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X-ray absorption fine structure studies on La$_{1-x}$Sr$_x$FeO$_3$

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Introduction

The issue of metal insulator transitions (MIT) in transition metal oxides has been investigation intensely for many decades, yet the phenomena is not completely understood till date. One of the many ways to realise such a transition is by doping an insulator with charge carriers, either electrons or holes. This has been most easily achieved by heterovalent substitution, where an ion with one oxidation sate (say La^{3+}) is replaced with another ion with a different oxidation state, for example Sr^{2+}, as in La$_{1-x}$Sr$_x$CoO$_3$ [1] and La$_{1-x}$Sr$_x$TiO$_3$ [2]. If the electronic system remains homogeneous, in spite of the inevitable presence of chemical inhomogeneity at the microscopic level due to chemical substitution, the parent insulating system, say LaTiO$_3$ or LaCoO$_3$, should transform to a metallic state with substitutional doping. However, the extent of doping required in reality to bring about this transition is substantial in every case, the exact amount being system dependent. In certain cases like La$_{1-x}$Sr$_x$FeO$_3$ [3] and La$_{1-x}$Sr$_x$CrO$_3$ [4], the system remains insulating for possible doping. Thus combining these observations with the preceding discussion, it appears clear that electronic inhomogeneity must play a significant role in determining the exact nature of metal-insulator transition in such chemically doped systems. In order to probe such effects, we have carried out a detailed investigation of La$_{1-x}$Sr$_x$FeO$_3$ employing x-ray absorption technique which is known to be influenced by local electronic and geometric structures.

Experiment

Polycrystalline samples of La$_{1-x}$Sr$_x$FeO$_3$ with x = 0, 0.1, 0.2, 0.3, 0.4, 0.5 and 0.67 were prepared by solid state synthesis using stoichiometric amounts of high purity starting materials La$_2$O$_3$, SrCO$_3$ and FeC$_2$O$_4$. 2H$_2$O. X-ray absorption measurements were carried out at the beam line BL-10B and BL-9A to cover the Fe K, Sr K and La L$_3$ absorption edges. Experiments were performed at temperatures ranging from 25 K to 300 K.

Results and discussion

Figure1 shows the Fe K-edge XANES spectra of La$_{1-x}$Sr$_x$FeO$_3$ collected at 25 K. The pre-edge, shoulder and white line is marked by P, S and W respectively in the figure. W and S are ascribed to dipolar 1s to np transitions where as P is ascribed to a transition from 1s to 3d [5]. It is clear from the figure that there is no drastic change in the spectra with hole doping. Thus, the Fe valency remains essentially the same across the series. Derivative spectra of the pre-edge region is shown in the inset (a).

Preliminary analysis of the Fe K EXAFS region was carried out using the nearest neighbour shell. Relative mean square displacement (RMSD) of bond lengths with respect to temperature for various compositions are shown in the inset (b) of figure1. Fitting the data using correlated Einstein model, Einstein frequency and relative static mean square displacement are extracted for each x value. More refined data analysis is now being carried out.
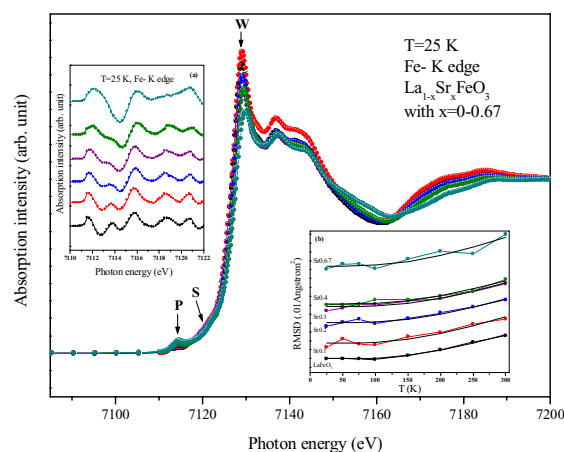
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