

Experiment Title : Dynamics in half doped manganites	Proposal Number 4-01-645
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Proposer (to whom correspondence will be addressed)

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DEEN PASCALE

Suggested keyword number **4-01**

This proposal is :

A new proposal.
 A continuation proposal.
 A resubmission.

The main research area of your proposal is

Biology Chemistry Physics Materials Methods and instrumentation
 Engineering Soft condensed matter Other :

Industry : **NOT Related to industrial applications**

Instrument requiredDays	Requested starting time :
D7 12	1. Jan/Feb 2. Mar/Apr 3. May/Jun
IN4 4	4. Jul/Aug 5. Sep/Oct 6. Nov/Dec
	Unacceptable Dates :

Sample availability **already available**

Sample description

Substance/Formula : **Nd_{0.5}Ca_{0.5}MnO₃**

Mass (in mg) : **10000**

Size (in mm³) :

State : **powder**

Surface area :

Space group :

Unit cell dimension :

a =

b =

c =

T (k) =

α =

β =

γ =

Sample container :

Safety aspects

The sample is : **TOXIC**

Is there any danger associated with the proposed sample or its preparation at ILL ?

Yes Uncertain No If Yes or Uncertain, please give details of the risks associated :

Is the sample a transuranium sample Yes No

Experimental details

Energy / wavelength range : **4.8Å D7; 1.1Å IN4**

Resolution in energy or wavelength :

Range of momentum transfer :

Resolution in momentum transfer :

Sample environment equipment (supplied by ILL)

Environment equipment : **cryofurnace 1.8 - 573 K**

Temperature range (stability) : **100 ÷ 500 K**

Pressure range :

Magnetic-field strength (stability)

Is there any danger associated with ancillary equipment ? Yes Uncertain No

If Yes or Uncertain, please give details of the risks associated :

To be filled in by ILL

Sample environment code

Comments by Health Physics Officer and Safety Engineer

CF

Abstract

Charge ordering (CO) in manganites RE_{1-x}DI_xMnO₃ (where, RE stands for rare earth element and DI for divalent ion) only occurs for a narrow range of doping x, around 0.5, and few combinations RE-DI. Nowadays, it is one of the main issues for these compounds.

In a recent elastic experiment on Nd_{0.5}Ca_{0.5}MnO₃ on the D7 spectrometer in a wide temperature range, we have evidence of developing of magnetic fluctuations crossing the CO transition. We would like to clarify the nature of such fluctuations by means of ToF measurements with polarisation analysis on D7 and characterise the spin fluctuation spectral width on the ToF IN4 spectrometer.

LOW ENERGY DYNAMICS IN HALF-DOPED MANGANITES

a) Scientific Background

The so-called half-doped manganite, $RE_{0.5}DI_{0.5}MnO_3$ (where, RE stands for rare earth element and DI for divalent ion) represents the most complex compound within the general system $RE_{1-x}DI_xMnO_3$ ($0 \leq x \leq 1$). Since the early days [1], it was soon clear that a superior complexity of this composition existed because of a non-unique bonding arrangement of the atoms within a fixed crystallographic structure, resulting [2] in an antiferromagnetic-insulator phase competing with a conductive-ferromagnetic one. Then, after the discovery of the CMR phenomenon, a charge-orbital ordering model was proposed and fully corroborated [3]. However, the charge ordering (CO) picture has been re-called into question as a result of highly accurate experiments and data analysis. XANES at the Mn K-edge in $La_{0.5}Ca_{0.5}MnO_3$ [4] and high resolution neutron diffraction on $Pr_{0.6}Ca_{0.4}MnO_3$ [5] have turned out to be incompatible with Mn^{+3} and Mn^{+4} ions arrangement and suggested an intermediate valence state for Mn. In the latter work, in particular, has been also pointed out the difficulty in making a good quality single crystal with the $x = 0.5$ concentration. Fortunately, compositions with $0.4 \leq x \leq 0.6$ have same general features.

We have recently been focusing on $Nd_{0.5}Ca_{0.5}MnO_3$ powder sample that show the same general characteristics of $Pr_{0.6}Ca_{0.4}MnO_3$. In particular, we have performed very recently an elastic experiment on the D7 spectrometer in a wide temperature range from 180K up to 400K where the susceptibility shows a peak attributed generally to the charge ordering [4]. As shown in *Fig.1*, in the “charge ordering” temperature range, the magnetic scattering diminished as the temperature increases with a magnetic signal developing at low Q for low temperatures. This particular picture depends on the fact that the magnetic fluctuations are of high frequency, and the magnetic signal goes outside of the energy window of the instrument following a Q-square behaviour.

b) Proposal

In order to investigate the nature of the spin dynamical properties, their evolution with temperature and their behaviour across the CO phenomenon, we propose to use D7 with the ToF option and xyz polarization analysis to probe $S(Q,\omega)$ and $S(Q)$ to separate the fluctuating from the non-fluctuating magnetic component. In addition, we intend to characterise the spin-fluctuation spectral width on the thermal ToF spectrometer, IN4 in order to quantify the integrated moment measured within the time-window of D7.

We ask 12 days on D7 using $\lambda = 4.8 \text{ \AA}$ (10 days for 5 temperatures; 2 days for calibrations), and 4 days on IN4 with $\lambda = 1.1 \text{ \AA}$ (3 days for a sample and 1 day for calibrations) in the temperature range 100K-500K

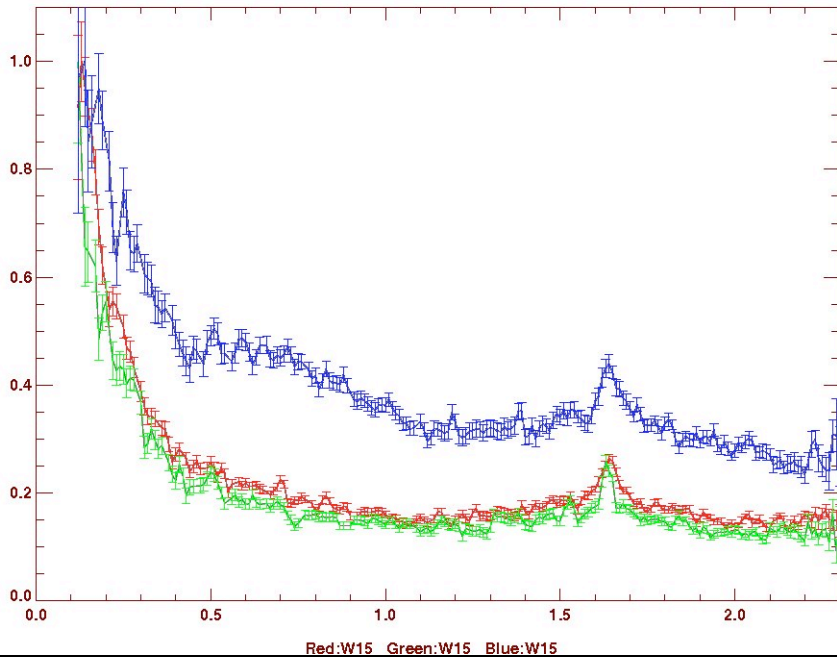


Fig.1 Magnetic component vs $Q(\text{\AA}^{-1})$ measured at different temperatures: blue at 180k; red at 252K; green at 400 K

References

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Proposal:	4-01-645	Council:	10/2006
Title:	Dynamics in half doped manganites		
This proposal is a new proposal			
Research Area:	Materials		
Industry:	Not related to industrial application		

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	BP 220	New neutron user? No
	38043	New ILL user? No
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Instrument	Req. Days
D7	12
IN4	4

Publication:

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