Experimental Report

30/10/2013

Proposal: **5-31-2202** **Council:** 4/2012

Title: Structural and Magnetic Phase Diagram of La2O(3-x)F(x)Fe2Se2 and LaREO3Fe2Se2 (RE= rare earth)

This proposal is a new proposal

Researh Area: Physics

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Samples: La2O(3-x)F(x)Fe2Se2
LaDyO3Fe2Se2
LaHoO3Fe2Se2
LaTbO3Fe2Se2
LaErO3Fe2Se2
LaYO3Fe2Se2

Instrument	Req. Days	All. Days	From	To
D1B	5	2	31/10/2012	02/11/2012

Abstract:

The cuprate oxides appear to teach us that what we need for high-TC superconductivity is an S=1/2 antiferromagnetic Mott insulator ground state where the transition metal resides in a square planar geometry. The newly discovered iron pnictide superconductors violate this notion as the parents phase ground state is metallic and the Fe ion resides in a tetrahedrally coordinated site. Despite this differences they are many features of the pnictides that are shared with the cuprates, such as high TC values, proximity to a magnetically ordered state and a linear temperature dependence of the resistivity. Recent work has shown that the oxo-selinide compound La2O3Fe2Se2 provides for a similar local environment of the Fe-ion to that found in the Fe-superconductors but is an antiferromagnetic Mott insulator that undergoes a structural transition at TN=90K. We varied this compound by using F for O and we induced strain by using mixed rare earts. The resulting solid solution follows the expected Vegard's Law and TN decreases with doping. We propose to determine the structural and magnetic phase diagram of this new solid solution over 5 days using D1B

Structure and Magnetic Transitions of Doped Iron Oxo Selenides

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INTRODUCTION

The cuprate oxides superconductors (SC) show an $S = \frac{1}{2}$ antiferromagnetic Mott insulator ground state where the transition metal resides in a square planar geometry. In the iron pnictide SC the parent's phase ground state is metallic and the Fe ion resides in a tetrahedrally coordinated site. Despite these differences there are many features of the pnictides that are shared with the cuprates, such as high T_C values, proximity to a magnetically ordered state and a linear temperature dependence of the resistivity. Despite the fact that the parent phases of the know Fe-superconductors are metal, the physics of these materials reveal more and more an interplay between itinerant and localized magnetism. It may be that the notion of a distant Mott insulator ancestor of these materials lurks possibly close by. Indeed recent work has shown that the oxy-selinide compound $La_2O_3Fe_2Se_2$ provides for a similar local environment of the Fe-ion to that found in the Fe superconductors[1][2]. However these materials are antiferromagnetic Mott insulators that undergo a structural transition at T_N=90K[2]. Of clear interest is here is the electronic doping of this compound in order to investigate if interesting electronic behavior emerges.

EXPERIMENTS

We measured seven samples at room temperature: $La_{1-x}Cd_xO_3Fe_2Se_2$ with x=0.1, 0.2, 0.4 (named LaCd01, LaCd02, LaCd04), $La_2O_{3-y}F_yFe_2Se_2$ with y=0.2 and 0.4 (named LaF02 and LaF04), $LaNdO_3Fe_2Se_2$ (named LaNd) and $Nd_2O_3Fe_2Se_2$(named Nd) with a wavelength of 2.52 Å and no collimation. Further we made four temperature dependent scans with LaCd02, LaF02, LaF04 and LaNd from 2 K to 300 K.

RESULTS

The results of the Rietveld refinements of the 300 K diffractions is shown in Table I. The length of the unit cell axis of the Cd doped samples do not change a lot while the F doped samples show a steady decrease of a and c. Also the LaNd and the Nd samples show the expected decrease. As the oxygen and iron atoms are fixed only the position of La/Cd and Se along the c-axis may vary. The distance between La and Se and the angle between Se-Fe-Se has been detected indicative of the SE and the magnetic properties. Here it is clearly visible that the Cd doping does not have a big effect in contrast to the doping of F as shown in Figure 1.

	LaCd01	LaCd02	LaCd04	LaF02	LaF04	LaNd	Nd
a (Å)	4.0814 (1)	4.0845 (1)	4.0875 (2)	4.0697 (2)	4.0590 (2)	4.0457 (1)	4.0232 (1)
c (Å)	18.640 (1)	18.640 (1)	18.633 (2)	18.574 (2)	18.562 (2)	18.558 (1)	18.488 (1)
V (Å^3)	310.50 (2)	310.97 (2)	311.33 (3)	307.64 (2)	305.82 (3)	304.57 (2)	299.25 (2)
La z (c)	0.1845 (2)	0.1851 (2)	0.1854 (4)	0.1843 (4)	0.1853 (4)	0.1861 (2)	0.1871 (2)
Se z (c)	0.0972 (2)	0.0969 (2)	0.0973 (3)	0.0989 (3)	0.0988 (3)	0.0982 (2)	0.0997 (2)
d (La-Se) (Å)	3.313 (4)	3.323 (4)	3.324 (3)	3.286 (5)	3.288 (3)	3.295 (7)	3.272 (6)
ang (Se-Fe-Se) (deg)	96.8 (1)	97.0 (1)	96.85 (5)	95.85 (6)	95.74 (4)	95.8 (1)	95.0 (1)
R_{wp} (%)	3.67	3.76	4.19	2.61	3.38	4.56	3.31
χ^2	3.64	5.51	5.67	4.74	4.03	6.3	4.67

TABLE I: Results from neutron Rietveld refinements of La2O2Fe2OSe2 at 300 K. The Space group we used was $I_{4/mmm}$ (No. 139), the general positions of the atoms are: La/Cd ($\frac{1}{2}$ $\frac{1}{2}$ z), Fe ($\frac{1}{2}$ 0 0), O(1)/F ($\frac{1}{2}$ 0 $\frac{1}{4}$), O(2) ($\frac{1}{2}$ $\frac{1}{2}$ 0), Se (0 0 z)

The refinement of the atomic occupation was difficult on the Cd doped samples as the error for the La/Cd position was too high, so we could not confirm the Cd content of our samples. On the other hand the refinement of the occupation of the F doped samples was possible. O(1) makes with Fe a 2D sheet comparable with the Cu-O sheets in the Cu superconductors, while O(2) resides in the sheet separating La-O-La layer. When F is refined in the 300K diffractions on the O(1) position $\chi^2 = 4.03$ what is significantly better than on the O(2) position with $\chi^2 = 4.22$ for LaF04 or $\chi^2 = 4.74$ (O(1) position) and $\chi^2 = 5.14$ (O(2) position) for LaF02, respectively. This indicates that the F is placed within the Fe sheet.

The temperature dependent scans did not show structural changes between 2 and 300 K. The magnetic order at 2K shows an antiferromagnetic order of the Fe atoms with a propagation vector of $k = (\frac{1}{2}0\frac{1}{2})$, according to the undoped compound. The transition temperature of the F doped

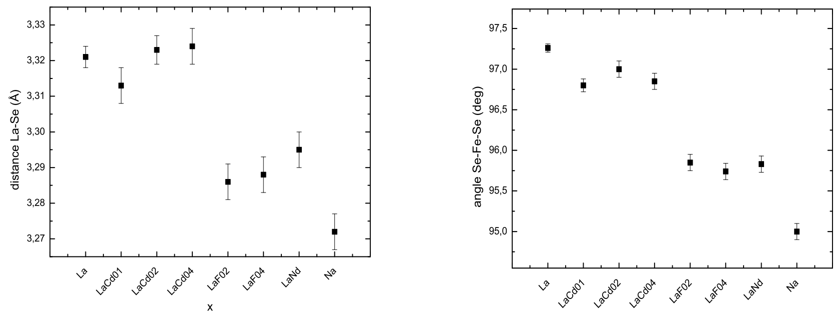

FIG. 1: Values of the distance (Å) between La/Cd and Se and angle (deg) between Se-Fe-Se at 300 K.

samples decreases with doping from 79 K to 73 K (90 K for the undoped sample) what is is accordance with new susceptibility measurements. The LaCd02 sample show an increased $T_N = 107K$, for the LaNd sample T_N is 84 K as shown in Figure 2.

The LaF02 sample further showed a magnetic reflection with a T_N of 120 K and a changing wavenumber with temperature that can not be fitted so far.

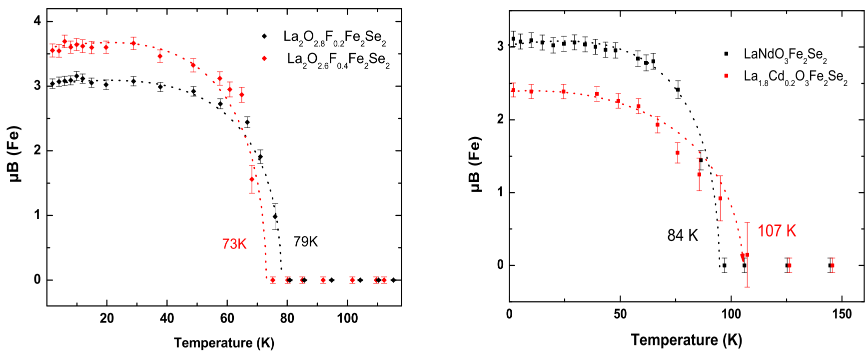

FIG. 2: Temperature dependence of the magnetic order of Fe in LaF02 and LaF04 (left panel) and LaCd02 and LaNd (right panel)

[1] Jian-Xin Zhu, *Phys. Rev. Lett.* **104**, 216405 (2000)

[2] David G. Free and John S. O. Evans, *Phys. Rev. B* **81**, 214433 (2010)