Precision investigation of modern crystalline materials by neutron diffraction method

1) The goal of project: increasing the knowledge of students up to users level of neutron diffraction method.

2) During time of school students get Introducing into methods, real or model measurements and data treatment: getting information about crystal system and unit cell parameters, atomic positions and thermal vibrations, microstresses and grain sizes (it is particularly important if have deals with nanocrystalline material). And refinement of magnetic structure is as additional seminar.

3) The work of students includes: sample preparation up to neutron powder diffraction requirements, data treatment by Rietveld method and preparation of final report. The results will be presented as answers to questions related to the course (individual questions).



Fig.1. HRFD diffractometer (<u>http://uc2.jinr.ru/pano/lnf/exp_zal1.html</u>).

4) Required level for students: at least 4th year of University. A general knowledge of crystal structures with the basic principles of diffraction phenomena is desirable.



Fig.2. Comparison of neutron diffraction patterns of the $YBa_2(Cu,Fe)_3O_7$ powder sample obtained in a high-resolution mode at HRFD (top part) and with a resolution usual for an IBR-2 diffractometer (bottom). The data are processed by Rietveld method.

5) Basic references:

1. A.M. Balagurov "High resolution Fourier diffraction at the IBR-2 reactor" Neutron News, 16 (2005) 8-12.

2. Young, R.A., ed. (1993). The Rietveld Method. Oxford: Oxford University Press & International Union of Crystallography.

3. Lovesey, S. W. (1984). Theory of Neutron Scattering from Condensed Matter; Volume 1: Neutron Scattering. Oxford: Clarendon Press.

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

6) up to 4 persons

7) PhD. Ivan Bobrikov, researcher, Frank Laboratory of Neutron Physics, Condensed Matter Department

http://flnp.jinr.ru/124/1/223/