



Short Communication

# Electronic Structure of Iron- Pnictide $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ Superconductor Using X- Ray Absorption Spectroscopy

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## Abstract

In this paper electronic structure of Fe- based superconductor  $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$  ( $x = 0.2$ ) has been studied using polarized X-ray absorption spectroscopy measured at ELLETRA synchrotron Trieste, Italy. The XAFS spectra for Sm  $M_{4,5}$ , Fe  $L_{2,3}$  and O K- edge has been analyzed and the results are explained to show the possible hybridization responsible for superconductivity in these compounds, which may be assumed due to a charge transfer from Sm-O layer to the Fe-As layer as a result of fluorine doping.

**Keywords:** Electronic structure, X- ray absorption,  $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ , superconductivity, density of states, charge transfer.

## Introduction

All the high temperature superconductors belong to the special category of materials, i.e. strongly correlated materials, which are characterized by strong interactions between electrons. However, cuprates and in pnictides, the mechanism behind superconductivity is still far from being well understood but It is believed that iron pnictides lies between the strongly correlated cuprates and the weakly correlated conventional superconductors. The discovery of iron based superconductors  $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$  [1111 family compounds] with critical temperature 26K has led to a great breakthrough in the research of high temperature superconductivity<sup>1</sup>. This new discovery has generated a great interest in this new class of materials for the high  $T_c$  research. Immediately, the  $T_c$  has been enhanced up to 50K by replacing La using rare earth elements<sup>2-5</sup>. A  $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$  ( $x=0.2$ ) superconductor still remains the high temperature superconductors (54K) in rare earth family. In these compounds superconductivity occurs by electron doping of  $\text{F}^-$  as a substitution for  $\text{O}^{2-}$ . This doped electron transfers to the FeAs layer to enhance the charge difference between the layers. The phase diagram and transport properties of  $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$  have been studied by Liu et al<sup>6</sup> and concluded that superconductivity emerges at  $x=0.10$  and optimal doping takes place at  $x=0.2$  with the highest  $T_c=54$  K.

## Methodology

The  $\text{Sm}M_{4,5}$ , Fe  $L_{2,3}$  and O k- edge x-ray absorption were performed on the powder samples  $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$  ( $x= 0.2$ ) prepared using the solid state reaction method. This compound crystallizes in the  $\text{ZrCuSiAs}$ -type structure with space group

$P4/nmm$ . In this structure, two dimensional layers of edge-sharing FeAs tetrahedral alternate with sheets of edge-sharing SmO tetrahedral and the differences between the ionic nature of these bonds, this two-dimensional structure is formed, where ionic layers of  $(\text{SmO})^+$  alternate with metallic layers of (FeAs). The x-ray absorption measurements were made at the Bear beam line of Elettra Synchrotron Radiation Facility, Trieste, Italy on Sm  $M_{4,5}$ , Fe  $L_{2,3}$ , and O K absorption edges in Total yield mode of detection employing the measurement of surface electrical current using the Keithley electrometer. The intensities of all the spectra are normalized by the incident beam intensity monitored just before the target on a gold foil. The sample was repeatedly scraped with a diamond file to obtain clean surfaces.

## Results and Discussion

In figure 1, Sm  $M_{4,5}$  edge XAS, two main peaks with satellites on the low energy side are observed clearly for our sample. The main peaks of Sm at 1077.46 eV and 1102.13 eV are related to the transitions from an atomic like  $f^0$  ( $\text{Sm}^{+4}$ ) ground state configuration<sup>7</sup>. The Satellite peaks may be originates from the transitions of 4f states in the conduction band. The  $M_{4,5}$  edges exhibit sharp near edge features as a result of strong atomic  $d^{10}4f^n \rightarrow d^94f^{n+1}$  transition which contain a wealth of spectroscopic information<sup>8</sup>.

Figure 2 shows the O K edge spectra with spectral fine structure details labeled as A, B, C, D, E and F. These various small structural details give the signature of hybridization between Sm and O. The O k edge is sensitive to the chemical environment around the x- ray absorbing atom and strongly depends on the oxidation state. Other peaks may be attributed due to the electric

transition from O 1s core levels into the empty O 2p hole states hybridized with the Sm dominated f, d<sub>eg</sub> and d<sub>t2g</sub> levels<sup>9</sup>.

are weak and broad shoulders in the Fe L<sub>2,3</sub> spectra as shown in the figure 3.

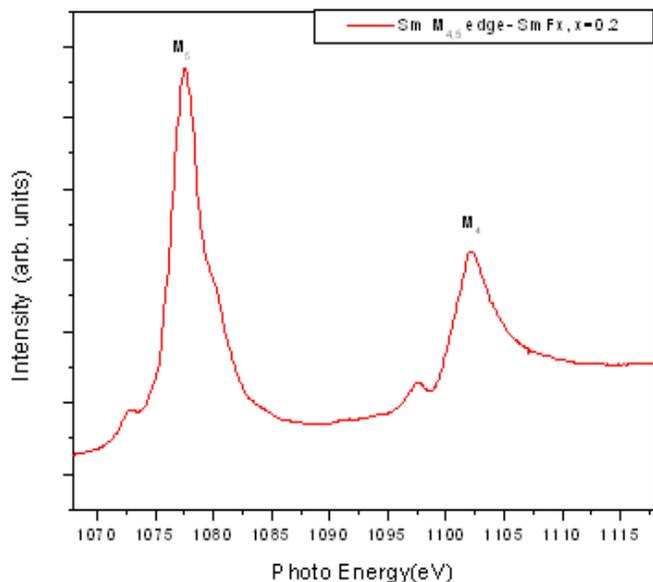


Figure-1

Normalized Sm M<sub>4,5</sub> edge x-ray absorption spectra measured on polycrystalline sample of SmO<sub>1-x</sub>F<sub>x</sub>FeAs(x=0.2).

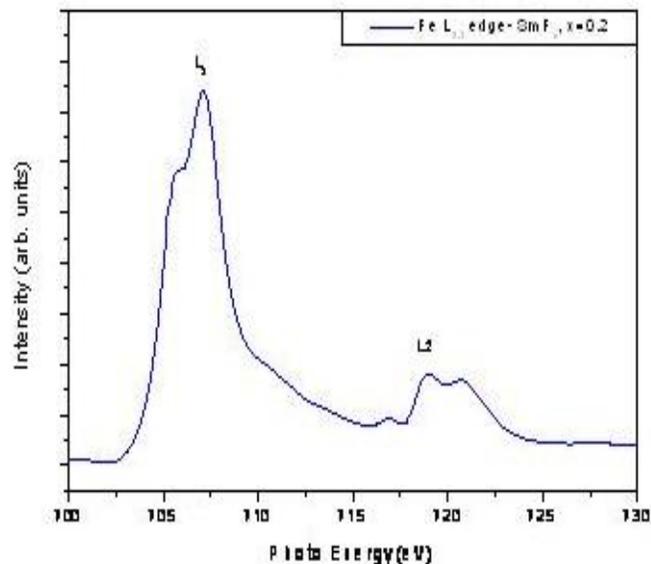


Figure-3

Normalized Fe L<sub>2,3</sub> edge x-ray absorption spectra measured on polycrystalline sample of SmO<sub>1-x</sub>F<sub>x</sub>FeAs(x=0.2).

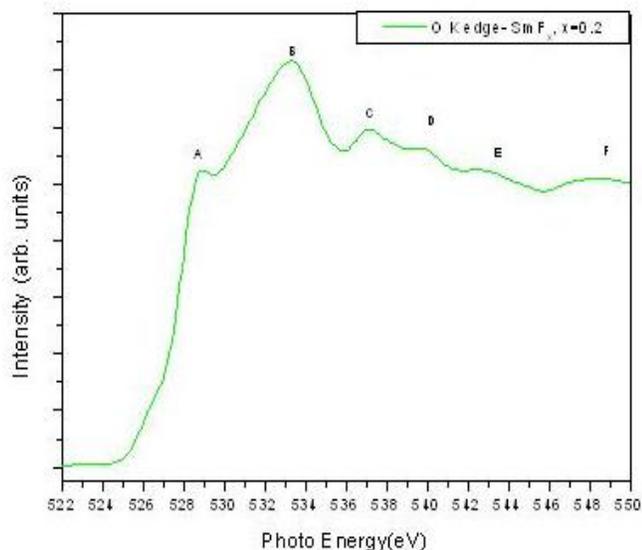


Figure-2

Normalized O k-edge x-ray absorption spectra of SmO<sub>1-x</sub>F<sub>x</sub>FeAs(x=0.2) sample.

The Fe atoms in Fe-As layer (the layer responsible for superconductivity) are bounded tetrahedrally with As. The dipole transition Fe 2p electrons (2p<sup>6</sup>3d<sup>6</sup>) → empty Fe 3d (2p<sup>3</sup>3d<sup>7</sup>) states, due to spin orbital coupling splits Fe into two peaks having energies at 706.78eV (Fe 2p<sub>3/2</sub> → Fe 3d), 719.45eV (Fe 2p<sub>1/2</sub> → Fe 3d). Along with the main peak, there

The presence of these shoulders indicates the covalent nature of Fe and As conduction electrons in the FeAs plane. The satellite appeared in the spectrum reflects the localized character of the Fe 3d electrons in this compounds. The splitting in the 2p<sub>1/2</sub> (L<sub>2</sub>) peak may be appeared due to the charge transfer from Sm-O plane. The As 3p orbital together with the Fe 3d orbitals are the main contributors to the density of state of the system and the spin d<sub>yz</sub> and d<sub>x<sup>2</sup>-y<sup>2</sup></sub> orbitals contribute to Fermi's level states. Hence we can say that the entire phenomenon of superconductivity in these compounds is due to square lattice of Fe within the Fe-As layer<sup>10,11</sup>.

### Conclusion

In summary, we have investigated Sm M<sub>4,5</sub>, Fe L<sub>2,3</sub>, O K edge XAS of SmO<sub>1-x</sub>F<sub>x</sub>FeAs (x= 0.2) system. The O K edge shows a possible hybridization between oxygen and Sm as indicated in the spectra and is involved in the long range mixing into FeAs hybridized state. Fe L<sub>2,3</sub> edge shows the shoulder, which indicate the covalent nature of Fe and As conduction electrons. The splitting of L<sub>2</sub> edge spectra is expected due to the charge transfer from Sm-O plane. The various features arises due to the hybridization is explained to understand the electronic structure of the compound.

### References

1. Kamihara Y., Watanabe T., Hirano M. and Hosono H., Iron-Based Layered Superconductor La [O<sub>1-x</sub>F<sub>x</sub>]FeAs

- ( $x=0.05-0.12$ ) with  $T_c = 26$  K, *Am. Chem. Soc.*, **130**, 3296-3297 (2008)
- Wang X.C., Liu Q.Q., Lv Y.X., Gao W.B., Yang L.X., Yu R.C., Li F.Y. and Jin C.Q., The superconductivity at 18 K in LiFeAs system, *Solid State Commun.*, **148**, 538-540 (2008)
  - Rotter M., Tegel M. and Johrendth D., Superconductivity at 38 K in the Iron Arsenide  $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$ , *Phys. Rev. Lett.*, **101**, 107006-4p (2008)
  - Wen H.H., Mu G., Fang L., Yang H. and Zhu X., Superconductivity at 25K in hole-doped  $(\text{La}_{1-x}\text{Sr}_x)\text{OFeAs}$ , *Europhys Lett.*, **82**, 17009-5p (2008)
  - Ogino H., Katsura Y., Horii S., Kishio K. and Shimoyama J., New iron-based arsenide oxides  $(\text{Fe}_2\text{As}_2)(\text{Sr}_4\text{M}_2\text{O}_6)(\text{M} = \text{Sc}, \text{Cr})$ , *Supercond. Sci. Technol.*, **22**, 085001-5 (2009)
  - Liu R.H., Wu G., Wu T., Fang D.F., Chen H., Li S.Y., Liu K., Xie Y.L., Wang X.F., Yang R.L., He C., Feng D.L. and Chen X.H., Phase Diagram and Quantum phase transition in Newly Discovered Superconductors:  $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ . Con-mat, arXiv, **0804**, 2105 (2008)
  - Putti M., Pallecchi I., Bellingeri E., Cimberle M. R., Tropeano M., Ferdeghini C., Palenzona A., Tarantini C., Yamamoto A., Jiang J., Jaroszynski J., Kametani F., Abramov D., Polyanskii A., Weiss J.D., Hellstrom E.E., Gurevich A., Larbalestier D.C., Jin R., Sales B.C., Sefat A.S., McGuire M.A., Mandrus D., Cheng P., Jia Y., Wen H.H., Lee S. and Eom C.B., New Fe-based superconductors: properties relevant for applications, *J. Supercond, Sci. Technol*, **23**, 034003-10 (2010)
  - Yuan H.Q., Singleton J., Balakirev F.F., Baily S.A., Chen G.F., Luo J.L. and Wang N.L., Nearly isotropic superconductivity in  $(\text{Ba},\text{K})\text{Fe}_2\text{As}_2$ , *Nature*, **457**, 565-568 (2009)
  - Chen S.Y., Lu Y.H., Huang T.W., Yan D.C. and Dong C.L., Oxygen Dependent magnetism of  $\text{CeO}_2$  nanoparticles prepared by thermal decomposition method, *J. Phys. Chem. C*, **114**, 19576- 19581 (2010)
  - Yang W.L., Sorini A.P., Chen C.C., Moritz B., Lee W.S., Vernay F., Velasco P.O., Denlinger J.D., Delley B., Chu J.H., Analytis J.G., Fisher I.R., Yang J., Lu W., Shen Z.X. and Devereaux T.P., Evidence for weak electronic correlations in iron pnictides, *Phys. Rev. B*, **80**, 014508-10 (2009)
  - Bondino F., Magnano E., Malvestuto M., Parmigiani F., McGuire M.A., Sefat A.S., Sales B.C., Jin R., Mandrus D., Plummer E.W., Singh D.J. and Mannella N., Evidence for Strong Itinerant Spin Fluctuations in the Normal State of  $\text{CeFeAsO} (0.89\text{F}(0.11))$  Iron-Oxypnictides, *Phys. Rev. Lett.*, **101**, 267001-4 (2008)