Low Temperature Study of the Complex Magnetic Order in Yb_{0.9}Sr_{0.1}MnO₃ Using Neutron Diffraction

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Objectives

Why YbMnO₃ Perovskites ? Complex magnetic structure Using neutron diffraction at very low temperatures

Introduction

- The unusual magneto-electric transport properties of rare earth manganites, as a result of doping with divalent element, are very rich topic for research.
- These compounds have $R_x A_{1-x} MnO_3$ chemical formula and have been formed with the perovskite-like structure in different crystal systems starting from the simple cubic
- Moreover, they showed very wide range of applications in spintronics magnetic storage media, chemical sensors, photocatalysis.
- These wide scale of applications reflect the rich properties of such compounds.
- Crystal structure paly very important role in the variation of these properties.
- The crystal structure depends on which rare earth element is used to form the perovskite.

Introduction

- The ionic radius of selected rare earth element controls the type of crystal system.
- ▶ If the rare earth in *R*MnO₃ is Y, Ho, Yb or Er with smaller ionic radius, these compounds considered as muliferroic materials where multiferroic materials display the simultaneous coexistence of (anti)ferromagnetism, ferroelectricity, and ferroelasticity.
- ► The most probable crystal system in such materials is the hexagonal structure where Mn atoms are located at the center of the MnO₅ bipyramids whose vertices are occupied by oxygen atoms.
- One O(3) and two O(4) atoms are on the equatorial plane of the MnO₅ polyhedra while O(1) and O(2) are located at apical positions.
- The bipyramids are linked by the corner-sharing equatorial oxygens.

- The displacement of each atom occurs when the temperature decreases below T_N and may lead to models are done to understand the unusual electric and magnetic transport.
- Based on the double exchange model and other theoretical methods Aliaga et al. showed that the half doped manganites have resistivity changing from an insulator to a metal phase in a first order manner depending on two parameters; temperature and applied magnetic field.
- Using Monte Carlo simulations to give description for the double-exchange model where the lattice distortion resulted in cooperative Jahn-Teller effect in 2d lattice was used.
- Also, a transition from insulator phase to metal phase has been observed.
- A dynamic version of the Ising model based on the exchange interactions fluctuate in time between two exchange interaction taking into consecration the distribution of magnetically doped insulating oxides.
- There are free spins associated with transition metal ions that occupy the Zn sites in zinc oxide.
- The mixed crystal structure in rare earth perovskite was recently reported
- In the present work, strontium doped ytterbium manganite was studied using neutron diffraction at very low temperature as well as theoretical model was presented

Experimental & theoretical calculations Details

Materials: Preparation and Characterization Neutron Diffraction Measurements Calculation using Monte Carlo Simulation

Materials: Preparation and Characterization

Preparation: we used coprecipitation method

Co-precipitation method was used to prepare Nano-crystalline $Yb_{0.9}Sr_{0.1}MnO_3$ from the initial pure chlorides of ytterbium, strontium and manganese. These chlorides reacted with pure sodium hydroxide according to the required molar ratio. The obtained powder after precipitation process was washed many times by distillated water until all sodium chloride dissolved in water and removed. The resulted powder after washing has been dried. The annealing process for the pressed powder in disc form was at 850 °C for 12h.

Characterization

The XRD test of the formation of perovskite-like structure was carried out using Panalytical X'pert pro MPD. The elemental analysis, EDXS spectrum, and SEM micrograph were done using Field Emission Scanning Electron Microscope FESEM–JEOL (JSM-5600) with acceleration voltage 15kV and magnification of 43000. Ising model in $Yb_{0.9}Sr_{0.1}MnO_3$

Neutron Diffraction Measurements

The neutron diffraction measurements were performed using high resolution powder diffractometer (superposition multi-detector type neutron diffractometer) which installed on neutron beam channel No.9 of the WWR-M Reactor in Petersburg Nuclear Physics Institute PNPI, Russian Academy of Science.

Ising model Calculations in Yb_{0.9}Sr_{0.1}MnO₃

► Ising model calculation for the complex crystal structure and magnetic types of the strontium doped ytterbium manganite; namely Yb_{0.9}Sr_{0.1}MnO₃, is done.

► The possible magnetic structures are estimated from the experimental results and symmetry consideration of each crystal system form is given in this work to explain the different magnetic behaviors in the hexagonal and the orthorhombic phases.

This magnetic structure represents a frustrated magnetic structure with a canted-spin ordering of Mn magnetic moments in plane of Γ 2-type. Mn ions form well-separated triangular layers parallel to (*ab*) plane, with antiferromagnetic exchange interaction between the spins of the most nearest neighbors, which make the Mn spin subsystem of low-dimensional and frustrated. The phase with orthorhombic crystal structure shows magnetic structure presumably *C*-type formation

Results & Discussions





XRD and EDAX of Yb0.9Sr0.1MnO3

Results & Discussions



SEM Image

ND



Refined ND pattern



Intensity (arb. units)



Calculation results



Conclusions

- ► The mixed crystal structure, orthorhombic/hexagonal, in the nanocrystlaline size of Yb_{0.9}Sr_{0.1}MnO₃ is found with crystallite size of 85nm.
- The orthorhombic phase content decreases with heat treatment of Yb_{0.9}Sr_{0.1}MnO₃ from 45% to 5%.
- The mixed antiferromagnetic ordering of the hexagonal and orthorhombic phases of $Yb_{0.9}Sr_{0.1}MnO_3$ is approved with T_N near 87K.
- The absence of ytterbium contribution to the magnetic ordering of Yb_{0.9}Sr_{0.1}MnO₃ in the low temperature range up to 2.5K.
- Theoretical calculations using Monte Carlo simulation for Ising model confirmed the existence of both C and Γ2 magnetic types

Acknowledgement

Thank you very much For Your attention



