| | Experiment title:<br><br>Temperature dependent electronic excitations in the FeTe$_{1-x}$Se$_x$ chalcogenides by RIXS | Experiment number:<br><br>HE- 3463 |
|---|---|---|
| **Beamline**:<br><br>ID16 | **Date of experiment**:<br><br>from: 01 Sep. 2010    to: 07 Sep. 2010 | **Date of report**:<br><br>18-February-2013 |
| **Shifts:**<br><br>18 | **Local contact(s)**:<br><br>Laura Simonelli | *Received at ESRF:* |

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## Report:

The aim of this experiment was to investigate the electronic structure of FeSe$_{1-x}$Te$_x$ compound which has the simplest crystal structure among the unconventional Fe-based superconductors.

We performed resonant inelastic x-ray scattering (RIXS) [1] measurements, tuning the incoming energy around the Fe K-edge. The RIXS technique is one of the most powerful probes of the charge and spin correlation functions multiplied by a resonant enhancement factor [2, 3]. Figure 1 shows the two dimensional RIXS maps, intensity versus incident energy and energy transfer, for the FeSe$_{1-x}$Te$_x$ samples with different Te substitution levels. Within the experimental resolution (0.9 eV) we do not see any clear inelastic features on top of the fluorescence. On tuning the incoming energy to the pre-edge, a distinct resonance of an inelastic feature around 4–5 eV of energy transfer is found. This corresponds to the charge transfer from the occupied to the unoccupied bands, and clearly appears as a well defined peak in the integrated intensity plot (figure 1(b)). With decreasing temperature, the intensity of the inelastic features increases, consistently with the temperature dependence of the partial fluorescence yield (PFY) spectra. The occupied and unoccupied bands, represented respectively by the satellite emission lines and absorption spectra, are plotted on the same energy scale for FeSe and FeTe in figure 1(c). There is a significant x-ray emission spectral weight overlapping with the XAS pre-peak quadrupole transition due to Fe 3d–chalcogen p state hybridization. Moreover, the charge transfer energy for the FeSe is of the order of 5 eV, and decreases continuously with increasing Te content, being about 4 eV for the FeTe. The change in the charge transfer appears to be related to the different polarizabilities of the Fe–chalcogen bonds. Indeed, the polarizability of Te (5.5 Å$^2$) is higher than that of Se (3.8 Å$^2$), and hence a lower charge transfer energy is expected for FeTe due to a wider orbital extension. In addition, the asymmetry of the charge transfer peak profile in FeTe could also be due to the higher polarizability of Te with respect to that of Se, revealing a rather symmetric peak profile in the case of FeSe (the nearest orbitals of Se and Te to the Fermi level are of p symmetry, more extended in the Te). Finally, changing hybridization between the Fe 3d states and the chalcogen p orbitals is also evident from the changing spectral weight of charge transfer excitation with decreasing hybridization.

The obtained results provide important information on the hybridization of Fe 3d and chalcogen p states and on the charge transfer in the FeSe$_{1-x}$Te$_x$ chalcogenides, a useful experimental feedback for realistic models to describe the electronic properties of these materials.
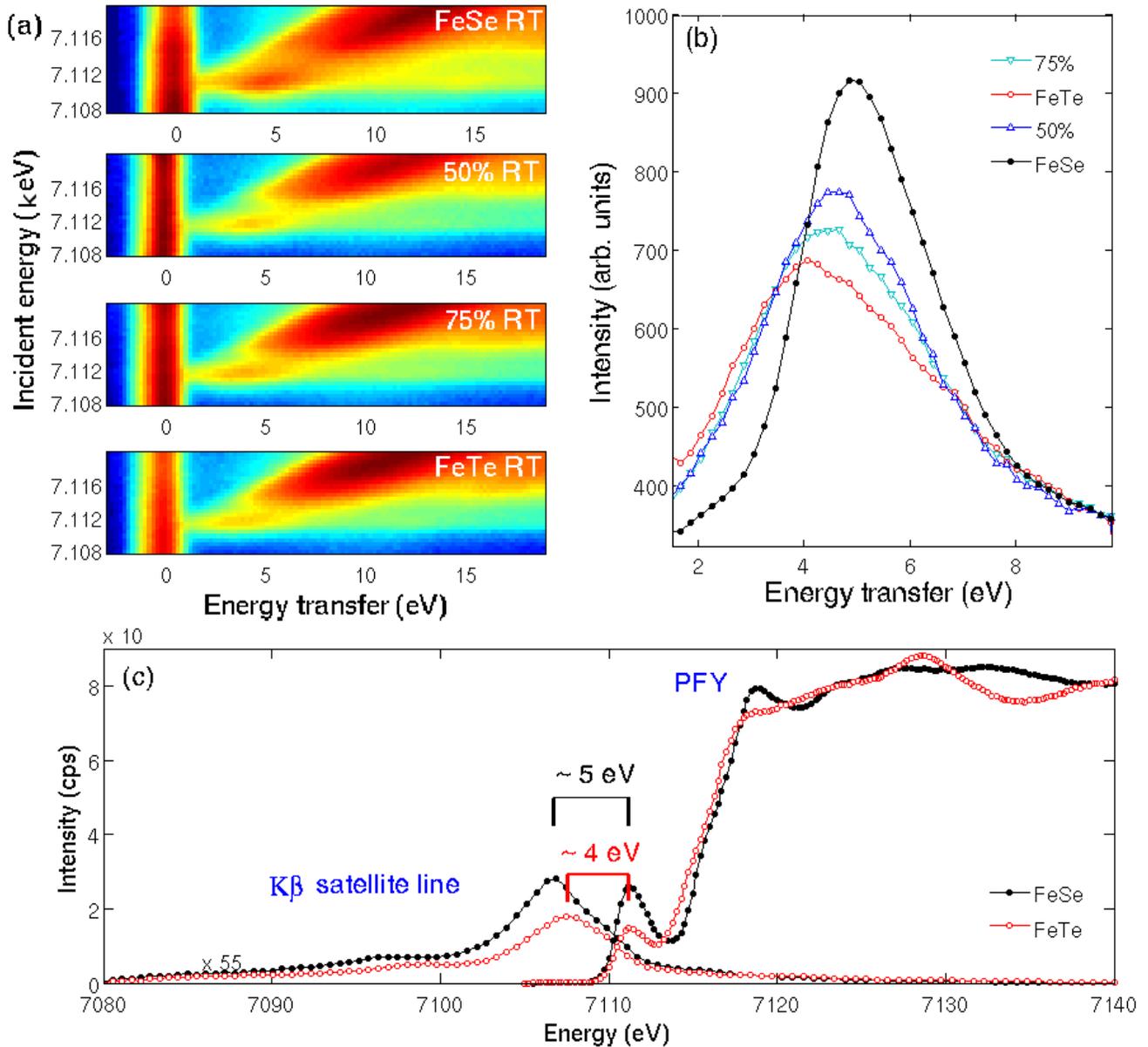
Figure 1. (a) The RIXS plane for samples with different Te substitution levels. (b) On tuning the incoming energy to the pre-edge a distinct resonance of an inelastic feature around 4–5 eV of energy transfer is found. (c) Occupied and unoccupied bands, represented respectively by the K satellite lines and partial fluorescence yield spectra, are plotted on the same energy scale axis for FeSe and FeTe.

## References

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