The crystal and magnetic structure of advanced oxide materials: neutron diffraction studies

Nadezhda Belozerova

1. Introduction. Progress in modern condensed matter physics and the development of modern technologies in recent decades is inseparably connected with the studies of complex oxide materials, since in this class of compounds was discovered such important phenomena as high temperature superconductivity, colossal magnetoresistance effect, the metal-insulator transition, charge and orbital ordering, ferroelectricity, magnetoelectric effect, spin crossover, etc. Neutron diffraction is the most direct and informative method of studying the magnetic ordering in crystal materials. Functional oxides of transition metals are convenient model systems for the study of basic rules of physical phenomena in oxide magnets, so new experimental data will be important to clarify modern concepts of the microscopic mechanisms of formation of physical properties and phenomena observed in these compounds. As an example, recently, the structural and magnetic ordering of Pb_2FeSbO_6 was studied by means of neutron powder diffraction in the temperature range from 5 to 300 K. At low temperature T_N~30 K the long-range antiferromagnetic ordering in the Pb_2FeSbO_6 compound was observed.

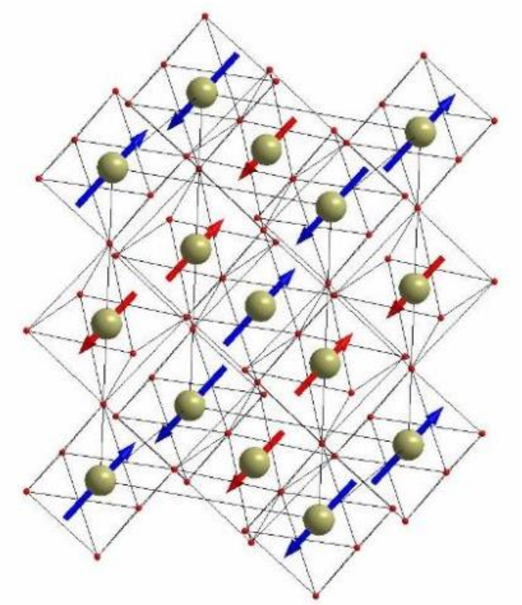

Figure 1. *The schematic representation of a magnetic structure of Pb_2FeSbO_6 compound at low temperatures. The iron atoms inside oxygen octahedra and corresponding magnetic moments are shown. The blue and red arrows mark the magnetic moments of Fe ions in crystallographic iron site (0, 0, 0) and antimony site (0, 0, ½) respectively.*

The corresponded propagation vector describes the antiferromagnetic order of iron ions as q = [½, ½, 0]. The mechanisms of formation of this antiferromagnetic phase are discussed in the framework of the hypotheses about the existence of domains with fully cation ordered phase and a disordered one. From the point of view of the increase of a piece of knowledge of students about magnetic oxides and the opportunities of neutron diffraction method, we propose a course focused on a knowledge about neutron diffraction experiments, treatment of diffraction experimental data, obtaining the basis of analysis of the crystal and magnetic structure of complex oxides.

2. Description of the project

During the project, it is planned to perform neutron diffraction experiments on DN-6 diffractometer, treat the obtained experimental data using Rietveld method, and obtain parameters of crystal and magnetic structure including interatomic distances, valence angles and the formation of magnetically ordered phases, and those basic dependences.

3. Experimental

The Joint Institute for Nuclear Research has a world-class scientific facility the IBR-2 high-flux pulsed reactor. The Frank Laboratory of Neuron Physics at JINR (Dubna, Russia), which basic facility is the IBR-2 high flux pulsed reactor, has more than twenty years of experience in the development in the neutron diffraction methods. By means of this research method, it is planned to achieve the main goal of the project – to determinate the structural mechanisms of the formation of the magnetic properties of several magnetic oxides. Neutron diffraction is a reliable experimental method for obtaining data on the crystal and magnetic structure of complex oxides. A new high-brilliance diffractometer DN-6 combining higher incident neutron flux and wide aperture of detector system have been developed in recent years. The DN-6 neutron diffractometer for high pressure research is located on the 6b beamline of the IBR-2 high flux pulsed reactor.

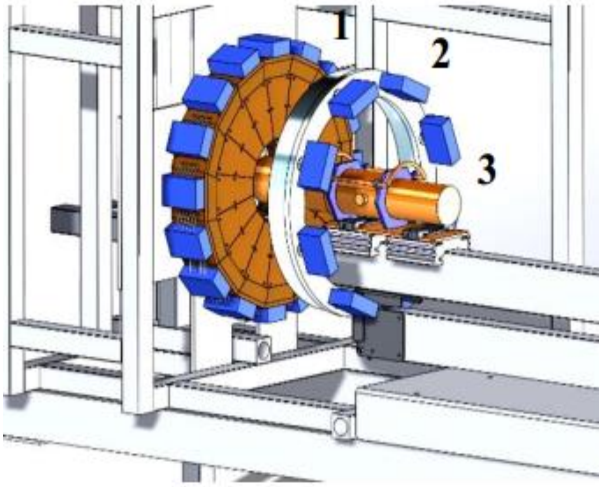

Figure 2. *Enlarged schematic layout of detector and sample environment systems of the DN-6 diffractometer. The 90-deg. scattering angle detector section (1), the low scattering angle detector section (2), the horizontal cryostat (3) and sample and high-pressure cells holders fixed on the movable slider are shown. The diffractometer components are mounted on a mechanical support cage.*

The pulsed regime of the IBR-2 reactor operation provides neutron diffraction measurements at the DN-6 diffractometer using a time-of-flight (TOF) mode. There are two detector sections of the circular form installed at different scattering angles at the DN-6 diffractometer. The horizontal cryostat based on a closed-cycle helium refrigerator is used for the low- temperature experiments in the range 5-320 K. The design of the cryostat provides the possibility of cooling the highpressure cells with different constructions. The DN-6 diffractometer provides possibilities for routine studies of broad classes of materials with ordinary neutron scattering lengths and average magnetic moment values over the significantly extended high pressure range. During the last years, a number of studies focused on the pressure and temperature induced modifications of the crystal structure, and magnetic order in different materials have been performed.

4. Requirements for the level of student training

Students should know the basic principles of condensed matter physics, be guided in the principles of diffraction methods, have basic skills of working with typical scientific software.

5. Recommended literature

1. Kozlenko D.P., Kichanov S.E., Lukin E.V., Savenko B.N. “The DN-6 Neutron Diffractometer for High-Pressure Research at Half a Megabar Scale”, Crystals, 8 (2018) 331

2. Neutron powder diffraction by Richard M. Ibberson and William I.F. David, Chapter 5 of Structure determination form powder diffraction data IUCr monographphs on crystallography, Oxford scientific publications 2002

3. A. V. Belushkin, D. P. Kozlenko, and A. V. Rogachev, Synchrotron and neutron-scattering methods for studies of properties of condensed matter: Competition or complementarity? J. Surf. Invest. 5, 828 (2011).

6. The number of participants of the project: up to 3 persons

7. The project leader from JINR:

Dr. Belozerova Nadezhda, Researcher, Condensed Matter Department Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research