Fe-*K* edge Resonant Inelastic X-ray Scattering in Single Crystal $PrFeAsO_x$

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The fresh discovery of high-Tc superconductivity in the iron oxypnictides [1] has generated a profusion of studies about their electronic structure. Still, there remain essential ambiguities that have yet to be addressed, such as the importance of the electron correlation effects, stressing the need for further in-depth studies. We here report on the first measurement on iron oxypnictides using resonant inelastic x-ray scattering (RIXS), a fine probe of the electronic structure, at the Fe-*K* edge. We chose the superconductor $PrFeAsO_{0.7}$ (critical temperature Tc=42 K) and its parent compound PrFeAsO, which belong to the so-called 1111 family. The experiment was performed at the Taiwan beamline BL12XU at SPring-8. The incident undulator beam was monochromazited via a Si(111) double-crystal monochromator, and the scattered beam was analyzed with a 1-m bent Si(531) crystal for $PrFeAsO_{0.7}$ and Ge(620) for PrFeAsO. The total energy resolution was estimated to be approximately 1 eV.

The incident energy dependence of the RIXS spectrum across the Fe-*K* edge is plotted in Fig. 1 as a function of loss energy, which is defined as the difference between the incident (E_1) and the emitted photon (E_2) energies. The spectra between E_1=7110 and 7117.5 eV were collected on $PrFeAsO_{0.7}$ at Q=[0 0 6.5], and those between E_1=7120 and 7131 eV on PrFeAsO at Q=[0 0 6.7]. The vertical offset of the spectra is scaled to the E_1 axis of the absorption spectrum on the left panel. Both spectra at E_1=7110 and 7112.5 e V exhibit a feature at E_1-E_2=4 eV which drifts linearly with E_1 above the pre-edge. Above the main edge, a feature with a closely ressembling behavior is observed to stay at E_1-E_2=4 eV between E_1=7120 and 7124 eV while its loss energy position tracks linearly with E_1 above 7124 eV.
An enlarged plot of this latter feature is presented in Fig. 2, as a function of loss energy in the left panel and photon energy in the right panel. For clarity, the elastic peak is not shown in the latter plot. Both plots confirm the pure Raman character of the feature between E_1=7120 and 7124 eV, switching to a fluorescence-like behavior at constant E_2=7120 eV for higher E_1. We note there seems to be some residual spectral weight around E_1-E_2=4 eV up to E_1 =7131 eV. Based on a comparison with calculated density of states [2], we ascribe the 4-eV Raman feature to the charge transfer excitation between As *4p* and Fe *3d*. This feature was found to be nondispersive and identical for $PrFeAsO_{0.7}$ and PrFeAsO.

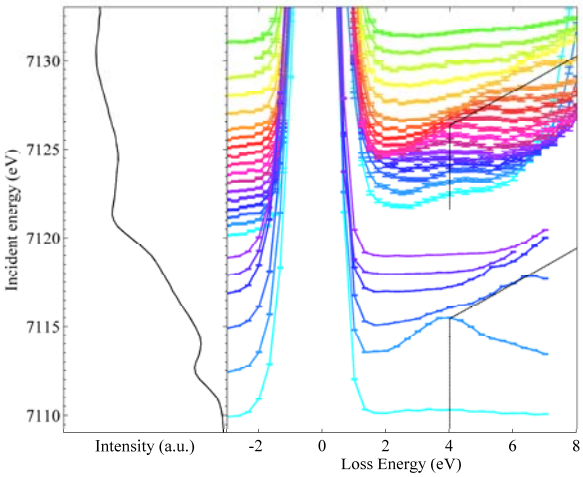

Fig. 1: Fe-*K* absorption spectrum (left panel) and RIXS spectra as a function of E_1 across the edge (right panel) for $PrFeAsO_{0.7}$ (E_1=7110-7117.5 eV) and PrFeAsO (E_1=7120-7131 eV). The dashed lines indicate the crossover between Raman and fluorescent behaviors.

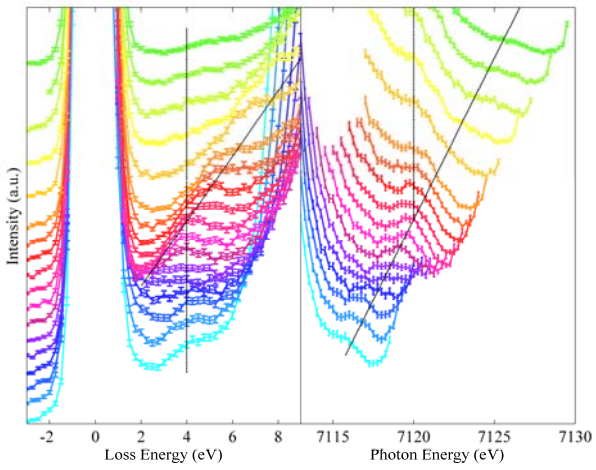

Fig. 2: Enlarged plot of the RIXS spectra in the E_1=7120-7131 eV range, as a function of loss energy (left panel) and photon energy (right panel).

[1] Y. Kamihara *et al.*, J. Am. Chem. Soc. **130**, 3296 (2008).
[2] S. Ishibashi *et al.*, J. Phys. Soc. Jpn. **77**, 053709 (2008).