

# **Book of Abstracts**

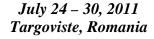
The 3rd Joint Seminar JINR - ROMANIA on Neutron Physics for Investigation of Nuclei, Condensed Matter and Life Science, Targoviste, Romania July 24-30 2011



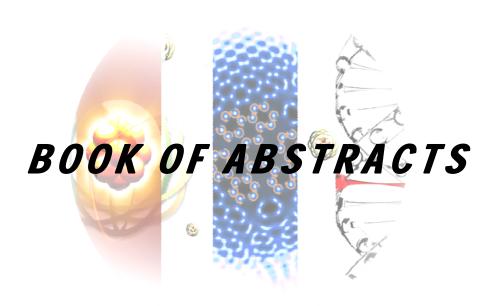












Editors: Ion V. Popescu, Cristiana Radulescu, Claudia Stihi

> Bibliotheca Publishing House Targoviste, 2011

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- I. Ion V. POPESCU (ed.)
- II. Cristiana RADULESCU (ed.)
- III. Claudia STIHI (ed.)

# THE 3<sup>rd</sup> JOINT SEMINAR JINR-ROMANIA ON NEUTRON PHYSICS FOR INVESTIGATIONS OF NUCLEI, CONDENSED MATTER AND LIFE SCIENCES

www.icstm.ro/JSJR3

## JULY 24-30, 2011 TARGOVISTE – ROMANIA

## The Seminar is jointly organized by:

Valahia University of Targoviste, Romania



Joint Institute for Nuclear Research, Dubna, Russia



National Institute for R & D in Electrical Engineering, ICPE-CA, Bucharest, Romania



*under the patronage of:* Romanian Ministry of Education, Research, Youth and Sport



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Valahia University of Targoviste,

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Romania I. Nita Valahia University of Targoviste, Romania

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#### AIMS AND SCOPE

It is well known that neutrons are a powerful instrument for investigation of nuclei and condensed matter. In recent years, neutrons proved their applicability in such dynamic fields of research as biotechnology, nanostructures, environmental chemistry and others.

Frank Laboratory of Neutron Physics (FLNP) is one of the seven JINR Laboratories. It possesses two active neutron sources: the modernized fast pulsed IBR-2 reactor and the Intense Resonance Neutron source (IREN). A set of 13 high-performance instruments, that are constantly being upgraded, are available for your experiments at the FLNP site, some other completely new instruments being presently under construction. A team of qualified and dedicated staff comprised by scientists, engineers and technicians is ready to assist you throughout the experiments at each instrument. A wide range of scientific themes for experimental works are available for undergraduates, masters and PhD students.

The general objective of the school-seminar is to consolidate collaboration between FLNP JINR and Romania.

The educational seminar is aimed at:

• presenting the most advanced scientific projects being processed in FLNP JINR and in various Romanian partner institutions;

• enabling young researchers to get involved, to present and to publish their original results;

• encouraging students to carry on scientific activity after graduation;

• enlarging the staff comprised by Romanian scientists (assistant as well as senior researchers) hired by JINR within the long term employment contracts.

The scientific program of the educational seminar for young scientists is targeted at covering several basic fields in the investigations of which the FLNP JINR staff members are taking active part and Romanian scientists has a special interest:

✓ Nuclear physics

✓ Life sciences

✓ Physics of nanosystems

✓ Structure and dynamics of functional materials

✓ Complex liquids and polymers

✓ Molecular biology and pharmacology

 $\checkmark$  Structure of rocks and minerals

✓ Engineering diagnostics

 $\checkmark$  Electronics and automatics of experimental installations

FLNP is proud to have active cooperation agreements with almost 200 scientific institutes and universities of 40 countries from all over the globe and willing to enlarge its collaborating activity.

Are you a physicist, a chemist, a materials scientist, a biologist, a geologist, a specialist in electronics? Then, we are looking forward to see you in Targoviste where you can learn more about the FLNP JINR opportunities.

Dr. Eugen Anitas	– BLTP JINR, Dubna, Russia		
	– IFIN-HH, Magurele, Romania		
Prof. Alexander V. Belushkin	- Director of FLNP, JINR, Dubna, Russia		
Dr. Maria Balasoiu	– FLNP JINR, Dubna, Russia		
	– IFIN-HH, Magurele, Romania		
Dr. Ivan A. Bobrikov	– FLNP JINR, Dubna, Russia		
Dr. Sergey B. Borzakov	– FLNP JINR, Dubna, Russia		
Acad. Prof. Emil Burzo	- Member Presidium Romanian Academy		
	- Member PAC Committee Solid State Physics		
	IUCN Dubna		
Dr. Otilia A. Culicov	– INCDIE ICPE – CA, Romania		
	– JINR, Dubna, Russia		
Prof. Octavian Duliu	- University of Bucharest, Romania		
Assoc. Prof. Antoaneta Ene	- Dunarea de Jos University of Galati, Romania		
Prof. Marina Frontasyeva	– FLNP JINR, Dubna, Russia		
Dr. Yu. M. Gledenov	– FLNP JINR, Dubna, Russia		
Dr. Ion Ionita	– INR, Pitesti, Romania		
Dr. Sorin Dumitru Ilie	- CERN TE/VSC/CSA, Switzerland		
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Dr. Pavel V. Sedyshev	– FLNP JINR, Dubna, Russia		
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Dr. Traian Zaharescu	- INCDIE ICPE - CA, Bucharest, Romania		
Dr. Alexandr V. Vinogradov	– FLNP JINR, Dubna, Russia		

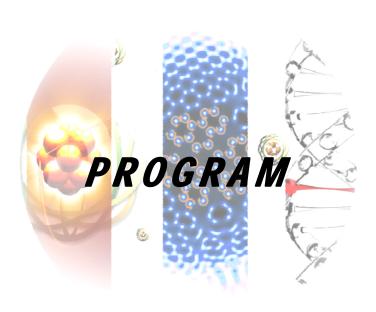
## PLENARY SPEAKERS

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## YOUNG PARTICIPANTS

Raul Erhan	– FLNP JINR, Dubna, Russia		
	– IFIN-HH, Magurele, Romania		
Lilia Anghel	– FLNP JINR, Dubna, Russia		
	- Institute of Chemistry of ASM, Moldova		
Alexandr Korokin	– FLNP JINR, Dubna, Russia		
Konstantin Mukhin	– FLNP JINR, Dubna, Russia		
Anatolii Nagornyi	– FLNP JINR, Dubna, Russia		
	- Taras Shevchenko National University of Kiev, Ukraine		
Maxim Bulavin	– FLNP JINR, Dubna, Russia		
Oleksandr Tomchuk	– FLNP JINR, Dubna, Russia		
	- Taras Shevchenko National University of Kiev, Ukraine		
Inga Zinicovscaia	– FLNP JINR, Dubna, Russia		
	- Institute of Chemistry of the ASM, Moldova		
Cristian Dragolici	– IFIN-HH, Magurele, Romania		
Alina Sion	- Dunarea de Jos University of Galati, Romania		
Dorin Bibicu	- Dunarea de Jos University of Galati, Romania		
Anca Gheboianu	- ICSTM, Valahia University of Targoviste, Romania		
Iulian Bancuta	- ICSTM, Valahia University of Targoviste, Romania		
Dorin Let	- ICSTM, Valahia University of Targoviste, Romania		
Andreea Stancu	- ICSTM, Valahia University of Targoviste, Romania		
Ioana Dulama	- ICSTM, Valahia University of Targoviste, Romania		
Alin Bucurica	- ICSTM, Valahia University of Targoviste, Romania		
Andrei Chilian	- ICSTM, Valahia University of Targoviste, Romania		
Geanina Stanescu	- ICSTM, Valahia University of Targoviste, Romania		
Simona Mihai	- ICSTM, Valahia University of Targoviste, Romania		
Roxana Bancuta	- ICSTM, Valahia University of Targoviste, Romania		
Lucica Toma	- ICSTM, Valahia University of Targoviste, Romania		
Marinela Voicu	- Valahia University of Targoviste, Romania		

Raluca Stirbescu	- PhD Physics School, University of Bucharest, Romania
Ovidiu Nitescu	- PhD Physics School, University of Bucharest, Romania
Delia Patroi	- ICPE-CA, Bucharest, Romania
Cristina Cirstea	- ICPE-CA, Bucharest, Romania
Dorinel Talpeanu	- ICPE-CA, Bucharest, Romania
Eugen Manta	- ICPE-CA, Bucharest, Romania
Florentina Albu	- ICPE-CA, Bucharest, Romania
Victor Stoica	- ICPE-CA, Bucharest, Romania
Cristian Morari	- ICPE-CA, Bucharest, Romania
Virgil Marinescu	- ICPE-CA, Bucharest, Romania
Mihai Iordoc	- ICPE-CA, Bucharest, Romania
Simona Pasareanu	- ICPE-CA, Bucharest, Romania
Catalin Rusu-Zagar	- ICPE-CA, Bucharest, Romania
Petru Vlaic	- Babes Bolyai University, Cluj-Napoca, Romania



Sunday 24 <sup>th</sup> of July	Arriving participants Dinner		
Monday 25 <sup>th</sup> of July	8.00 - 9.00	Breakfast	
	Valahia Univers	ity of Targoviste, Confe	rence Hall
	9.15 - 10.00	Registration	
	10.00 – 10.30	Opening ceremony	Prof. dr. Ion Cucui – Rector of Valahia University of Targoviste, Romania Prof. dr. Nicolae Zamfir – General Director of IFIN-HH, Magurele, Romania Prof. dr. Alexander V. Belushkin – Director of FLNP-JINR, Dubna, Russia Prof. dr. Ion V. Popescu – Director of ICSTM – UVT, Targoviste, Romania
	10.30 - 11.00	Neutron research at JINR-FLNP	Prof. dr. Alexander V. Belushkin
	11.00 - 11.15	Presentation of Valahia University of Targoviste	Dr. Laura M. Gorghiu Dean of Faculty of Sciences and Arts, Valahia University of Targoviste, Romania
	11.15 - 11.30	Coff	ee break

## PROGRAM

Prof. dr. Alexander V. Belushkin, Prof. dr. Nicolae V. Zamfir		
11.30 - 11.45	Presentation of ICSTM-UVT	Prof. dr. Gh. Valerica Cimpoca – Technical Director of ICSTM, Targoviste, Romania
11.45 - 12.00	JINR – Romania history of collaboration	Dr. Otilia A. Culicov INCDIE ICPE – CA, Bucharest, Romania and Scientific secretary of FLNP JINR, Russia
12.00 - 12.30	Neutron scattering in Romania	Maria Balasoiu Otilia A. Culicov, Ion Ionita,
12.30 - 13.30	The IBR-2 reactor: history and status	Dr. Alexandr V. Vinogradov
13.30 - 15.00	L	unch
Prof. dr.	Marina Frontasyeva, Prot	f. dr. Ion V. Popescu
15.00 - 15.30	Nanocarbons – Properties and Applications	Prof. dr. Wilhelm Kappel General Director of INCDIE ICPE – CA, Bucharest, Romania Iulian Iordache
15.30 - 16.30	NAA for life sciences and material science at FLNP JINR	Prof. dr. Marina V. Frontasyeva
16.30 – 17.30	Instrumental neutron activation analysis applications to environmental and geological studies – A joint Romanian – Russian Project	Prof. dr. Octavian G. Duliu
17.30 - 18.00	Discussions an	nd closing session
17.50 10.00		
	11.30 - 11.45 $11.45 - 12.00$ $12.00 - 12.30$ $12.30 - 13.30$ $13.30 - 15.00$ $Prof. dr.$ $15.00 - 15.30$ $15.30 - 16.30$ $16.30 - 17.30$	11.30 - 11.45Presentation of ICSTM-UVT $11.45 - 12.00$ JINR - Romania history of collaboration $12.00 - 12.30$ Neutron scattering in Romania $12.00 - 12.30$ Neutron scattering in Romania $12.30 - 13.30$ The IBR-2 reactor: history and status $13.30 - 15.00$ LProf. dr. Marina Frontasyeva, Prof $15.00 - 15.30$ Nanocarbons - Properties and Applications $15.30 - 16.30$ NAA for life sciences and material science at FLNP JINR $16.30 - 17.30$ Instrumental neutron activation analysis applications to environmental and geological studies - A joint Romanian - Russian Project

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Tuesday 26 <sup>th</sup> of July,	8.00 - 9.00	Breakfast		
	Valahia Univers	ity of Tragoviste, Confe	erence Hall	
Chairs	Prof. Dr. Radu Setnescu, Dr. Sergey A. Kulikov			
L5	9.15 - 10.15	(n, p) and (n, $\alpha$ ) reactions induced by resonance and fast neutrons	Dr. Yu M. Gledenov	
L6	10.15 - 11.15	Magnetoresistive manganese based perovskites	Prof. dr. Emil Burzo	
	11.15 - 12.00	Coffee break	and Poster session	
L7	12.00 - 12.45	Radiative capture of neutrons: fundamental investigations and applications	Dr. Sergey B. Borzakov	
L8	12.45 - 13.30	Analytical applications of thermal and 14 MeV neutron activation analysis in metallurgical industry	Dr. Antoaneta Ene	
	13.30 - 15.00	I	Lunch	
Chairs		Prof. Dr. Emil Burzo, Dr. Sergey B. Borzakov		
L9	15.00 - 16.00	Development of cryogenic moderators for neutron sources	Dr. Sergey A. Kulikov	
L10	16.00 – 17.00	Neutron activation analysis on reference materials from intercomparison runs (environmental and biological samples)	Dr. Ana Pantelica	

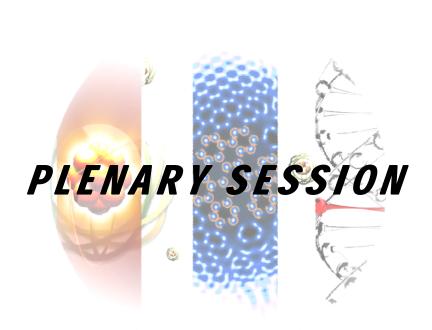
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THE 3 <sup>rd</sup> JOINT SEMINAR JINR-ROMANIA ON NEUTRON PHYSICS FOR
INVESTIGATIONS OF NUCLEI, CONDENSED MATTER AND LIFE SCIENCES

	17.00 - 19.00		town Targoviste, Princely ower, Dealu Monastery	
	19.00 - 20.00	Dinner		
Wednesday 27 <sup>th</sup> of July	8.00 - 9.00	Breakfast		
	9.00 - 21.00	Excursion and barbeque – Hanul din Meri, Buciumeni		
Thursday 28 <sup>th</sup> of July	8.00 - 9.00	Breakfast		
	Valahia Univers	sity of Tragoviste, Conf	erence Hall	
Chairs	Dı	r. Ana Pantelica, Dr. Pavel V. Sedyshev		
L11	9.15 - 10.15	Synchrotrons versus neutrons. Competitive or complimentary?	Prof. dr. Alexander V. Belushkin	
L12	10.15 - 11.00	Current status and future needs of nuclear analytical techniques and their applications	Prof. dr. Marina V. Frontasyeva	
	11.00 - 12.00	Coffee break and Poster Session		
L13	12.00 - 12.45	Investigations of ferrofluids and magnetic elastomers by means of small angle neutron scattering method	Dr. Maria Balasoiu Alexander I. Kuklin	
L14	12.45 - 13.30	High resolution neutron diffraction in Dubna. Examples of applications	Dr. Ivan A. Bobrikov, Anatoly M. Balagurov Valeriy G. Simkin	

	13.30 - 15.00	L	unch	
Chairs	Prof.	f. Dr. Octavian Duliu, Dr. Ivan A. Bobrikov		
L15	15.00 - 16.00	Using Q-Space Focusing in Thermal Neutrons Spectrometry To Get Improved Resolution Performances	Dr. Ion Ionita	
L16	16.00 - 16.30	Data acquisition and control systems for the IBR-2 spectrometers complex	Dr. Elena I. Litvinenko,	
	16.30 - 16.45	Coff	ee break	
L17 L18	16.45 - 17.30 17.30 - 18.00	On the behavior of the organic polymer materials in nuclear radiation fields Radiation induced chemical effects on some perfluorocarbon fluids	Prof. dr. Radu Setnescu Dr. Sorin Ilie, Prof. dr. Radu Setnescu	
	20.00	Gala	ı Dinner	
Friday 29 <sup>th</sup> of July	8.30 - 9.30	Breakfast		
	Valahia Univers	ity of Tragoviste, Confe	rence Hall	
Chairs	Dr. Antoaneta Ene, Dr. Elena I. Litvinenko			
L19	9.45 - 10.45	Radiation modifications induced in polymers. Synthetic polymers	Dr. Traian Zaharescu	

L20	10.45 - 11.45	Investigations of the parity violation in neutron reactions with lightest nuclei	Dr. Pavel V. Sedyshev et. al.
	11.45 - 12.00	Coff	èe break
L21	12.00 - 13.00	How to collaborate with JINR – technical aspects	Dr. Otilia A. Culicov
	13.00 - 13.30	Dise	cussions
	13.30 - 15.00	Ι	unch
	15.00 - 15.30	Closing ceremony and conclusions	Prof. dr. A. V. Belushkin Dr. Calin Oros Dr. Laura Monica Gorghiu Dr. Otilia Culicov
	15.30 - 16.00	Certificate awarding ceremony	Prof. dr. Marina Frontasyeva Dr. Otilia A. Culicov Dr. Cristiana Radulescu Dr. Claudia Stihi
	16.00 10.00		
	16.00 - 19.00	Free time or	Sport activities
	19.00 - 21.00	E	vinner
Saturday 30 <sup>th</sup> of July	8.00 - 9.30	Breakfast	
	9.30	Departure of	JINR participants



# NEUTRON RESEARCH AT THE FRANK LABORATORY OF NEUTRON PHYSICS

## ALEXANDER V. BELUSHKIN<sup>1</sup>

**Abstract.** IBR-2 reactor operated by Frank Laboratory of Neutron Physics is the main basic facility at JINR dedicated to condensed matter research. The IBR-2 is a fast pulsed reactor. Its main distinctive property, which makes it differ from other nuclear reactors, is the mechanical modulation of the reactivity by means of a movable reflector. IBR-2 is the most intense pulsed neutron source in the world (IAEA-TECDOC-1439, February 2005). Producing a record neutron flux of 1016 n/cm<sup>2</sup> /s in the pulse, the IBR-2 reactor is also an economical and relatively inexpensive facility. The IBR-2 reactor is mainly used for investigations in the fields of condensed matter physics (solids and liquids), biology, chemistry, Earth and materials science. Some recent highlights from IBR-2 research will be presented.

In 2008 the Laboratory put into operation the IREN facility – power electron linac which is used to produce very short neutron pulses from heavy metal target. This facility is already in use for some applied research and education and is planned to be upgraded for basic research in nuclear physics in near future. Some results from this facility will be presented with an emphasis on common research with Mongolia.

Laboratory has a long and fruitful collaboration with Russian Space Research Institute. Common experiments aimed for searching water on Mars, Moon have been realized and results will be reported.

Last, but not least, information on the applied research activities in the fields of ecology, biotechnology, and engineering research will be outlined.

<sup>&</sup>lt;sup>1</sup> Frank Laborarory of Neutron Physics, Joint Institute for Nuclear Research, 141980, Dubna, Moscow Region, Russia.

# FLNP-ROMANIA HISTORY OF COLLABORATION

# OTILIA ANA CULICOV<sup>1,2</sup>

**Abstract.** The majority of Romanian scientist (7 of 12) working at JINR as representatives of different Romanian research institutes are FLNP stuff members. More than Romanian universities and research institutes are today involved in collaboration with FLNP. This fact reflects the sustained interest of Romanian research community in use of neutrons in condensed matter fundamental and applied studies, in nuclear physics and life sciences. Some aspects of FLNP-Romania history of collaboration since FLNP foundation up today are presented.

<sup>&</sup>lt;sup>1</sup> INCDIE ICPE-CA, 030138, Bucharest, Romania

<sup>&</sup>lt;sup>2</sup> Frank Laborarory of Neutron Physics, Joint Institute for Nuclear Research, 141980, Dubna, Moscow Region, Russia.

## LO

# NEUTRON SCATTERING IN ROMANIA

# MARIA BALASOIU<sup>1,2</sup>, OTILIA A. CULICOV<sup>1,3</sup>, ION IONITA<sup>4</sup>

**Abstract.** The neutron physics in Romania started in 1957 along with the construction of the VVR-S Nuclear Reactor, at the Institute of Atomic Physics (IFA), founded in 1956 from the Institute of Physics of the Romanian Academy (Bucharest, 1949). The founder and the first director of the Institute of Atomic Physics was Professor Horia Hulubei.

The Nuclear Research Reactor VVR-S located in Magurele-Bucharest, was designed for research and radioisotope production. It was commissioned in 1957 and operated without any event or accident for forty years until the shut down in 1997. In 2002, by the Romanian government decision, it was permanently shutdown for decommissioning.

The physics of neutrons was at that time one of the newest research directions just after the Second World War. The founder of the Romanian neutron scattering school is Professor Dorel Bally.

He was involved in the development of new nondestructive control methods in Romania. He set up and led for many years the Laboratory of Physics of Low Energy Neutrons at IFA Bucharest. He obtained important results concerning the influence of the local order on the X-ray spectra, confirmed later by the results of EXAFS method, and on the critical neutron scattering on the ferromagnets. His data relevant to the penetration depth of the neutrons, in the total reflection, appeared in the International Table of the Brookhaven National Laboratory.

Some of the more representative results obtained by Romanian physicists along the time in the field of neutron scattering and applied neutron physics are:

> Development of high performance instruments by using focusing effects;

<sup>&</sup>lt;sup>1</sup> Joint Institute for Nuclear Research, 141980, Dubna, Moscow Region, Russia.

<sup>&</sup>lt;sup>2</sup> Horia Hulubei National Institute of Physics and Nuclear Engineering, 077125, Magurele, Romania.

<sup>&</sup>lt;sup>3</sup> INCDIE ICPE-CA, 030138, Bucharest, Romania.

<sup>&</sup>lt;sup>4</sup> Institute for Nuclear Research, 115400, Mioveni, Romania.

- Critical magnetic scattering;
- Advancements in the theory of neutron diffraction;
- > Dynamics of gases adsorbed on activated charcoal;
- > Dynamics of simple and molecular liquids by neutron scattering;
- Small angle neutron scattering studies of magnetic fluids;

 $\succ$  Phase transition in hydrogen bonded molecular crystals by quasielastic neutron scattering;

Neutron activation analysis.

# L1

## THE IBR-2 REACTOR: HISTORY AND STATUS

## ALEXANDR V. VINOGRADOV<sup>1</sup>

**Abstract.** The IBR-2 fast pulsed reactor had been operated more than 22 years with no accidents. These years of regular, continuous operation of the IBR-2 have demonstrated its high reliability in operation. After this period of successful work the reactor its rated resource has been exhausted by 2007. In this connection the reactor modernization program has elaborated for the period up to 2010.

The concept of the IBR-2 reactor modernization involved carrying out work including development, manufacturing and installation of the main reactor equipment. At the same time, accounting for the experience of reactor operation and physical research, the given concept contained a number of novel technical solutions that substantially improve operation and physical reactor characteristics, which permits one to assert that actually in the process of modernization a new IBR-2M reactor is being created.

In the end of 2010 all work planned in a frame of the modernization was done and start-up of the reactor in accordance with the elaborated programs has been begun. Main directions of the paper: general description, main characteristics of the IBR-2 before modernization; main works of the modernization program; programs of the physical start-up and first power of the reactor; parameters of the reactor after modernization; utilization plan of the reactor.

<sup>&</sup>lt;sup>1</sup> Frank Laborarory of Neutron Physics, Joint Institute for Nuclear Research, 141980, Dubna, Moscow Region, Russia.

# NANOCARBONS – PROPERTIES AND APPLICATIONS

## IULIAN IORDACHE<sup>1</sup>, <u>WILHELM KAPPEL<sup>1</sup></u>

Abstract. Elemental carbon in the  $sp^2$  hybridization can form a variety of amazing structures. Apart from the well-known graphite, carbon can build closed and open cages with honeycomb atomic arrangement. Carbon nanoparticles occur in five different basic forms: diamond, graphite, fullerenes, nanotubes and nanocones. In addition to these basic forms, nanocarbon also occurs in less geometrically perfect forms such as amorphous nanoparticles, nanohorns and helical structured particles. In this lecture, will be discussed the structure, properties, and potential applications of most of these novel carbons. It is also interesting to examine how the various forms of nanocarbons are related to one another, and the conditions under which one form transforms to another. From the vast amount of research that has been carried out over the last decade, it is apparent that some of these nanocarbons would have extremely unique properties that might be of value for specific applications that are being contemplated by various researchers. As an example, progress in the synthesis, processing and integration of ultra-thin conducting carbon films, graphene and nanotubes for applications such as interconnects, transistors, spintronics and sensing is just only a direction that deserves to be mentioned. One of the important challenges of research on nanocarbons is the development of advanced technologies that allow the construction of complex devices based on such structures. On the aother hand, the real breakthrough for this technology would be new processing methods to produce such novel structures in commercial quantities.

L2

<sup>&</sup>lt;sup>1</sup> INCDIE ICPE-CA, 030138, Bucharest, Romania.

# L3 NAA FOR LIFE SCIENCES AND MATERIAL SCIENCE AT FLNP JINR

## MARINA V. FRONTASYEVA<sup>1</sup>

**Abstract.** Among the broad spectrum of the constituent trends of the Life Sciences at JINR such as nuclear medicine and pharmacy, radiation biology, radioecology, radioisotope production - radioanalytical investigations play a special role due to the long-term experience in multielement instrumental neutron activation analysis (INAA) at the reactor IBR-2 of FLNP, JINR.

Principles of INAA are briefly described for better understanding if its role and place in the Life Sciences and Material Science. INAA is presently being used in several projects on air pollution studies using biomonitors (moss, lichens, tree bark). The results for some selected areas of Central Russia, South Urals, Kola Peninsula and countries of Eastern and Southern Europe (Bulgaria, Bosnia, Croatia, Macedonia, Poland, Romania, Serbia, Slovakia, Thrace Region (the European Part of Turkey), Western Ukraine are reported to the European Atlas of Heavy Metal Atmospheric Deposition edited every 5 years under the auspices of the UNECE (United Nations Economic Commission for Europe). Similar studies have been carried out in Asia: Vietnam, Mongolia, and China. Applied to the analysis of air filters, INAA is successfully used in assessing quality of London underground air, Sahara desert impact on the Greater Cairo Area, etc.

The analytical possibilities of NAA are favorably used in biotechnologies, (i) for investigation of bacterial leaching of metals, including uranium and thorium, out of low-grade ores, rocks and industrial wastes; (ii) in the development of new pharmaceuticals based on blue-green algae Spirulina platensis. INAA is used to trace technological process of microbial synthesis of silver and gold nanopartiocles. Occupational health studies are carried out at several fertilizer plants in Russia, Uzbekistan, Poland, Romania, Denmark and the Netherlands in the framework of the 5<sup>th</sup> Programme COPERNICUS. The quality of foodstuffs grown in some

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contaminated areas of Russia is investigated in the framework of IAEA Coordinated Research Programme. In Material Sciences high-purity Al, Ge, Si, Cu and synthesis of artificial diamonds and boron nitride are being studied.

Possibilities of scientific collaboration and present studies with the Romanian scientists reviewed.

# L4 INSTRUMENTAL NEUTRON ACTIVATION ANALYSIS APPLICATIONS TO ENVIRONMENTAL AND GEOLOGICAL STUDIES – A JOINT ROMANIAN - RUSSIAN PROJECT

## OCTAVIAN G. DULIU<sup>1</sup>

Instrumental Neutron Activation Analysis (INAA), in spite of newly developed mass spectrometric methods, represents one of the most sensitive and accurate multi-elemental analytical technique with multiple applications in environmental as well as earth sciences.

By taking into account its multiple variants, INAA could be used to detect up to 74 different elements with a minimum detection limit varying between 0.1 to 103 g/kg, without any preliminary preparation such as acid digestion orµ column separation. The only limitation regards the use of intense neutron sources such as nuclear reactors or spallation generators, able to deliver neutron at fluency debts over 1012 neutrons/cm2s. Although the number of such generators is limited, the IBR-2 pulsed reactor of the I.M. Frank Neutron Physics Laboratory of the Joint Institute of Nuclear Research (JINR) at Dubna (Russian Federation) showed to be one of the best of its kind, perfectly suitable for INAA.

For these reasons, within more cooperation programs between the University of Bucharest and the JINR-Dubna, in the past five years it was possible to investigate by INAA a significant number of samples belonging to different geological formations such as igneous and metamorphic rocks from Romanian Carpathian and Macin Mountains, euxinic sediments from Black Sea, recent sediments from proglacial Balea and Volcanic St. Ana Lakes, both located in Carpatian Mountains, ancient sediments and halite from Slanic-Prahova salt mine, manganese nodules and abyssal clay from Clarion-Clipperton North Pacific abyssal plain.

By using some univariate and multivariate statistical methods of analysis such as time series analysis, cluster as well as principal component

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analysis, it was possible to evidence a multitude of apparently hidden properties of investigated media.

This fruitful cooperation was materialized by six papers published in well known ISI journals, two Ph.D. theses and more communications to renowned international conferences as well as wining the third prize of the 2010 JINR contest.

Without the essential contribution of devoted researchers such as Carman Cristache, Otilia Culicov, Marina Frontasyeva, Serghei Lyapunov, Gheorghe Oaie, Calin Ricman and Stefan Szobotka, the remarkable results obtained during these programs would not be achieved.

## L5 (n, p) AND (n, α) REACTIONS INDUCED BY RESONANCE AND FAST NEUTRONS

## YU M. GLEDENOV<sup>1</sup>

Abstract. A survey of recent experimental results on resonance and fast neutron induced (n, p) and (n,  $\alpha$ ) reactions is presented. The experimental data (cross sections, energy spectra, angular distributions, proton and alpha widths) are important to both nuclear reactor technology and basic physics. For example, the study (n, p) and (n, $\alpha$ ) cross sections is necessary to estimate radiation damage due to hydrogen and helium production, nuclear heating and transmutations in the materials of fission and fusion reactors, some of these cross sections are crucial for a better understanding of many scenarios of nucleosynthesis. They have also been used to study several topics in nuclear structure, fundamental symmetries and mechanism of the interaction of neutron with nuclear.

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# MAGNETORESISTIVE MANGANESE BASED PEROVSKITES

## EMIL BURZO<sup>1</sup>

Abstract. The La<sub>1-x</sub>Pb<sub>x</sub>MnO<sub>3</sub> perovskites, with  $0.24 \le x \le 0.40$ , were obtained by solid state reaction. These crystallize in rhombohedral structure having **K3c** space group. The magnetizations, at 4.2 K, increase from 3.15 µB/f.u. (x=0.24) up to 3.60 µB/f.u. (x=0.40), as the lead content is higher. The contributions of superexchange and double exchange mechanisms to exchange interactions were evaluated. The Curie temperatures vary from 285 K (x=0.24) to 384 K (x=0.4). A new type of transition has been seen around 42 K. The frequency dependence of the transition temperatures reveals an uncommon spin glass type behaviour. The type of transition changes as the Pb content increases. The observed behaviour was attributed to lone pair effects. The temperature and field dependences of the magnetoresistivities (MR) were studied. The MR values up to 50 % were obtained.

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## RADIATIVE CAPTURE OF NEUTRONS: L7 FUNDAMENTAL INVESTIGATIONS AND APPLICATIONS

## SERGEY B. BORZAKOV<sup>1</sup>

**Abstract.** The investigations of the neutron radiative capture by light and heavy nuclei are observed. The parity nonconserving effects are described. The perspectives to study the P-even and time nonconserving effects on the IREN facility are discussed. The possibility to use neutron resonance reactions for determination of the element content in the samples are described also.

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# ANALYTICAL APPLICATIONS OF THERMAL AND 14 MEV NEUTRON ACTIVATION ANALYSIS IN METALLURGICAL INDUSTRY

## ANTOANETA ENE<sup>1</sup>

Due to the increased demand for ultrapure metals and alloys and requirements for knowledge of toxic emissions, along with the increasing use of new sources of raw materials (new deposits, industrial by-products, wastes), it is necessary to carefully analyze the distribution of impurity elements between the main products and by-products of metallurgical processes. Special attention should be given to the elements that are harmful both to metallurgical products and to the environment. Trace and minor elements existing in the raw materials (ores, coal and secondary resources) can remain in the final products as residual elements and influence their properties, so that their transfer during metallurgical operations must be thoroughly investigated.

The work presents some applications in ferrous metallurgical industry of instrumental neutron activation analysis (INAA), using thermal and fast (14.7 MeV) neutrons.

Thermal neutron INAA was applied at VVR-S nuclear reactor from IFIN-HH Bucharest-Magurele to investigate the compositional scheme of raw materials and final products involved in metallurgical industry at Iron and Steel Works at Galati (Romania) and the transfer of minor and trace elements: a) from the converter charge to the metallic bath during the two stages of the steelmaking process in LD converter - refining and deoxidation - and b) from the blast-furnace charge to pig iron and slag during ironmaking process.

A study of the capabilities of 14 MeV INAA for alkali determination in ores used in iron and steel industry with respect to the interferences of all useful nuclear reactions has been accomplished. The reaction interferences hold an important role in alkali analysis. A calculus relation is presented for

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the first order interferences which appear in alkali determination from raw materials using the pertinent nuclear reactions of 14 MeV neutrons on Na and K. The ore samples were irradiated with the aid of the neutron generator facility from Activation Laboratory, Nuclear Unit, Iron and Steel Works of Galati. Also, 14 MeV INAA was applied for the determination of gold in alluvial deposits and auriferous rocks in Romania, being a rapid and sufficiently sensitive method for the determination of gold traces (the minimum concentration of gold required for an economic extraction is 20 ppm). There have been studied the spectral interferences which appear in the determination of gold in alluvial sands and auriferous rocks and alkali in iron ores, due to the other elements present in the samples, with the aid of the original field spectrum of gamma-rays emitted by the irradiated sample in the absence of any ambient interaction, considered as a radiation field produced in vacuum by a point source, which maintains the energetic and angular characteristics of the disintegrations taking place in the source. This spectrum depends on the resulted radionuclides from the nuclear reactions between the fast neutrons and the existing elements in the sample, their concentrations and the experimental times (activation, cooling and measuring).

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#### CRYOGENIC MODERATORS FOR NEUTRON SOURCES

#### SERGEY KULIKOV<sup>1</sup>

**Abstract.** Nowadays neutron scientists in many research centers are trying to increase neutron performance of instruments by optimizing source environment. This way is much cheaper than increasing current of accelerators for spallation sources or reactors power and can significantly improve neutron flux at a sample. One of elements of source environment is a neutron moderator. Cold neutron moderators are complicated devices and their development is still in evolution.

The review of the work will be dedicated to the problems which are exists with cold neutron moderators in general. One of the main problems is a choice of moderating material. It has to satisfy to different demands such as:

- to have a good moderation properties;

- to be safe and easy in operation;
- to have a good resistance to radiation etc.;

An attempt to summaries some results received in the field of development of cold moderators for neutron sources and a project of elaboration of a complex of cold neutron moderators at the IBR-2M research reactor are to be presented.

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# NEUTRON ACTIVATION ANALYSISL10ON REFERENCE MATERIALS FROM<br/>INTERCOMPARISON RUNS(ENVIRONMENTAL AND BIOLOGICAL SAMPLES)

#### ANA PANTELICA<sup>1</sup>

Abstract. An overview of using the Instrumental Neutron Activation Analysis (INAA) technique in our laboratory to determine major, minor and trace elements in mineral and biological samples from international intercomparison runs organised by IAEA Vienna, IAEA-MEL Monaco, pbanal Košice, INCT Warszawa and IPNT Kraków is presented. Neutron irradiation was carried out at VVR-S reactor in Bucharest (short and longterm irradiation) during 1980-1997 and at TRIGA reactor in Pitești (long irradiation) during the later period. The following type of materials were analysed: soil, marine sediment, uranium phosphate ore, water sludge, copper smelting flue dust, and fly coal ash, yeast, milk, whey, cereal flour (rye, wheat, and corn), soya bean flour, marine animal tissue (mussel, garfish and tuna fish), as well as vegetal tissue (seaweed, cabbage, spinach, alfalfa, algae, tea leaves, herbs, and tobacco leaves). The following elements were investigated: Ag, As, Au, Ba, Br, Ca, Cd, Ce, Co, Cr, Cs, Eu, Fe, Hf, Hg, K, La, Lu, Mo, Na, Nd, Ni, Rb, Sb, Sc, Se, Sm, Sn, Sr, Ta, Tb, Th, U, W, Yb and Zn of long-lived radionuclides, as well as Al, Ca, Cl, Cu, Dy, Mg, Mn, Ti, and V of short-lived radionuclides (45 elements). Our laboratory data for various matrix samples are presented over against the intercomparison certified values. The intercomparison exercises offer to the participating laboratories the opportunity to test the accuracy of their analytical methods as well as to acquire valuable Reference Materials/ standards for future analytical applications.

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L11 SYNCHROTRONS VERSUS NEUTRONS. COMPETITIVE OR COMPLIMENTARY?

#### ALEXANDER V. BELUSHKIN<sup>1</sup>

Abstract. In present days both synchrotron radiation and neutron scattering are used for the study of different aspects of condensed matter properties. Synchrotron radiation interacts with electron shell of the atoms. Neutrons scattered by atomic nucleus and, due to the large magnetic moment, can "feel" magnetic properties of matter. These differences allow both methods to address some specific fields of research where they do not compete to each other. However, in many important areas both methods are applicable and question is raised whether it is necessary to avoid duplication and to concentrate efforts on development just one method and to sacrifice the other. If one compares the properties of synchrotron sources and neutron facilities, the first win in all categories. Nothing negative can be said about the X-rav synchrotron sources. They are simply wonderful! They are continuously getting smaller and brighter. They are partially coherent. One can vary the size of the beam without intensity loss and, whenever necessary, reduce beam coherence. Compared to synchrotrons neutron sources are "lousy", they are large and not highly directional. A different type of interaction with matter makes some advantages for one or another method. But relative advantages appear to be not of crucial importance:

- *Radiation damage*. Neutrons do not hurt. Neutrons allow studying biological objects in vivo. X-rays are bad for all soft matter systems – care must be taken to avoid sample damage: changing beam position on the sample (possible due to the small beam size), keep the sample "frozen" (bio-samples), checking the sample quality before and after the experiment. These are serious complications but they do not prevent scientists from obtaining high quality and useful data;

- Absorption. High energy X-rays alleviate absorption problems and allow to study not only surface but bulk properties. However, due to the heat

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load deposited in the sample by X-rays, it is impossible to perform experiments at very low temperatures (below ca. 1K);

- *Brightness*. Contrary to SR, single nanoparticle object can not be studied with neutrons, only big assemblies of nano's can be probed.

If one takes into account that today synchrotron radiation allows performing measurements in many fields traditionally investigated by neutron scattering methods, then at first glance it looks like neutrons cannot survive the competition. Present report analyses differences for both methods when they applied to the same scientific problems. It is shown that deeper analysis of differences dependent on particular experimental methods used for the study of the same scientific problems makes both methods complimentary and that they never will be able to replace each other, but rather need to be used in synergy to obtain most comprehensive picture of the scientific problem under study.

#### CURRENT STATUS AND FUTURE NEEDS OF NUCLEAR ANALYTICAL TECHNIQUES AND THEIR APPLICATIONS

#### MARINA V. FRONTASYEVA<sup>1</sup>

Abstract. According to the IAEA classification, we define nuclear analytical techniques (NATs) as those that use nuclear reactions, radioactive decay, or nuclear instrumentation to investigate properties of matter. This definition extends from the well-established radiochemistry, neutron activation analysis (NAA), and prompt-gamma activation analysis (PGAA) to advanced methods at the limits of science and technology, and includes the applications of these techniques to the determination of composition and structure of matter for science and technology. The broad range of nuclear analytical techniques share a set of advantages over competing methods: (i) highly penetrating probe and response radiation; (ii) independence of chemical state and of analytical blank; (iii) nondestructive character, and (iv) sensitivity. NAA in particular is in regular use worldwide to perform elemental analysis of as many as forty elements in a variety of materials important to industrial process development and control, human health, environmental protection, and cultural heritage. Although NAA is a mature and since 2007 is a primary analytical technique, several developing extensions to the method promise greater applicability to the analysis of large ultrapure solids and extremely heterogeneous samples. There is an urgent demand for the determination of ultra-fine (nano) particles in the environmental studies and an understanding of their health impact.

New developments in analytical techniques and applications: Over 200 small and medium charged-particle accelerators are in use in many countries for PIXE and other ion beam analysis techniques.

Their applications in materials and life sciences are expanding, especially with microbeam facilities which allow imaging in two or three dimensions (more than 40 operational  $\mu$ -beam facilities available at this moment). Charged-particle activation analysis (with or without

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radiochemistry) can be a complementary technique to NAA for the determination of particular elements in different matrices (biological, environmental, and certain technologically advanced materials). In the version of TLA (thin layer activation) this technique is effective for wear and corrosion studies on moving mechanical equipments for industrial applications and the assessment of the performances with time of human prostheses as well. There is a remarkable growth in the number and availability of particle accelerators related to the rapid expansion of diagnostic and therapeutic nuclear medicine procedures, notably positron emission tomography (PET), single-photon emission tomography (SPET), (including hybrid systems with CT or MRI), functional diagnosis, molecular imaging, and metabolic radionuclide therapy. Analytical techniques based on synchrotron radiation are emerging which can provide qualitative and quantitative information on in-vivo elemental composition, structure, and molecular imaging. As many as ten of the new large facilities are dedicated to the biomedical sciences.

The role of trace elements in health and environmental studies: NATs are playing a significant role in understanding the mechanism of cancer, cardiovascular disease, and diabetes, as well as of brain-gut interactions related to satiety and obesity. Artificially produced radioactive tracers, characterized by short half-life and high specific activity, are finding several applications in the life sciences, in particular in occupational and environmental toxicology, in metallobiochemistry and nanotoxicology as well as in living organisms (cell cultures, plants, animals, and fishes).

#### L13 INVESTIGATIONS OF FERROFLUIDS AND MAGNETIC ELASTOMERS BY MEANS OF SMALL ANGLE NEUTRON SCATTERING METHOD

#### MARIA BALASOIU<sup>1,2</sup>, ALEXANDER I. KUKLIN<sup>1</sup>

**Abstract.** For 20 years, at the Frank Laboratory of Neutron Physics in cooperation with the National Institute of Materials Physics (Bucharest), Institute of Space Sciences (Bucharest), Laboratory of Magnetic Fluids, CFATR of Romanian Academy (Timisoara Division), National Institute for Research and Development of Isotopic and Molecular Technologies (Cluj-Napoca), West University of Timisoara, Department of Electricity and Magnetism, Horia Hulubei Institute of Physics and Nuclear Engineering (Bucharest), investigations of ferrofluids and magnetic elastomers by means of small angle neutron scattering methods are running.

Neutron scattering in the study of magnetic materials presents a number of advantages arising from the peculiarities of the interaction of neutrons with matter.

The presence of the neutron magnetic moment leads to the fact that along with the scattering of neutrons on atomic nuclei (nuclear scattering) the so-called magnetic scattering occurs due to the interaction of the neutron magnetic moment with the magnetic moments of electronic shells of atoms.

Among the main results obtained on the base of the experimental data measured at YuMO-SANS instrument at the beginning of 90's in investigation of ferrofluids must be mentioned the following:

(i) the use of contrast variation technique for obtaining a new method for the separate determination of the nuclear and magnetic contributions of the small angle scattering of nonpolarized neutrons;

(ii) the obtaining of both physical and magnetic radii of the nanoparticle with the same experimental method, without applying a perturbative external magnetic field;

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(iii) the demonstration with a direct method that the two radii are not equal, the magnetic radius beeing smoller than the physical one.

Combination of magnetic and elastic properties of magnetic elastomers leads to diverse phenomena exhibited in magnetic fields and opens new possibilities for technological applications. Various structures could be formed inside the material or the already existing structures would be changed due to the application of a magnetic field. A new rubber material containing anisotropically magnetized nanoclusters with the use of ferrofluids is proposed. By means of small angle neutron scattering specific variations of the structure factor and interparticle correlation length with the particle concentration and the magnetic field imposed during polymerization are found and modeled.

## HIGH RESOLUTION NEUTRONL14DIFFRACTOMETER IN DUBNA.EXAMPLES OF APPLICATIONS

#### IVAN A. BOBRIKOV<sup>1</sup>, ANATOLY M. BALAGUROV<sup>1</sup>, VALERIY G. SIMKIN<sup>1</sup>

**Abstract.** High Resolution Fourier Diffractometer (HRFD) is a neutron reverse time-of-flight Fourier diffractometer intended for precise structural studies of powders, investigation of phase transitions in powders and single crystals and residual stress investigations in bulk samples and advanced materials at a resolution level of about 0.001 or even better. HRFD, the first neutron Fourier diffractometer at a pulsed neutron source, combines a high neutron flux at sample position,  $\sim 8*10^6$  n cm<sup>-2</sup> s<sup>-1</sup>, provided by the IBR-2 high flux pulsed reactor, and a high resolution over a wide range of d-spacings. The presentation deals with description of HRFD and examples of structural experiments.

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#### L15 USING Q-SPACE FOCUSING IN THERMAL NEUTRONS SPECTROMETRY TO GET IMPROVED RESOLUTION PERFORMANCES

#### ION IONITA<sup>1</sup>

Abstract. In neutron spectrometry the optimal use of the available neutrons is of the greatest importance. The general philosophy to do it is to maximize the neutron flux at sample by using neutron guides, supermirrors, or spatial focusing effects involving flexible configurations and curved crystals. A different approach, is to obtain the required optimum experimental conditions not by getting focused beams at sample or anywhere else, but only by decreasing as much as possible the scan variable variances. A Q-space focusing configuration is characterized by highresolution even when no spatial focusing exist at sample position or anywhere else or is used quite open beam without any Soller collimators; only coarse collimators should be used to reduce the background level. This is possible just by decreasing the scan variable variances. The following steps should be followed; - to define the scan variable - to define the significant spatial variables as are the monochromator and sample width for example - to express the scan variable, using specific geometry characteristics and the existing correlation between variables, through the spatial variables - to cancel the significant contributions to the scans variable variances by canceling the important variables coefficients, from the scan variable expression; when correlation between variable exists, as is the case for these kind of experimental configurations, such a coefficient has more then one term, not all of the same sign, appearing the possibility to be cancelled and therefore to cancel entirely the corresponding contribution of this spatial variable to the line-width.

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#### DATA ACQUISITION AND CONTROL SYSTEMS FOR THE IBR-2 SPECTROMETERS COMPLEX

#### ELENA I. LITVINENKO<sup>1</sup>

Abstract. Development of data acquisition systems, computing and information infrastructure is a key to a successful program of research of condensed matter at the IBR-2. Improvement of measurement techniques, the growing number of managed and controlled parameters, increasing the number and complexity of the detectors used in the experiment, increasing demands on accuracy and speed of the data acquisition equipment, the need for a remote (from anywhere in the local area network) management of the spectrometer and the experiment subsystems have put forward new requirements to the automation system experiments, which can not be satisfied in full without the modernization of the existing hardware and software environment, computing and information infrastructure. Selected technical solutions must take into account the development trends of microelectronics and computer technology, i.e. it should be a system "of tomorrow".

FLNP has the long-term program to develop new generation of the data acquisition systems for IBR-2 spectrometer complex. The goal of the program – to create such electronics and software for data acquisition, data accumulation and data treatment that would be adequate to the word level of the FLNP spectrometers. Such a goal can be reached only with the modern technical tools, software and information technologies, as well as the unified approach to the system design.

User mode spectrometer of IBR-2 puts additional demands on the systems of data acquisition: the simplicity of development and user-friendly graphical interface, access to measurement results on the Internet, etc.

The main problems in creating new data acquisition systems for neutron spectrometers are reliability, cost, development time, and

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commissioning, as well as the ability to quickly adapt systems to changing requirements of the experiment.

Adaptability is essential, because provides the necessary flexibility to meet the requirements (sometimes unknown) future experiments.

The modernization project for the control systems of the IBR-2 spectrometers includes projects of the unified control system of stepper motors, actuating mechanisms, the sample-changing systems, motor-based beam choppers.

New developments of the software for the experiment control on the IBR-2 spectrometers are concentrated on the software package Sonix+. It the long-term project, which includes interfaces to the detectors, motors (goniometers, slits, platforms, collimators), temperatures controllers (refrigerators, stoves), etc. and is used already on several neutron instruments at the FLNP JINR (http://sonix.jinr.ru/). The software for data acquisition from the modern position-sensitive detectors with delay line readout includes the software interface to the DeLiDAQ-1 PCI board (http://wwwinfo.jinr.ru/~elitvin/DeLiDAQ/) and will include in the nearest future the software interface to the next generation of the DeLiDAQ electronics with USB interface.

#### ON THE BEHAVIOUR OF THE ORGANIC POLYMER MATERIALS IN NUCLEAR RADIATION FIELDS

#### RADU SETNESCU<sup>1,2</sup>

**Abstract.** The main topics are: interaction of ionizing radiation with the matter - physical and chemical effects, radiation degradation and stabilisation of polymers, applications of radiation technologies in materials synthesis and transformation, lifetime of organic materials in radiation fields - durability evaluation. A review of the literature data concerning each topic is presented. Examples of original data illustrating the experience in the field of the scientists of Valahia University, National Research and Development Institute for Electrical Engineering (ICPE-CA) Bucharest and University of Bucharest are also included.

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#### RADIATION INDUCED CHEMICAL EFFECTS ON SOME PERFLUOROCARBON FLUIDS

#### SORIN ILIE<sup>1</sup>, <u>RADU SETNESCU</u><sup>2,3</sup>

**Abstract.** Perfluorocarbon fluids - mainly  $C_6F_{14}$  and  $C_3F_8$  – used as coolants within High Energy Physics Detectors in the Large Hadrons Collider (LHC) at CERN, irradiated in different conditions, were characterized using FT-IR spectroscopy, GC and specific surface analysis methods. The identification of the impurities and establishing their role in radiation hardness of the coolant fluids are described. Thus, the presence of different H containing molecules and oxygen strongly influenced the radiation behavior of the fluids, such as the radiation-induced hydrofluoric acid yield, low molecular weight products and polymers resulting upon the irradiation process. The applicability of different purification procedures is also discussed.

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#### RADIATION MODIFICATIONS INDUCED IN POLYMERS. SYNTHETIC POLYMERS

#### TRAIAN ZAHARESCU<sup>1</sup>

Abstract. The radiation processing of polymers receives a large attention because of the modification induced by high energy exposure may be controlled and frozen on a certain level. The structural changes found by sensitive investigation procedures are the background for further applications. The radiolysis mechanisms that explain the routes of reactions will be presented in relation with the molecular configurations of irradiated substrates. The general overview on the intimate processes correlated with the resulting physical and chemical properties of irradiated polymers is discussed.

A special attention in this presentation will be paid to ethylenepropylene elastomers, whose large application areas ask it. The correspondences between irradiation doses and resulting mechanical, physical and chemical characteristics will be commented starting from the original experiments carried out in our laboratory. The radiation resistance of polymer matrix will be presented after the highlighting effects of chemical parameters (level of oxidation, type of antioxidant, irradiation environment, formulation).

The similitude between different polyolefins subjected to the action of  $\gamma$ -rays will be analyzed.

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#### **EXPERIMENTAL INVESTIGATION OF** SPATIAL PARITY VIOLATION EFFECTS IN INTERACTION OF THE POLARIZED NEUTRONS WITH LIGHT NUCLEI WITH THE PURPOSE OF DETERMINATION OF WEAK MESON-NUCLEON COUPLING CONSTANTS

#### V. A. VESNA<sup>1</sup>, YU. M. GLEDENOV<sup>2</sup>, V. V. NESVIZHEVSKY<sup>3</sup>, A. K. PETOUKHOV<sup>3</sup>, <u>PAVEL V. SEDYSHEV<sup>2</sup></u>, T. SOLDNER<sup>3</sup>, E. V. SHULGINA<sup>1</sup>, O. ZIMMER<sup>3</sup>

Abstract. Two experiments on the measurement of the parity violation effects are presented: measurement of an asymmetry of triton emission At with respect to neutron spin in the  $6\text{Li}(n,\alpha)3\text{H}$  reaction with cold polarized neutrons and measurement of an asymmetry of  $\gamma$ -quanta emission A $\gamma$  with respect to neutron spin for the transition  $7\text{Li}^* \rightarrow 7\text{Li} + \gamma(\text{M1})$ ,  $E\gamma = 0.478$  MeV following the reaction  $10\text{B}(n,\alpha)7\text{Li}$  induced by cold polarized neutrons. The aim of works is determination of the weak  $\pi$ -meson exchange constant  $f\pi$ , associating with neutral currents in electroweak nucleon-nucleon interactions. Parity violation in NN interactions has been observed in various processes involving few-nucleon systems and more complex nuclei. While the observation of parity violation in proton-proton scattering is a manifestation of charged weak currents in accordance with theory, no observation has yet been claimed for neutral weak current contributions in NN-interaction in nuclei.

To perform a statistically significant measurement of these asymmetries, the sensitivity needed is close to 10-8. Experiments were carried out at the high-intensity neutron reactors: the WWR-M reactor in the Petersburg Nuclear Physics Institute (Gatchina, Russia) and at the reactor of the Institut Laue-Langevin (Grenoble, France). The total flux of polarized

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neutrons was equal  $(3 - 5) \cdot 10^{10}$  s<sup>-1</sup>. The incident neutrons were mainly absorbed in samples providing count rate of ~10<sup>10</sup> s<sup>-1</sup>.

The experimental technique for the measurement of very low P-odd effects is described: detectors and electronics for the event registration in current mode, the special data acquisition procedure and method for compensation in the reactor power fluctuations and elimination of the possible fake effects, special test experiments.

The obtained asymmetry values are At =  $(-8.8 \pm 2.1) \cdot 10^{-8}$  and A $\gamma = (0.0 \pm 2.6) \cdot 10^{-8}$ . The constraints for the coupling constant  $f\pi$  derived from these result are analyzed.

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#### HOW TO COLLABORATE WITH FLNP – TECHNICAL ASPECTS

#### OTILIA ANA CULICOV<sup>1,2</sup>

**Abstract.** The Joint Institute for Nuclear Research (JINR) is a world-known centre where the fundamental research is successfully integrated with development of new technologies, application of the latest techniques, and university education.

The Frank Laboratory of Neutron Physics (FLNP) is one of the seven JINR Laboratories. The scientific activity of the Laboratory focuses on two fields of science, namely nuclear physics and condensed matter research with neutrons.

The greater part of all investigations is carried out in close collaboration with the JINR member states, as well as with international associates. FLNP is proud to have active cooperation agreements with almost 200 scientific institutes and universities of 40 countries from all over the globe and apply efforts in order to offer larger access to FLNP facilities (IBR-2 reactor and IREN) for the specialists from JINR member states.

Collaboration between scientists from JINR member states with FLNP research groups has multiple mechanisms. Their technical aspects, including the FLNP user policy, JINR social and cultural facilities and some features specific to Romanian – JINR collaboration are presented.

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#### PFN DATA ANALYSIS IN SPONTANEOUS FISSION

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Abstract. The main motivation of the present work was investigation of the nature of anomalous (from the point of view of modern theory) dependence of the average PFN number on the total kinetic (TKE) energy of the fission fragments (FF) using modern digital signal processing (DSP) approach. A twin Frisch-grid ionization chamber (TGIC) was used for FF mass and kinetic energy spectroscopy. A fast neutron detector (ND) with NE213 (or analog) scintillation liquid was used for PFN time-of-flight measurement. Correlated FF kinetic energies, their masses, an angle between fission axis and the PFN, the PFN velocity all were measured with help of eight channel setup of synchronized waveform digitizers (WFD), having 100 MHz sampling frequency and 12 bit pulse height resolution. Special modifications in the data analysis procedure brought to reasonable agreement between experimental results and theoretical calculations. In the first time the linear dependence of the average number of PFN on TKE in the range of (140 - 220) MeV was demonstrated.

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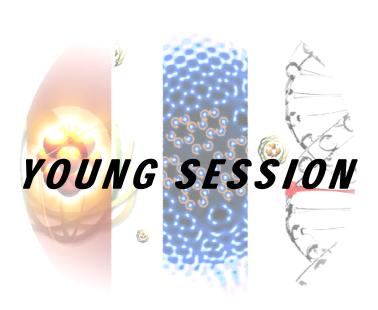
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#### 123 NEUTRON DIFFRACTION INVESTIGATIONS OF RESIDUAL STRESSES FOR THE INDUSTRY CARRIED OUT AT FLNP JINR

#### ANDREI V. TAMONOV<sup>1</sup>

Abstract. Residual stresses are stresses, which exist inside some solid body at absence of any kinds of external forces and temperature fields. As usual, these stresses arise in details due to various manufacturing processes and as consequence they exist practically in all details and constructions. Nowadays designers and engineers can analyse a construction for durability, but they can't take into account that technological processes of manufacturing have created rather great residual stresses in a detail. Therefore, it is absolutely necessarily to posses methods which would allow to measure residual stresses in details after all technological processes of manufacturing. One of such methods is the high-resolution neutron diffraction.

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#### P01 MODELING OF SMALL-ANGLE NEUTRON SCATTERING CURVES FROM MAGNETIC FLUIDS TAKING INTO ACCOUNT PARTICLE ANISOTROPY

#### <u>ANATOLII V. NAGORNYI</u><sup>1,2</sup>, M. V. AVDEEV<sup>1</sup>, V. I. PETRENKO<sup>1,2</sup>, V. L. AKSENOV<sup>1,3</sup>, L. A. BULAVIN<sup>2</sup>

**Abstract.** Ferrofluids (magnetic fluids) are liquid dispersions of magnetic nanoparticles covered with surfactants for preventing their coagulation in different conditions. Structure investigations of ferrofluids are of great interest from both the fundamental and application viewpoints.

Synthesis of magnetic liquid is a complex process that requires high quality of the resulting sample. That is why the relevant topic is the quality control of the obtained ferrofluid. To study the structural parameters of liquids are widely used by small-angle neutron scattering experiments. Data interpretations of such experiments are carried out using a core-shell model under the assumption that the particles have a spherical shape as usual. However, in some cases there is some inconsistency between experimental data and the model in Guinier region, which is often explained by the small aggregation. This work is an attempt to describe this discrepancy by taking into account the shape anisotropy of particles.

The possibility for modeling small-angle neutron scattering from ferrofluids taking into account the anisotropy of magnetic nanoparticles is considered. The spectra were obtained by the computer simulation of the scattering from the ferrofluids based on polydisperse magnetite particles coated with a single surfactant layer and dispersed in H-benzene or Dbenzene. From the given analysis the limits of the polydisperse core-shell model has been determined.

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#### **P02** TECHNOLOGICAL SUPPORT OF MODEL OF CRYOGENIC PELLETIZED NEUTRON MODERATOR OF IBR – 2 M REACTOR

#### MAXIM BULAVIN<sup>1</sup>, V. ANANIEV<sup>1</sup>, A. BELYAKOV<sup>1</sup>, A. BOGDZEL<sup>1</sup>, A. VERHOGLYADOV<sup>1</sup>, E. KULAGIN<sup>1</sup>, S. KULIKOV<sup>1</sup>, A. KUSTOV<sup>1</sup>, K. MUKHIN<sup>1</sup>, T. PETUKHOVA<sup>1</sup>, A. SIROTIN<sup>1</sup>, A. FEDOROV<sup>1</sup>, E. SHABALIN<sup>1</sup>, D. SHABALIN<sup>1</sup>, V. SHIROKOV<sup>1</sup>, M. SITNIK<sup>1</sup>

Abstract. Complex of cryogenic pelletized neutron moderators is a part of the plan of IBR-2M modernization. Cryogenic moderator represents a chamber filled with working material in the form of frozen balls (pellets) of mixture of aromatic hydrocarbons (mesitylene and m-xylene). Charging the chamber with pellets is doing by conveying them with flow of cold helium at temperature about 30-40K. Such moderator is a very complicated facility demanding optimization of engineering parts and verification of all system integrity on a special experimental model. The major purpose of the full-scaled model is performing experiments to recognize an optimal regime of charging a simulating chamber of the moderator by working material. Loading the chamber and serviceability of the model is provided by basic technological components and control systems: a cryostat with helium circulator (blower), temperature control system, vacuum system, metering device, the system detecting of balls, visualization of loading the chamber with pellets.

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#### **MODELING OF SANS SPECTRA FROM** FRACTAL STRUCTURES IN DETONATION NANODIAMOND DISPERSIONS

### <u>OLEKSANDR TOMCHUK</u><sup>1,2</sup>, M. V. AVDEEV<sup>1</sup>, V. L. AKSENOV<sup>1,3</sup>, L. ROSTA<sup>4</sup>, L. A. BULAVIN<sup>2</sup>

Abstract. Detonation nanodiamond (DND) is formed during an explosion of oxygen-imbalanced explosives in the absence of any extra carbon source. DND particles are ultra-fine single crystals of cubic diamond with diameters within 5-10 nm, thus offering nanosized diamond, apparently a highly attractive material in nanotechnology including biomedical applications. Small-angle neutron scattering (SANS) reveals fractal structures in two kinds (dry powders and liquid colloidal solutions) of DND dispersions. In this work we discuss several models to describe SANS curves in terms of the fractal approach basing on deterministic and stochastic growth mechanisms. The polydispersity of basic structural units is taken into account as well.

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#### P04

#### EPITHERMAL NEUTRON ACTIVATION ANALYSIS FOR BACTERIAL TRANSFORMATIONS OF CHROMIUM

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Abstract. Indigenous bacteria can be successfully used to either detoxify or immobilize toxic heavy metals. These bacteria are under continuous investigation, and in-depth molecular understanding has been developed for some of them. However, up to date the dependence between the ability of bacteria to reduce or immobilize metals and their elemental compositions is not clear yet. For the first time epithermal neutron activation analysis method (ENAA) has been applied to determine the elemental content of bacteria before (control) and after exposure to different loadings of chromate. As a model, Cr(VI)-reducer bacteria of Arthrobacter genera, isolated from polluted basalts from both the Republic of Georgia and the USA, was used. Were determined concentration of elements: Na, Al, Cl, K, Fe, Co, Zn, As, Br, Rb, Sr, Sb, Ba, Th, U. In the cells treated with Cr(VI) significant alterations in the concentrations of some elements playing essential role in the life processes of microorganisms were observed. To understand the mechanisms of microbial resistance to Cr(VI) electron spin resonance (ESR) spectrometry was used to trace the formation and behaviour of chromium species (Cr(V)/Cr(III)) in bacterial cells. The concentrations from 12 to 19 elements were determined in the bacterial cells.

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#### P05

## NEUTRON SCATTERING METHODS USED TO INVESTIGATE THE RADIOACTIVE WASTE CONFINEMENT

#### CRISTIAN A. DRAGOLICI<sup>1</sup>, F. DRAGOLICI<sup>1</sup>

Abstract. The management of the radioactive waste, as it is performed at IFIN-HH, implies the conditioning in a cement matrix as an embedding, stable, disposal material. Neutron scattering methods are a powerful and direct method for investigating the static and dynamic properties of materials manifesting disordered structure. They offer the possibility to analyze the substance without disturbing its natural environment. In the study of the cement matrix guasielastic neutron scattering and small angle neutron scattering methods were used. Hydrogen containing molecules are involved in microscopic diffusive motions that can be most effectively studied by quasielastic incoherent neutron scattering while solid and liquid systems, phase transformations, germination and grows flaws and defects and generally any inhomogeneity's occurred in a range of 10 to 1000Å are most suitable studied by small angle coherent scattering. This paper highlights the work performed in investigation by neutron scattering of the cement paste used for radioactive waste conditioning.

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#### P06

#### HEAVY METALS IN SOILS NEAR AN INDUSTRIAL PLANT IN GALATI, ROMANIA: IMPLICATIONS FOR THE POPULATION HEALTH RISK

#### ALINA (BOSNEAGA) SION<sup>1</sup>, A. ENE<sup>1</sup>, L. GEORGESCU<sup>1</sup>

Abstract. Decades of industrial activity and popularization have developed many environmental pollution problems. Due to the toxicity and the ability of heavy metals to accumulate in the biota, pollution with these elements is a serious problem. An important difference between these metals and other pollutants is the fact that these are not biodegradable. Information about the total concentration of the heavy metal alone is not sufficient to assess the environmental impact being necessary to find ways to explain the metal behavior. The current study characterizes the migration index and enrichment factor of trace metals nearby an industrial site from Galati city, Romania. The quantitative analyzes were carried out by nuclear related technique X-Ray Fluorescence (XRF) using a Niton XLT analyzer from 700 series and the following metals were chosen to be studied: As, Cr, Cu, Pb and Zn. These elements are specific pollutants for industrial sites, their concentrations exceed the legal norms in almost all the sampling points. The migration index (MI) value indicates a high or a low mobility of the element. Usually the MI depends on the pH values, the texture of the soil, the concentration of sulfur and (oxy)hidroxy Fe/Mn, the level of pollution etc. A high value of the enrichment factor (EF) indicates an anthropic origin of the metal. High values for EF where calculated for all the studied elements. These facts indicate that the pollution with As, Cr, Cu, Pb and Zn is serious and can affect the health of the population, by infiltrations in the underground waters, and by atmospheric depositions.

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#### AUTOMATIC SYSTEM FOR ANALYSIS OF METABOLIC DISEASE

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**Abstract.** Echography science plays an important role in medicine and life sciences. Echography analysis is a modern technique, effective and noninvasive, widely used in diagnosis and medical investigation. The steatosis (fatty) liver disease is an example of the investigation based on ultrasound imaging examination. Fatty liver disease is a large accumulation of the fat in liver cells. Physicians diagnose the fatty liver disease based on visual and analytical interpretation of the ultrasound imaging. In this study, we tried a classification between the two pathologies : normal liver and steatosis liver. The decision parameter is the Euler number. For the purpose of helping physicians in providing rapid and accurate diagnosis we present a software application for diagnose and investigation of steatosis diseases. Finally, a conclusion was drawn on the effectiveness of the tested method.

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#### **P08**

#### Bi-Te-Se THERMOELEMENTS STUDIES BY PIXE AND EDXRF METHODS

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**Abstract.** A good thermoelectric material should have high electrical conductivity and thermal power, and low thermal conductivity. For making the thermoelements with the appropriate characteristics is required to choose the material according on the application followed and temperature range. This requires different methods to study the structure of these materials, the amount of impurities contained in the material or alloy used. The quality and content of these materials are key factors in achieving high performance in thermoelectric conversion. This paper presents original contributions in the study of Bi-Te-Se thermoelements, using particle induced X-ray emission - PIXE and energy dispersive X-ray fluorescence – EDXRF techniques. The studied thermoelements are used in micro and optoelectronic systems, as well as in energy recovery applications.

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#### ANALYTICAL TECHNIQUE FOR AZOIC DYES CHARACTERIZATION

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**Abstract.** Quartz Crystal Microbalance (QCM) has found numerous applications in many fields including thin-film measurement, chemical analysis, gas sensor, humidity sensor and biosensor. Especially, the development of QCM for use in fluids or with visco-elastic deposits has dramatically increased the interest towards this technique.

QCM device will be used for measurements of adsorption of synthesized copolymer. The gold sensor has been recognized as excellent indicator of mass changes because of the direct relationship between mass change and resonant frequency response. New maleic anhydride (MA) copolymer with styrene (S) modified by condensative coupling reaction with azo photochrome dye (H<sub>2</sub>N-C<sub>6</sub>H<sub>4</sub>-N=N-C<sub>6</sub>H<sub>4</sub>-R, with R = -CH<sub>3</sub>; -Cl; -Br; -I) was obtained and the results concerning structures were published. The selection of the MA copolymer is justify by MA tendency for forming alternant copolymers, what permits to obtain architectures with big degree of structural regularity as well as of the anhydridic group reactivity in reaction with primary amines. During the adsorption process the QCM measures a frequency change that can be associated to a mass change due to adsorption of the copolymer.

QCM was used to monitor in real-time the polymer adsorption followed by azoic dye adsorption and then copolymer adsorption as well as optimization of interaction processes and determination of solution effects on the analytical signal. Solutions of azoic dye  $(5 \cdot 10^{-4} \text{ g/L}, 5 \cdot 10^{-5} \text{ g/L} \text{ and } 5 \cdot 10^{-6} \text{ g/L in DMF})$  were adsorbed at gold electrodes of QCM and the sensor

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responses are estimated through decrease of QCM frequency. Also, the response of the sensor at MA-S copolymer (solution  $5 \cdot 10^{-4}$  g/L,  $5 \cdot 10^{-5}$  g/L and  $5 \cdot 10^{-6}$  g/L in DMF) is fast, large, and reversible.

This research showed that the QCM can be an alternative to study some physical and chemical properties of synthesized copolymer. Additionally, FTIR and NMR have been used to compare the properties of the polymer, copolymer and dye.

#### **P10**

#### STUDY OF BIOCHEMICAL PROCESSES INDUCED BY HEAVY METALS ACCUMULATION IN Zea Mays

#### <u>ANDREI CHILIAN</u><sup>1</sup>, I. V. POPESCU<sup>2,3</sup>, C. OROS<sup>2</sup>, C. RADULESCU<sup>2</sup>, A. GHEBOIANU<sup>1</sup>, R. BANCUTA<sup>1</sup>

Abstract. This study aims to follow the biochemical process from Zea mays in the presence of some heavy metals, as copper, zinc, nickel and lead at different concentrations. It is very well known that some elements, as carbon, hydrogen, oxygen, nitrogen, sulphur, phosphorous and chloride, named macroelements, participate at all biochemical processes from plants. Other elements (e.g. Br, Fe, Co, Mn, Cu, Mo, Se, F, Cr, Zn etc), which are in small concentrations and named microelements, have an important biological role in plants growth. By this work it is shown that are initiated classics biochemical reactions if the substrate is enriched with heavy metals (Cu and Zn) in small concentrations. If the concentrations of studied heavy metals are higher, then can be appeared secondary reactions (e.g. stopping, malformations) which can have negative effects on Zea mays growth. The biological importance of nickel and lead on plant growth was much lower, or these metals can take the vital functions of other metals which missing. The heavy metals analysis was achieved by gualitative and guantitative techniques (i.e. EDXRF and GF-AAS). The biochemical process was correlated with the influence of heavy metals added at different concentrations as well.

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### CONCEPTION OF THE PELLETIZED SOLID METHANE COLD NEUTRON MODERATORS

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Abstract. Solid methane is known as a priority cold neutron moderator. But, its very poor radiation resistance put obstacles in the way of installing it at high power neutron sources. A single way to do it seems to use small beads of solid methane continuous removable in a moderator chamber. One of possible conception of a pelletized solid methane moderator is presented together with some theoretical confirmations of solid beads continuously recharging techniques and experiments. As it is possible to make solid methane pellets.

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#### SANS AND SAXS STUDIES OF BIOMINERAL PARTICLES PRODUCED BY BACTERIA *Klebsiella Oxytoca*

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Abstract. An important area of research in nanotechnology deals with the synthesis of nanoparticles of different chemical composition, sizes and controlled monodispersity. Indeed, nanoparticles shape control is a recent addition to the list of demands being made of newly emerging synthesis methods. Currently, there is a growing need to develop environmentally benign nanoparticles synthesis methods that do not use toxic chemicals in the synthesis protocol. A promising new dimension in this field is the use of microorganisms for the production of inorganic nanoscale particles. This is not surprising given that many organisms, both unicellular and multicellular, are known to produce inorganic materials either intra- or extra-cellular. It was established that bacterium Klebsiella oxytoca creates different types of ferrihydrite nanoparticles as a result of variation of the growth conditions, whose differences were accurately identified by means of Mossbauer spectroscopy, static magnetic measurements analysis, scanning electron microscopy and small angle Xray scattering methods on dry powder and water dispersed samples. In the

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present work structural and stabilization properties of biogenic ferrihydrite water based dispersion of nanoparticles produced by bacteria *Klebsiella oxytoca* are investigated by means of SANS and SAXS methods.

# └ MATERIAL SURFACE INVESTIGATIONS, A REVIEW OF RESULTS CONCERNING THE APPLICATIONS OF SCANNING ELECTRON MICROSCOPY (SEM) BASED METHODS

# <u>VIRGIL MARINESCU</u><sup>1</sup>, LUCIA LEONAT<sup>1</sup>, MIHAI IORDOC<sup>1</sup>, RADU SETNESCU<sup>1,2</sup>

**Abstract.** This paper presents a review of original investigations and applications of Scanning Electron Microscopy (SEM) as a material surface analysis technique. The applications of SEM and Energy Dispersive Spectra of the characteristic X-Ray and even sectioning, lithography and microtomography 3D models using Ion Focus beam (FIB) are presented. Examples of surface morphology/ topography, compositional contrast, high resolution imaging at nanometer scale, elemental analysis and mapping of elemental concentration on different polymer, ceramic metal or composite materials are discussed.

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# CONTRIBUTIONS TO THE EVALUATION OF PRESSURIZED OXYGEN EFFECTS IN ACCELERATED THERMAL AGEING OF AN EVA COMPOUND

# <u>CATALIN RUSU-ZAGAR</u><sup>1</sup>, PASAREANU SIMONA<sup>1</sup>, GILDA RUSU-ZAGAR<sup>2</sup>

Abstract. The equipment used in nuclear power plant must always correspond to high standards of security. In order to maintain the conformity to the standards, the degradation state of the electrical insulation materials has to be known permanently. Accelerated thermal aging can be used to assess the lifetime of such insulations. The effect of oxygen pressure on the degradation rate of an EVA compound used as a cable jacket compared to the simple accelerated thermal aging was studied. Cable insulation degradation was evaluated based on DSC measurements, and verified by determining the elongation at break.

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# P15 MONTE CARLO SIMULATIONS OF NEUTRON OPTICAL ELEMENTS FOR A SANS SPECTROMETER AT THE IBR-2M PULSED REACTOR

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Abstract. We proposed a configuration for a new neutron small angle scattering instrument at the IBR-2M pulsed reactor using a combined moderator system. This system provides added-up spectra from the cold and thermal parts of the moderator. Our efforts have the purpose to obtain a better resolution and an increased neutron flux, as well as decreasing the neutron and gamma background for the small-angle neutron scattering instrument.

We suggest a combined collimation system composed of neutron optics elements (divergent or elliptical neutron guides) and further different configurations of multiple pinhole collimation system. Also, a stack of neutron lenses will be considered as an alternative option for improvement of the spectrometer. The performance of the final collimation system has been evaluated. The results proposed for the neutron optical devices and the extraction system for the SANS spectrometer were obtained using VITESS software package.

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# P16 SMALL-ANGLE SCATTERING FROM THE GENERALIZED SELF-SIMILAR VICSEK FRACTALS

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Abstract. An analytical approach for calculating the small-angle Xray or neutron scattering (SAXS/SANS) from generalized self-similar Vicsek fractals (GSSVF) is developed. The system considered is a massfractal, generated iteratively from a regular 3D Vicsek fractal structure. It's fractal dimension increases with increasing the value of the scaling factor. This dependency allows one to vary in this model the fractal dimension to any value between zero and two. Small-angle scattering (SAS) intensity is determined from a set of non-interacting, randomly and uniformly distributed GSSVF scatterers, where each scatterer represent a cluster composed of spherical subunits. We calculate a number of key features: form factor, fractal structure factor, radius of gyration, boundaries of fractal regions, intensity at zero angle, influence of polydispersity, radial and pair distribution functions. We show that the self-similarity property of the GSSVF is the source of the periodic pair distribution function on a double logarithmic scale. This demonstrates that an in depth structural characterization of nano/microsized GSSVF clusters with a hierarchical spatial organization can be achieved in terms of the scaling factor, in both reciprocal and real spaces.

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# STRUCTURAL, ELECTRONIC AND SPIN DEPENDENT TRANSPORT PROPERTIES OF FE/CAS/FE (001) HETEROSTRUCTURE

### PETRU VLAIC<sup>1,2</sup>, EMIL BURZO<sup>2</sup>

Abstract. The aim of present work is the ab-initio investigation of structural, electronic, magnetic and spins dependent transport properties of Fe/CaS/Fe (001) magnetic tunnel junction. The electronic structure calculations are performed by means of a self-consistent Green's function technique for surface and interfaces implemented within the tight-binding linear muffin-tin orbital method (TB-LMTO) in its atomic sphere approximation (ASA). The spin dependent transport properties in the current-perpendicular-to-plane (CPP) geometry are studied by means of the linear response of Kubo approach implemented within TB-LMTO formalism and including vertex corrections. The results show that electronic, magnetic and spin dependent transport properties are sensitive to Fe/CaS (001) interface structure. Total energy calculations suggest that the interface geometry with Fe atoms located above Ca and S sites is the most stable one. A small charge transfer produced by the band offset and mainly localized at Fe/CaS interfaces is evidenced. The interface iron magnetic moments are enhanced over the bulk value due to the low coordination number. A small antiferromagnetic coupling that rapidly decreases to zero is evidenced. Metal induced gap states (MIGS) in the nonconducting CaS spacer, having a fast decay with increasing barrier thickness and playing a fundamental role in spin dependent transport properties, are evidenced. In the ferromagnetic state the majority spin conductance dominated by electronic states close to |k||=0 decays faster than the minority spin one and almost at the same rate with both conductances in the antifferomagnetic state. The tunneling mechanism is mostly dominated by interface and interface resonate states. Tunneling magnetoresistance ratios up to 400 % are evidenced for the stable interface configuration while TMR values up to 5000 % are predicted for the interface configuration with iron atoms located above the hollow between Ca and S sites.

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# A FIRST-PRINCIPLE STUDY OF SOME FE/ALKALI HALIDES/FE TUNNEL JUNCTIONS

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Abstract. The nanostructured magnetic tunnel junctions (MTJs) are nowdays one of the most active area in the field of material science due to their potential applications in spintronic devices such as non-volatile magnetic random access memories (MRAM) and magnetic field sensors. In contrast with semiconducting and insulating amorphous AlOx based junctions, the MTJs with insulating nanocrystalline barriers opened the new field of archiving higher tunneling magnetoresistance (TMR) values as it is required for better device performances. Beside the extensively studied Fe/MgO/Fe MTJ [1-3] other alternative systems suitable for comparative studies and possible technical applications may be represented by Fe/NaCl/Fe [4,5] and Fe/NaBr/Fe heterostructures. A first-principles study of electronic, magnetic and spin dependent transport properties of Fe/NaCl(NaBr)/Fe (001) MTJs is presented. The ground state electronic structure calculations are performed by means of a self-consistent Green's function technique for surface and interfaces implemented within tightbinding linear muffin-tin orbital method (TB-LMTO) in its atomic sphere approximation (ASA) [6]. The spin dependent transport properties are studied by means of the linear response of Kubo approach implemented within TB-LMTO formalism [7]. The results evidence the formation of sharp Fe/NaCl(NaBr) interfaces and the enhancement of magnetic moments of interfacial iron atoms. Presence of metal induced gap states (MIGS) in insulating NaCl(NaBr) barriers are evidenced. A small ferromagnetic (antiferromagnetic) exchange couplings that rapidly decreases to zero with increasing barrier thickness is observed for Fe/NaCl(NaBr)/Fe heterostructures. For both NaCl and NaBr barriers, the main contribution to the conductance in the ferromagnetic state is given by the minority spin electrons. The TMR ratios rapidly increase with barriers widths and reach high values in the asymptotic regimes.

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"The important thing is not to stop questioning. Curiosity has its own reason for existing."

**ALBERT EINSTEIN**