ESRF	**Experiment title:** Local structure around Fe atoms in $FeSe_{0.1}Te_{0.9}$ high-temperature superconductor	**Experiment number**: HC-2843
Beamline: BM02	**Date of experiment**: from: 15 Feb 2017 to: 21 Feb 2017	**Date of report**: 09 / 09 / 2017
Shifts: 18	**Local contact(s)**: Nathalie Boudet, Nils Blanc, Marc de Boissieu	*Received at ESRF:*

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Report:

In this beamtime, we performed the first X-ray fluorescence holography (XFH) experiment at BM02. The original plan for this beamtime was to investigate Ce impurities in Ce doped Yttrium Aluminum Garnet (Ce:YAG, $Y_3Al_5O_{12}$), which is a synthetic crystalline material commonly used as radiation scintillator. However, with the current experimental setup, it was impossible to detect a sufficiently intense signal from the small amount of Ce impurities. Therefore, the sample was changed to $FeSe_{0.1}Te_{0.9}$.

$FeSe_xTe_{1-x}$ is one of the simplest Fe-based superconductors, and has intensively been studied concerning the interplay between structural or magnetic degrees of freedom and superconductivity. It is widely accepted that magnetic fluctuations play a very important role for their superconducting nature.

The measurements were performed in inverse mode by rotating two axes, the exit angle of $0° \leq \theta \leq 70°$ in steps of 1.00°, and the azimuthal angle continuously between $0° \leq \varphi \leq 360°$. The incident X-rays were focused onto the (001) surface of the sample. Fe $K\alpha$ fluorescence X-rays were collected using an XPAD 2D detector with a C-shaped graphite crystal energy-analyzer. The XFH signals were recorded at six different incident X-ray energies from 7.5 to 10.0 keV in steps of

0.5 keV, and close to the Fe absorption edge at 7.113 and at 7.129 keV. Each scan took about 6-10 h. Details of the XFH experimental technique can be found elsewehere [1]. Holographic oscillation data were obtained by subtracting the background from the measured fluorescent X-ray intensities and by normalizing them to the incident X-ray intensities. An extension of the holograms was carried out using the tetragonal crystal symmetry. The resulting holograms are shown in Fig. 1 for incident energies of 7.113 and 7.500 keV, respectively. Intense X-ray standing wave lines are visible in both holograms.

From the holographic patterns, 3D atomic configuration images can be reconstructed using Barton's algorithm by superimposing the holograms with the different incident X-ray energies, which can highly suppress the appearance of artificial signals. Details of the data analysis are given elsewhere [1,2]. These reconstructions will allow us to discuss the extent of the positional fluctuations of the constituent atoms and the positions of possibly different coexisting valence states of Fe, which would have a strong impact on the superconductivity properties of the material. More precisely, it is supposed that excess Fe atoms are intercalated in the crystal lattice and that they will negatively effect the superconductivity [3]. These atoms can be made visible by using the shift of the absorption edge for the different valence states, and they will be highly enhanced in the real space reconstructions from the hologram measured at 7.113 keV.

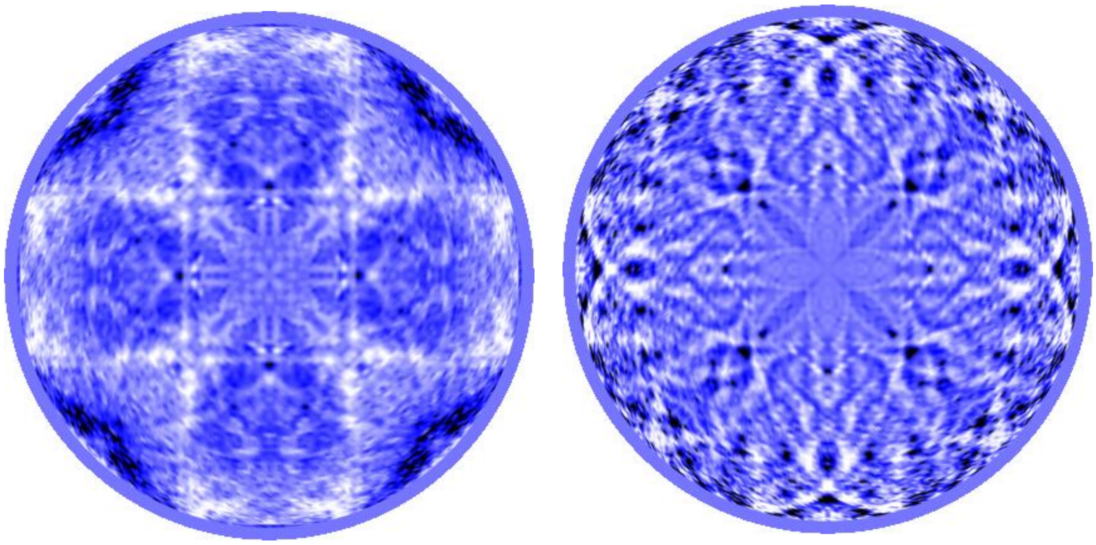

Fig. 1: Orthographic projections of the FeSeTe hologams measured close to the absorption edge at 7.113 keV (left) and at 7.500 keV (right). The holograms are centered at $\theta = 0°$, and the radial and angular directions indicate θ and φ, respectively.

References

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