SOME RESULTS OF NIMP-ROMANIA: POSSIBLE APPLICATIONS OF ESS IN MATERIALS PHYSICS
Neutron Scattering in Romania

- The neutron physics in Romania started along with VVRS Nuclear Reactor (1957).
- Unfortunately this machine was not upgraded and was shut down in 1997. At present time the majority of Romanian researchers are working abroad. However the neutron physics activity had continuity in Romania especially due to constantly collaboration with JINR Dubna, Russia.

Some more representative results obtained by Romanian physicists along the time:
- *The development of high performance instruments by using focusing effects*
- *Critical magnetic scattering*
- *Advancements in theory of Neutron Diffraction*
- *Dynamics of gases adsorbed on activated charcoal*
- *Dynamics of simple and molecular liquids by Neutron Scattering*
- *SANS studies of super-paramagnetic particle and magnetic fluids*
- *Phase transition in hydrogen bonded molecular crystals*
NATIONAL INSTITUTE FOR MATERIALS PHYSICS

Scope

*Basic and applied research in the field of:*
  condensed matter physics
  advanced functional materials
  nanomaterials and nanostructures

*Educational activities:*
  diplomas
  master dissertations
  PhD thesis

*Services:*
  advanced characterization
  prototypes
  consultancy
Present organization

5 research laboratories with 9 research teams:
- **L10-Multifunctional Materials and Structures**
  - Functional nanostructures
  - Complex Heterostructures and Perovskite Oxides
- **L20-Magnetism and Superconductivity**
  - Electronic Correlations and Magnetism
  - Superconductivity
- **L30-Physics of Condensed Matter at Nanoscale**
  - Si- and Ge–based nanomaterials and nanostructures
  - Surfaces, interfaces, thin films and single crystals. X-ray / electron spectroscopies and diffraction
  - Theory
- **L40-Optical Processes in Nanostructured Materials**
- **L50-Laboratory of Atomic Structures and Defects in Advanced Materials**
JEOL JEM ARM 200F
Cs-corrected Analytical High-Resolution Transmission Electron Microscope

Clean room

SEM-FIB
Complex cluster for surface physics:
MBE, RHEED, STM, XPS, LEEM

**Growth methods:**
- Wet chemical (sol-gel, solution bath deposition, Langmuir-Blodgett);
- mechanochemical (high energy ball milling);
- standard ceramic technology;
- spark plasma sintering;
- hot pressing;
- pulling machines for single crystals growth;
- hydrothermal and solvothermal growth;
- electrodeposition;
- melt spinning;
- MBE; RF-sputtering, PLD;
- clean room for nanostructures fabrications (photolithography, electron beam lithography, FIB).

RF-sputtering with in-situ characterization techniques: Auger, ellipsometry

PLD with excimer laser
**Characterization:**
- Structural: XRD; SEM; Raman; RES; Moessbauer; HRTEM, TEM, SAED; AFM, SPM.
- Physical properties: magnetism (VSM, MOKE, PPMS, SQUID); optical (luminescence, fluorescence, transmission-absorption-reflectivity, ellipsometry, near field optical microscopy); dielectric; superconducting; semiconductor (Hall); electric-photoelectric; ferroelectric and piezoelectric; trap investigations (DLTS); THz spectroscopy; broad band dielectric spectroscopy; a cluster for surface physics (XPS, SARPES, ARUPS, STM); a XAS spectrometer for EXAFS and XANES studies; etc.
Nanomaterials

Structural investigations related to synthesis of novel nanomaterials whose properties are determined by structural features at the nanolevel, are one of the most promising directions of application of neutron scattering. The possibility of simultaneous use of isotopic substitution of hydrogen for deuterium in a substance under investigation and magnetic neutron scattering for studying magnetic systems is of particular significance.

The behaviour of complex nanomaterials is frequently determined by key components, which are present in very small quantities. Detailed investigations of internal structure are necessary to study the behaviour of an individual component in multi-component structures.

Crystalline materials with special properties

The major factor of development of all branches of industries, power engineering, medicine, information technologies is the synthesis of novel nanosystems and materials with unique tailored properties, which can change their properties and structure depending on the environment conditions and controllable external influences.

Novel oxide materials among which are high-temperature superconductivity, colossal magnetoresistance effect, ferroelectricity have been recently synthesized. Neutron diffraction studies are the highest-precision method of the structure analysis of light-atom materials. With their help it became possible to reveal microscopic basis of physical properties of these compounds.
RECENT RESULTS INTERESTING FOR NEUTRON DIFRACTION AND ESS MEASUREMENTS
ENERGY MATERIALS

Storage materials are a broad class of materials that include hydrides, hydrates, metal-organic frameworks (MOF) and nanotubes, with an emphasis on reversible hydrogen storage, encapsulation of other small molecules, such as alkanes, and trapping of harmful gases, such as carbon dioxide.

Physical properties investigated by optical methods

Chemical properties: p type doping, functionalization
Carbon 40,2201, 2002

Electrochemical properties: n type doping, functionalization with organic compounds and polymers
Carbon 47, 1389,2009

Polymer/CNT composites
Polymer48,5279,2007

Semiconductor/CNT composites
J.Phys. Cond. Mat. 21,445801, 2009

Carbon nanotubes and composites

Applications

Energy storage
Small 2,1075, 2006

Non-linear optics
Phys. Rev. B72, 245402, 2005
**TiO$_2$ NANOSTRUCTURED THIN FILMS FOR PHOTO-CATALYTIC DEGRADATION OF ORGANIC POLLUTANTS**

TEM images of TiO$_2$ nanocrystals.

**CATALYSIS**

The ESS will facilitate routine, time-resolved measurements in fast catalytic processes at the gas-solid interface. These measurements at ESS has the potential to provide new insight into the structure and function of catalysts.

Phenol conversion degree CPh (%) after 5 h of UV illumination ($\lambda = 312$ nm) for the hydrothermally synthesized TiO$_2$ samples.
Multi-segment nanowires based photodetectors

Template method

Nanoporous membro+electrochem. Dep.

⇒ nanowire photodetectors

⇒ single bath deposition-easy to transfer to industry

Neutrons and X-rays are the most basic tools for characterizing these new materials. While X-rays often provide highly accurate information on complex symmetry, neutrons are best suited for accurately finding the position of atoms. These tools are indispensable for advancing understanding of novel materials and their properties. Neutron scattering provides information about the composition, phases, microstructure and stresses in materials in ambient conditions, as well as a function of some external parameters.

SEM-EDX analysis of the CdTe nanowires

Multi-segment nanowires based photodetectors
Metallic micro and nanotubes

Auto-catalytic deposition using the template method

Copper tubes prepared by electroless deposition in ion track templates
A few select examples are given below to support the wealth and breadth of neutron scattering in this field:

Thin film heterostructures based on metal oxide materials can display a broad range of physical phenomena including large spin polarisation, colossal magnetoresistance, electronic phase ordering, charge, orbital and spin ordering.

Magnetic domain structures, such as periodic antidot arrays, can be observed by grazing incidence scattering or small angle neutron scattering.

Emergent complex phenomena, such as fundamental magnetic and superconducting order, are studied on a microscopic level using diffraction and spectroscopic techniques.

Magnetic frustration and spin glasses display low frequency spin dynamics. These are typically probed by cold neutrons on chopper spectrometers, and backscattering instruments.
Magnetoresitive elements (spin valves). Exchange spring phenomena and interlayer magnetic coupling

Specific problems: extending the study of interfacial phenomena by neutron reflectometry in Fe free structures.
Ferromagnetic and antiferromagnetic films with compositional depth gradient

Specific problems: depth dependent structural changes and depth dependent spin structures

Additional interest:

- Ferromagnetic-ferroelectric interfaces
- Ferromagnetic-superconducting interfaces
- Internal spin structure in spinels perovskites
- Spin structure and structural disorder in magnetic nanoparticles for biomedical applications
- Structural and magnetic phase transitions in ferromagnetic shape memory alloys
SELF-ASSEMBLED CORE_SHELL COLLOIDAL MAGNETIC NANOPARTICLES

- Principle of the self-assembly

As-synthesized particles are coated by Oleic acid and oleyl amine

After thermal annealing, the organic groups decompose to carbonaceous coating. The exact nature of this coating has yet to be studied.

- Breakthrough in data storage, biomedicine, catalysis and nanoelectronics

Core-shell Ag-Co nanoparticles

\[ \text{Co}_2(\text{CO})_8 + 2\text{AgClO}_4 \rightarrow 2\text{Ag} + \text{Co} + 8\text{CO} + \text{Co} (\text{ClO}_4)_2 \]

APPLICATIONS

- Magnetic-conducting bimetallic nanosystems that exhibit GMR effect

- Use of patterned substrates with logic capabilities
An increased number of articles published in journals with high impact factor

An increased attractiveness for young researchers (around 30 new employees in the last 4 years, including from Diaspora)

New opportunities for international collaborations (NIMP had become partner in new FP7, Euratom, EUROCORE, COST, SCOPES, etc. projects); researchers from abroad start to come and work at NIMP (e.g. stages of PhD students from Latvia, France, Turkey, post-docs from UK, India, China)

NIMP had become an important player not only at national level, but also at European level
FOR NIMP RESEARCHERS

Neutron scattering is a unique and important complementary probe for the structure and dynamics of materials due to the neutron's penetration power and its sensitivity to the presence of light elements, in particular hydrogen.

The ESS, with its unparalleled brightness and innovative instrument suite, will be an indispensable tool to make breakthroughs in materials research.