Experimental report

16/11/2016

Proposal: 5-31-2285 **Council:** 10/2012

Title: Phase diagram of Mn-doped Iron Oxo-Selenides

Research area: Physics

This proposal is a continuation of 5-31-2147

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Samples: La2O3Fe{2-x}Mn{x}Se2

Instrument	Requested days	Allocated days	From	To
D20	6	3	07/05/2013	10/05/2013
			08/08/2013	09/08/2013

Abstract:

The cuprate oxide and the iron pnictide superconductors share many similarities but differ also in central characteristics. 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.
We use an iron oxo-selenide compound with similar structural and magnetic properties as the known iron superconductors. By doping the parent compound on different positions we want to understand the developement of the magnetic and electric properties in the iron selenides under different conditions.
In this experiment we want to investigate the temperature dependance of the crystallographic and magnetic structure of the La2O3Fe(2-x)Mn(x)Se2 series that show a very interesting magnetization curve with several transitions to finally map out a magnetic phase diagram for this system.

In the known iron pnictide and chalcogenide systems the Fe ion is tetrahedrally coordinated [1,2] and the environment is non-planar in contrast to the Cu superconductors where the Cu resides in a square planar geometry. Recent work has shown that the oxyselenide compound La2O3Fe2Se2 provides for Fe a similar local environment for the Fe-ion [3]. Doping attempts by Mn for Fe did not give any hint of a new superconducting class, though three different kinds of AF order were observed (see Fig. 1) [3,4]. As the transition between those orders was unclear we have focused on this problem. We have prepared a series of solid-solution systems La2O3(Fe1-xMnx)2Se2 (0<x<1) and performed a concerted magnetic thermal, electrical transport and X-ray and neutron diffraction measurements using D20 and D1B.

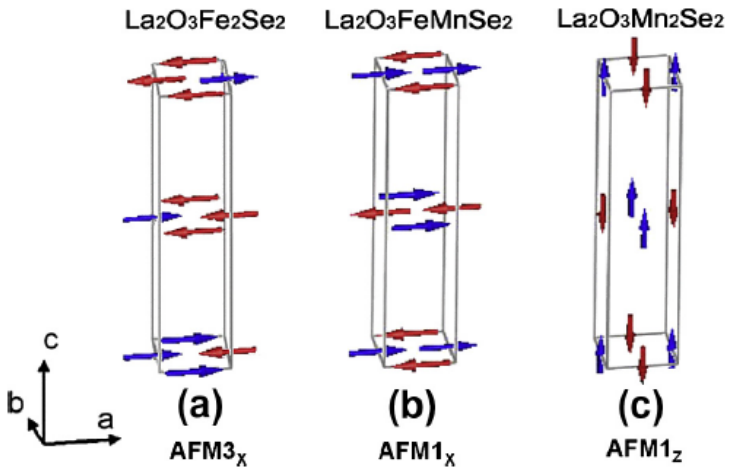

Fig. 1: Observed magnetic structure of La2O3(Fe1-xMnx)2Se2 (a) AFM3x as found in La2O3Fe2Se2, (b) AFM1x as found in La2O3FeMnSe2 and (c) AFM1z as found in La2O3Mn2Se2.

We have confirmed that all the systems crystallize in the tetragonal I4=mmm space group with no changes down to 2 K. The neutron diffraction at 2 K confirmed the finding of three different AF orders [7,19,20], and we were able to draw the phase lines between those orders. We were able to identify four different sections for the magnetic order in the solid solution as shown in Fig. 2.

First, in low-Mn region with x = 0.00 to x < 0.1 we find an AFM3x order with a strong splitting between the ZFC/FC magnetization measurements at low magnetic fields and a transition at temperatures above 300 K. In this part of the x-T phase diagram the magnetic phase transition temperature decreases with increasing Mn content.

In the second region, from x = 0.1 to x = 0.25, no long-range AF reflection is visible with neutron diffraction, while magnetization measurements show magnetic anomalies. Subsequent neutron measurements at HZB revealed a presence of a short-range order in this region.

The third region, from x > 0.25 to x = 0.9, shows the AFM1x order and a very strong splitting of the ZFC/FC magnetization measurement at low external magnetic fields with strongly negative values at 2 K on ZFC measurements.

In the fourth and last region, from x > 0.9 to x = 1.0, the magnetic spins show an AFM1z order and the ZFC/FC magnetization graphs indicate a low magnetic
competition.

The transition from AFM1x to AFM1z occurs in one step and does not result in significant changes in the amplitude of the magnetic moment compared to the transition from AFM3x to AFM1x (see Fig. 2).

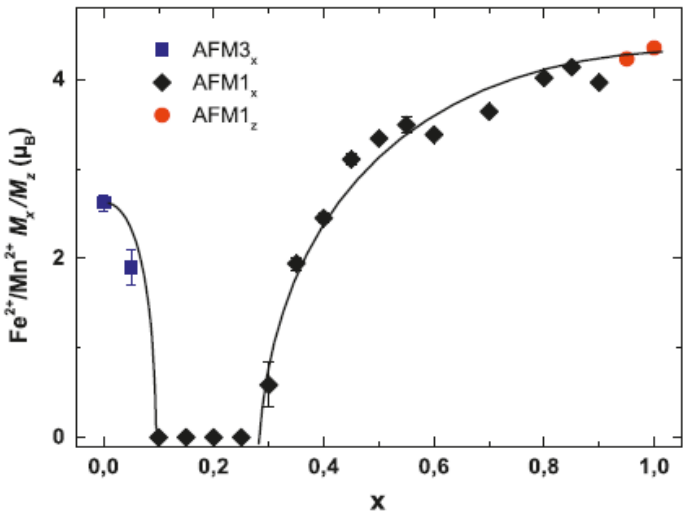

Fig. 2: The x dependence of the magnetic moment of La2O3(Fe1-xMnx)2Se2 measured at 2 K. Blue boxes refer to the AFM3x model, black diamonds to the AFM1x model and red circles to the AFM1z model. For the samples x = 0.10, 0.2 and 0.25 no long-range magnetic contribution was found.

While the a and c axes show a convex and concave shape with x, respectively, and a linearly increasing volume of the unit cell at 2 K, the position of La and Se, the distance between the magnetic layers and Se–La distances show nonlinear dependences. However, the angle between Se–Fe/Mn–Se changes linearly with x. This suggests that different mechanisms are triggering the structural and magnetic changes in the system.

Results of this study were published in S. Landsgesell et al., Acta Materialia **66** (2014) 232.

References

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[3] D.G. Free et al., Phys Rev B **81** (2010) 214433.
[4] S. Landsgesell et al., J. Phys: Condens Matter 25, (2013) 086004.