



Experiment title: Hydrostatic pressure effects on the local structure of the iron-selenide superconductor: An energy dispersive x-ray absorption spectroscopic study

Experiment number: HS 4787

Beamline: ID-24	Date of experiment: from:21 Nov. 2012 to: 21 Nov. 2012	Date of report: <i>Received at ESRF:</i>
Shifts: 18	Local contact(s): Carlo Marini	

Names and affiliations of applicants (* indicates experimentalists):

Boby Joseph (Sapienza University of Rome)
Carlo Marini (ESRF)
Laura Simonelli (ESRF)
Markus Bendele (Sapienza University of Rome)
Paolo Postorino (Sapienza University of Rome)

Report:

The local structure and the electronic properties of FeSe under hydrostatic pressure were studied by means of dispersive x-ray absorption measurements at the Fe K-edge (See figure 1 below). The pressure dependence of the x-ray absorption near edge structure features seems to follow the behavior of the superconducting transition temperature T_c (Figure 2). The local structure, that has an important impact on the superconducting properties, appears to fall into two regimes: the pressure dependence of the Fe–Fe bond distance shows a clear change in the compressibility at p around 5 GPa; in contrast, the Fe–Se bond distance decreases continuously with increasing pressure with a lower compressibility than the Fe–Fe bond (Figure 3). The results suggest that the pressure dependent changes in T_c of FeSe are closely related to the changes in local structure.

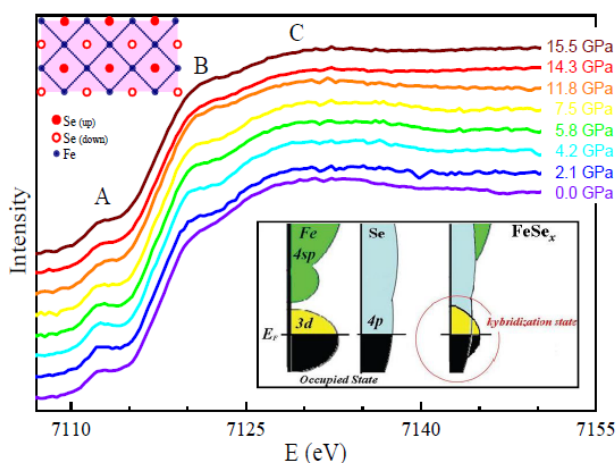


Figure 1: Fe K-edge x-ray absorption data of FeSe for selected pressures at room temperature. The data are vertically shifted for clarity in presentation. The upper inset shows a schematic view of the FeSe plane. The lower inset shows a schematic of the electronic structure (figure adapted from J. *Phys.: Condens. Matter.* [25 \(2013\) 425704](#))

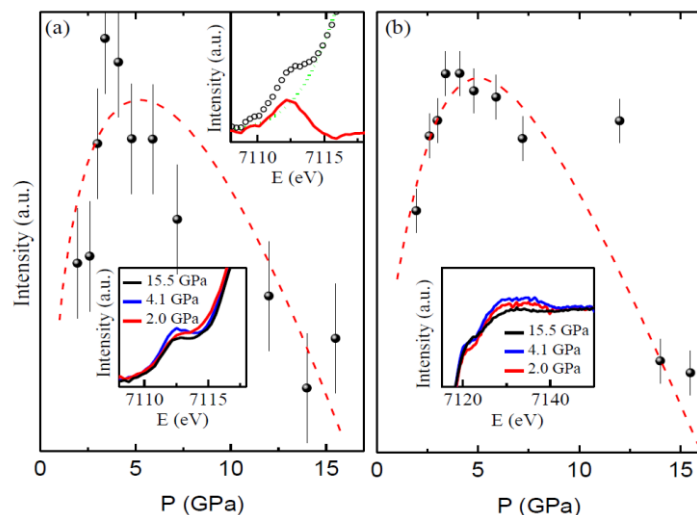


Figure 2: Pressure dependence of the integrated intensity of (a) the Fe K-edge pre-edge peak and (b) the feature C indicated in figure 1 of FeSe at room temperature. The dashed lines are guides to the eye. The lower insets in (a) and (b) show the normalized measured data of the respective features at three selected pressures. The subtraction of the background for the pre-edge integration is presented in the upper inset of (a).. (Ref: *J. Phys.: Condens. Matter.* [25 \(2013\) 425704](#))

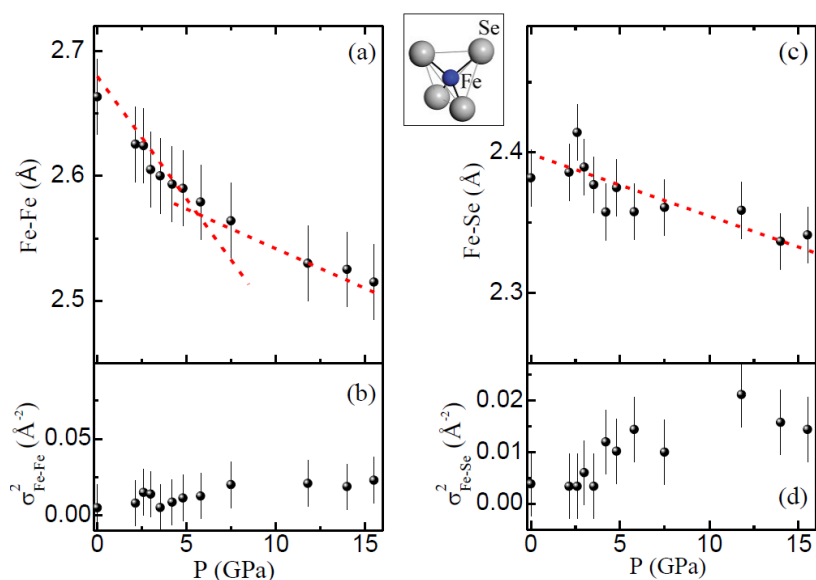


Figure 3: Pressure dependence of the Fe–Fe bond length (a) and Fe–Se bond length (c) of FeSe at room temperature. the corresponding MSRDS are shown in (b) and (d). The dashed lines are guides to the eye. The upper inset shows a schematic view of the FeSe₄ tetrahedron. (figure adapted from *J. Phys.: Condens. Matter.* [25 \(2013\) 425704](#))

The main results from the HS-4787 beamtime are published in

Dispersive x-ray absorption studies at the Fe K-edge on the iron chalcogenide superconductor FeSe Under pressure:

M. Bendele, C. Marini, B. Joseph, L. Simonelli, P. Dore, S. Pascarelli, M. Chikovani, E. Pomjakushina, K. Conder, N. L. Saini, P. Postorino

JOURNAL OF PHYSICS CONDENSED MATTER [25 \(2013\) 425704](#)

[doi:10.1088/0953-8984/25/42/425704](https://doi.org/10.1088/0953-8984/25/42/425704)