

## JOINT INSTITUTE FOR NUCLEAR RESEARCH Frank Laboratory of Neutron Physics

# FINAL REPORT ON THE SUMMER STUDENT PROGRAM

*Creating a database of inelastic and quasielastic neutron scattering spectra from NERA spectrometer* 

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### Abstract

In Frank Laboratory of Neutron Physics of the Joint Institute for Nuclear Research in Dubna scientists conduct their research about neutrons as elementary particles and also study other materials using neutrons. In FLNP there is fast pulsed reactor IBR-2M surrounded by the experimental facilities which uses neutron beam from reactor. One of experimental facilities is NERA. The NERA spectrometer is aimed to study inelastic and quasielastic neutron scattering with simultaneous control of the phase of the sample by neutron diffraction. This report is about a project which main task was creating a database of experimental results obtained from NERA spectrometer which is available at the website: neradb.jinr.ru.

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#### 1. Introduction

I was a participant of Summer Student Program 2016 at Frank Laboratory of Neutron Physics of the Joint Institute for Nuclear Research in Dubna for five weeks. During this time I learnt a lot about JINR and studied opportunities of research in JINR.

The purpose of my work was creating a database of inelastic and quasielastic neutron scattering spectra obtained from NERA spectrometer in Frank Laboratory of Neutron Physics. Project aimed to prepare a database which will display information such as: sample's name, experiment's author and author's affiliation, date of start and end of measurement, comments and information of publication of results. For some samples pictures of spectra are shown. It was assumed that the user of database will be able to search for a sample giving: sample's name, experiment's author or/and year of the measurement. Database should have an administrator's panel where administrator can change data, add new samples and delete sample. Database should be available as the website. I wrote html, php and css scripts and added them to the server: neradb.jinr.ru.

In this report I started from the basic information about Frank Laboratory of Neutron Physics. In next point I explained how fast pulsed reactor IBR-2M works and how NERA spectrometer works. In third section there is a short description of the project's realization. I ended by presenting results of my work and further steps that should be taken to finish the database.

#### 2. Information about NERA group

#### 2.1. Frank Laboratory of Neutron Physics

Joint Institute of Nuclear Physics consists of seven laboratories. One of them is Frank Laboratory of Neutron Physics (FLNP). Frank Laboratory of Neutron Physics was founded in 1957. FLNP has a lot of experience in creation and development of neutron sources. There are two neutron sources in FLNP: pulsed fast reactor IBR-2M and the Intense Resonance Neutron Source. There is also EG-5 – Van de Graaff accelerator. FLNP has also experience in using neutrons in fundamental and applied science. There are research about neutron as an elementary particle and also studies of other materials using neutrons. Many experiments are performed by the researchers from many countries. In FLNP ultracold neutrons were discovered. Enhancement of the space parity violation effect in neutron resonances was found.

#### 2.2. Reactor IBR-2M

In Frank Laboratory of Neutron Physics one of neutron sources is fast pulsed reactor IBR-2M with mechanical modulation of reactivity with a movable reflector. Reactor IBR-2 was put into operation in 1984 (1). The IBR-2M is a modernized version of the IBR-2 reactor. IBR-2M is a sodium-cooled reactor. Stationary thermal power of IBR-2M is 2MW. Fuel of IBR-2M is plutonium dioxide pellets. In core there are 69 fuels assemblies. Thermal neutron beam, which is used in experimental facilities is produced by thermalization of fast neutrons from reactor by water or mesitilene moderators. Frequency of power pulse is 5Hz. Thermal neutron flux density from the surface of the moderator in burst maximum is  $10^{16}$ n/cm<sup>2</sup>·s. Power pulse is generated when the blades pass opposite the core. The core of the reactor is shown in figure 1.



Figure 1. Scheme of the core of the IBR-2M reactor (2)

There are many neutron installations near IBR-2M reactor which are shown in figure 2. The IBR-2M instruments are (3):

- Diffraction: HRFD, DN-2, DN-12, DN-6, SKAT, EPSILON, FSD;
- Small-angle scattering: YuMO;
- Reflectometry: REMUR, REFLEX, GRAINS;
- Inelastic scattering: DIN-2PI, NERA;
- Neutron Activation Analysis: REGATA;
- Irradiation Facility.

Reactor is used to research in physics, structure and dynamics of functional materials, complex liquids and polymers, molecular biology and pharmacology, structure of rocks and minerals, engineering diagnostics, neutron-nuclear interactions and neutron activation analysis for life science.



Figure2. Experimental facilities (4)

#### 2.3. NERA spectrometer

The NERA Group is a part of Frank Laboratory of Neutron Physic of the Joint Institute for Nuclear Research in Dubna. The NERA spectrometer is aimed to study inelastic and quasielastic neutron scattering with simultaneous control of the phase of the sample by neutron diffraction. NERA spectrometer (Fig. 2) is used to investigate the dynamics and structure of condensed matter, particularly, of the substances exhibiting phase polymorphism. NERA spectrometer is also used to investigate substances in which phase transitions are accompanied by changes in the structure, lattice dynamics or in the character of stochastic motion of the molecules or molecular groups.





1 – Moderator, 2 – Background Choppers, 3 – Ni Guide Tube, 4 – Detector for High Intensity Diffraction, 5 – Detector for High Resolution Diffraction, 6 – He<sup>3</sup> Detectors (INS and QNS), 7 – Single Crystal QNS Analyzer, 8 – Pyrolytic Graphite INS Analyzer, 9 – Be-Filters, 10 – Collimators, 11 – VME control and operative visualization/analysis, 12 – VME Station (OS/9) Data Acquisition, 13 – EtherNet Data Transfer

#### 3. Realization and results

The main point of my work during Summer Student Program was creating a database for spectra from NERA spectrometer.

Assumptions:

- Database should include the following information: sample's name, experiment's author and author's affiliation, date of start and end of measurement, comments and information of publication of results;
- For some samples there are pictures of two spectra: INS/QENS and ND;
- User of database can search for a sample using: sample's name, experimentator's name or/and year of measurement;
- Database should have administrator's panel where administrator can change data, upload spectra, add new samples and delete a sample;
- Database should be available by the website.

Database was written in MySQL language. I used the CREATE DATABASE statement to create database Nera. I used the CREATE TABLE statement to create table Nera. In table Nera I created columns: ID, sample's name, experiment's author, author's affiliation, year, experimental start date, experimental end date, comments and publications. I described the data-type parameter specifies and the size parameter specifies for each column in table Nera.

I used SQL statements, specifically the INSERT command to write data into the database, the UPDATE command to edit data in database and the DELETE command to delete data from the database. I had to use the PHP code to send commands to the database. PHP is a script language which I used to handle the administration of MySQL database over the web. PHP code should be embedded inside HTML code. I used Total Commander to connect with server. I put HTML and PHP files into page: neradb.jinr.ru by this program.

The website page consists of three frames: banner, menu and main page (fig. 4). The banner displays superscription: Frank Laboratory of Neutron Physics, NERA database. Website's user can select three options in menu: list of samples, search and administration with results shown in main frame.



Figure 4. Main page

If website's user selects "List of samples", list of samples displays on main page (fig. 5). There are two ways for displaying list of samples. One is list of samples ordered by name, second is list of samples ordered by year.



When website's user selects a sample, sample's data from database and spectra display on main page (fig.6).

← → C 🗋 neradb.jinr.rd	J				
Frank Labo	Frank Laboratory of Neutron Physics				
NERA data	NERA database				
	2,5 - Lutidine				
List of samples	Experiment's author: Ireneusz Natkaniec				
	Affiliation: Adam Mickiewicz University, Poznan, Poland				
Search	Chemical formula:				
	Start date: 2013-01-27				
Administration	End date: 2013-01-28				
	Comment:				
	Publication:				
	INS seconds				
	Download				
	20. Jaka Hole, Y-180, UT GLIPPE all, 20. Jakaben Hole, Y-1001, UT GLIPPE all, 20. Jakaben, Hole, Y-001, UT G. 20. Jakaben, Hole, Y-1001, UT G. 20. Jakaben, Hole, Y-101, UT G. 20. Jakaben, Ho				
	N300 D-				
	300 D-				
	A A				
	990.0-				
	a p to sho sho sho sho sho sho sho sho				

Figure 6. Sample's data

After click on "Search" website's user can search the samples by name, author and year (fig.7). List of matching samples display on main page. If website's user selects sample, chosen sample's data display on main page.

←	→ C 🗋 ner	adb.jinr.ru			
	Frank Laboratory of Neutron Physics NERA database				
			Search		
	List of samp	les	Sample's name Experiment's author Year		
	Search				
	Administrati	on		Search	
Figure 7. Search panel					

If website's user clicks on "Administration", a window to log automatically opens (fig. 8).

Frank Laboratory of Neutron Phy	Wymagane uwierzytelnienie	
NERA database	http://neradb.jinr.ru wymaga nazwy użytkownika i hasła. Twoje połączenie z tą witryną nie jest prywatne.	
	Nazwa użytkownika:	
	Hasło:	
List of samples		
Search	Zaloguj się Anuluj	
Administration		

Figure 8. Administrator's panel

In administrator's panel (fig.9) there are options: add new sample (fig.10), upload spectra, edit sample (fig.11) and delete sample available only for logged-in users.



Figure 9. Administrator's menu

← → C 🗋 neradb.jinr.ru	1				
Frank Labo	Frank Laboratory of Neutron Physics				
NERA data	NERA database				
	Add sample				
List of samples					
Search	Sample's name Experiment's author				
Administration	Affiliation Chemical formula Year Start date				
	End date Comment Publication Save				

Figure 10. Add sample's data

F	> C 🗋 neradb.jinr.ru					
	Frank Laboratory of Neutron Physics					
	NERA database					
		Change data				
	List of samples	Sample's name	(NH4)2MoO2F4			
	Search	Experiment's author Affiliation	L. Smirnov			
	Administration	Chemical formula	(NH4)2MoO2F4			
		Year	2013			
		Start date	2013-10-21			
		End date	2013-10-21			
		Comment	18, 17g, T=225K			
		Publication	0			
			Save			

Figure 11. Edit sample's data

Results of my project are on the website: www.neradb.jinr.ru.

#### 4. Further steps

Now database contains only the data from year 2013, without spectra. There is some work to do, namely inserting the data from other years and adding spectra for all samples. I hope that database will be supplemented systematically by members of NERA Group.

#### 5. Bibliography

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- 2 http://flnp.jinr.ru/564/ (4.08.2016)
- 3 http://flnp.jinr.ru/img/27/1055\_Booklet\_FLNP.pdf (4.08.2016)
- 4 http://ibr-2.jinr.ru (4.08.2016)
- 5 http://flnp.jinr.ru/134/ (4.08.2016)

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