. Dallera et al., to be published in Phys. Rev. B.