



Experiment title:
Pressure and temperature dependence on the electronic structure in the $\text{FeSe}_{1-x}\text{Te}_x$ system by hard x-ray emission spectroscopy

Experiment number:
HE- 3594

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Report:

The aim of this experiment was to investigate the fundamental electronic properties of the $\text{FeSe}_{0.5}\text{Te}_{0.5}$, key member of the family of new iron-based superconductors. More in particular we investigated the electronic properties of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ compound at room and low temperatures and at 0 and 3 GPa. For this particular experiment $\text{FeTe}_{0.5}\text{Se}_{0.5}$ powder sample was mounted in a panoramic high-pressure cell kept in a cryogenic environment. The incoming and out-coming x-rays were passing through the Be gasket (Fig. 1).

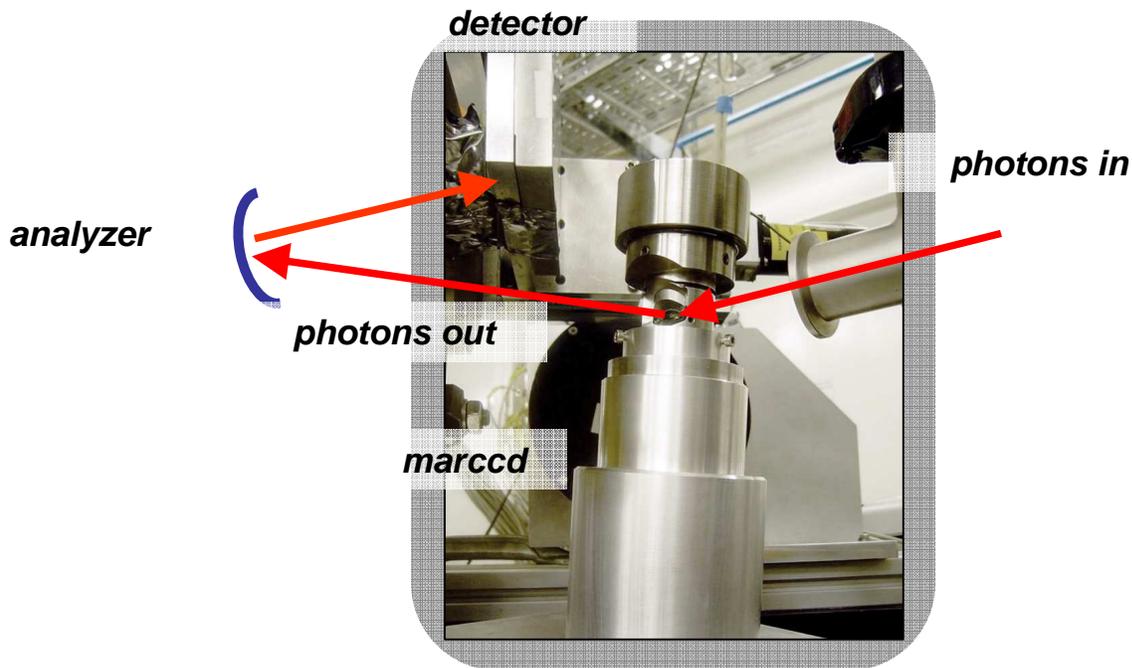


Fig. 1 X-ray path through the Be gasket.

We measured the Fe $K\beta$ emission line and the high-resolution Fe k-edge absorption spectra (PFY) (Fig. 2). No differences have been detected between spectra collected at room and low temperature, across the superconducting transition.

Instead pressure acts on the electronic structure moving the absorption pre-peak towards higher energies and reducing the Fe local magnetic moment (Fig. 2). Unfortunately by increasing further the pressure the gasket hole closed, making impossible to investigate higher pressures conditions.

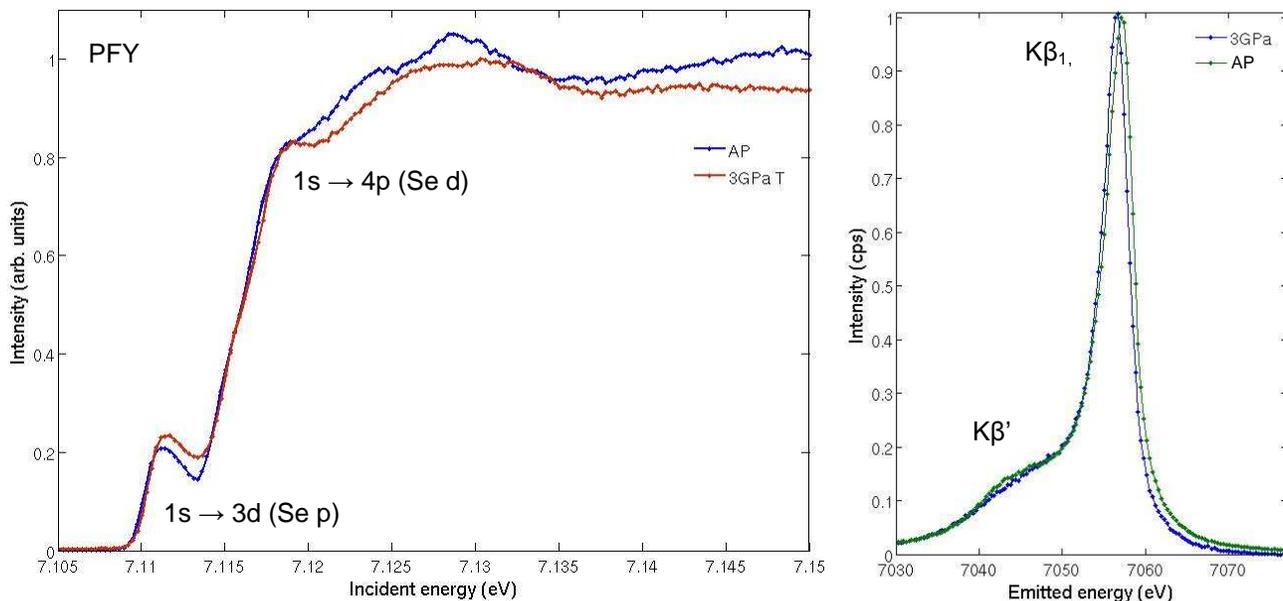


Fig. 2 (Left) High resolution Fe k-edge absorption spectra collected at ambient pressure (blue) and 3 GPa (red). (Right) Fe $K\beta$ emission line collected at AP (green) and 3 GPa (blue).

The shift of the pre-peak towards higher energies and the decrease of the Fe local magnetic moment by increasing the pressure are in agreement with the results obtained on the FeSe binary compound by J. M. Chen et al. [1]. Despite obvious difficulties in normalizing the spectra collected at different pressures, it seems that at 3 GPa the hybridization between Fe 3d and chalcogen-p orbitals, that strongly depend from the chalcogen height [2], increases. This is in contrast with the results published J. M. Chen et al. [1].

Anyway, in our case, thanks to the use of a bidimensional detector, we were able to identify a strong contribution coming from Fe impurities contained in the Be gasket, that can easily be responsible of this discrepancy.

The results obtained here give useful indications on the effect of pressure on the electronic structure that likely can help in clarify the role of electronic properties in the superconducting phenomena in this class of materials.

Anyway further experiments are required in order to cover the full temperature/pressure range where the structural or superconducting transition occur.

Finally we identify the use of the panoramic anvil cell, with the incoming and out-coming x-rays passing through the Be gasket, like a dangerous setup for this kind of experiments that can makes difficult the data analysis and questionable the results at high pressures.

References

- [1] J. M. Chen et al., Phys. Rev. B **84**, 125117 (2011)
- [2] L. Simonelli et al., J. Phys.: Condens. Matter **24**, 415501 (2012).