Studies of Condensed Matter Properties

I. Introduction

Current trends in development of scientific research are more and more focused on the interdisciplinary integration of various lines and methods of research. In studies of condensed matter properties, combination of nanotechnologies, biotechnologies, information technologies, and biomedical technologies on the basis of common methodological approaches may lead to appreciable advances and radically new fundamental and applied results.

Since JINR has a unique basis, great experience, and internationally acknowledged competence in such fields as nanosciences involving the use of neutron scattering, synchrotron radiation, and other complementary techniques, nanotechnologies involving the use of heavy ions, radiobiology, including genetic investigations, and a wide range of information technologies, integration of these researches will undoubtedly bear rich fruit. This is the idea underlying the JINR road map for studies of condensed matter properties.

The selection criteria for the currently central lines of research were as follows:

- an elaborated programme of research at the basic facilities of JINR with due regard for their unique and specific capabilities;
- clear prospects of research development for the nearest decade;
- proved interest of JINR Member States and other countries in the research;
- attractiveness of the research for young scientists;
- sufficiently large trained personnel;
- possibilities of realizing the goals within the JINR budget.

Additional criteria were the presence of their own basic and experimental facilities with similar parameters in the JINR Member States and a potential possibility of establishing at JINR centres for collective use of the facilities within the framework of the topical researches in question.

II. Research fields

1. Nanoobjects and nanotechnologies.

Theoretical studies of nanostructures

Current requirements of more sophisticated electronics and manufacture of electronic components of size beyond the capability limits of traditional lithography have led to noticeable progress in development of new nanoscale processor technology, for example, production of conductors of atomic size and devices based on the one-electron tunnelling effect, studies of spin-polarized electrons and magnetic nanostructures. This all holds much promise for production of electronics of new generation. Potential applications range from quantum computers and so-called safe quantum information to sensor devices operated under the action of a single particle. Unique nanosize samples open up new possibilities in various fields: computer storage, electricity transmission and heat transfer, microswitches, and high-sensitivity detectors.

Carbon nanostructures are of particular interest. For example, carbon nanotubes are thought of as possible components of MOSFET transistors and compounds. Their good emission characteristics allow them to be used in indicator panels while thin needle structures allow their use as probes in various microscopes. Good absorption characteristics of carbon nanoparticles, in particular hydrogen, may be used for development of new fuel devices. However, much has to be done to understand clearly and control their production in view of an arbitrary shape, topology, chirality, size, structure (e.g. single-wall in comparison with many-wall ones), arrangement, parallel wiring, integration into nanoelectronic systems, heat removal. In addition, it is necessary to understand connection of these materials on the molecular level.

For this reason, the key lines of research will include theoretical studies of electronic, thermal, and transport characteristics of various modern nanomaterials and nanostructures.

Experimental formation of nanoporous structures.

Production of nanoporous structures in polymers by the ion track method is both of fundamental and applied interest. Investigation of track etching in the nanometre radius range provides information on features of interaction of a high-energy heavy particle with a material. Investigation of the behaviour of the "track" nanopores allows a possibility of simulating processes occurring in biological ion channels. A lot of researches have been carried out in this field at various laboratories in the past decade.

Production of nanosize cluster structures by ion implantation.

Among the extensively developing methods for production of nanostructures, the ion implantation technology hold a particular place because, unlike all other methods, it allows formation of separation phases from practically any chimerical elements in any material. High-dose ion implantation is a well-established method for synthesis of nanostructures in solids in order to modify properties of materials, which find various applications in technology. Considerable study is being given to the use of ion implantation for solving nanotechnology problems.

Realization of these goals will provide effective conditions for creation of new materials with nanosize separations of the given phases with high volume density for their use in micro- and nanoelectronics, technologies for production of new materials with much new physical and chemical properties.

Use of ion tracks for production of nanoobjects.

Experiments based on specially developed technologies showed that metallic nanowires of various diameters and geometrical profiles can be formed and grown on massive backings. Metallization of the inner surface of an etched track makes it possible to produce systems of metallic microtubes. The studies have shown that unique one-dimensional metallic nanostructures with a high base ratio (diameter-to-length ratio) can be produced.

Template synthesis of metallic nanowires involves development of field electron emitters, biosensors, new materials for magnetic discs, magnetic sensors based on the giant magnetic impedance effect, anisotropic optical filters, synthesis of single-crystal rods for colloidal solutions, etc.

Neutron methods for diagnostics of nanostructures.

A general scientific trend is to place emphasis on the studies of materials and systems whose properties are dictated by the structural features at the nanolevel. Here the particular potential of neutron methods arises from the possibilities of using isotope replacement in the material under study (first of all hydrogen/deuterium) and magnetic scattering of neutrons. The general trend in development of neutron spectrometers is the use of new technological possibilities for significant improvement of their main parameters: luminosity and resolution. This allows earlier unfeasible experiments to be planned and carried out. The IBR-2 reactor is a pulsed neutron source with a record intensity and comparatively long pulses, which makes it different from all existing high-flux sources and should be taken into account when it is used for experiments. Condensed matter studies at pulsed reactors have been carried out at JINR for over 45 years. The most adequate experimental techniques have been developed and relations with the scientific centres in Russia and JINR Member States have been established over this period.

All these factors dictate the following choice of the topical lines of nanostructure research:

1. properties of the surface, interfaces, and low-dimension nanostructures;
2. structure of model and biological lipid membranes;
3. large-scale structure of non-crystalline materials: vesicles, polymers, colloidal solutions, etc.;

The planned investigations include studies of both non-magnetic systems (polymers, dendrimers, porous glasses, carbon nanomaterials and their liquid dispersions, biologically active compounds, liquid metals with admixtures) and magnetic systems (ferroliquids, heterostructures, low-dimension magnetic structures in thin metallic films). The common goal of the investigations is to determine parameters of the nanoobject structure (geometrical characteristics, polydispersity, specific surface, interparticle correlations, cluster formation, molecular dynamics) under different conditions of varying temperature, pressure, external magnetic field and to construct structure models for some complex nanomaterials.

2. Biomedical research

Radiation-genetic investigations

A strategic long-term objective in this field will be fundamental study of biological effect of accelerated heavy ions in a wide range of linear energy transfer (LET). Heavy charged particles are a rather convenient tool for studying inducing mechanisms of radiation-stochastic and radiation-genetic effects. The character of DNA damage induced by heavy charged particles (especially heavy ions) is different from the damaging effect of weakly ionizing radiation (e.g. gamma rays). One of the characteristic features of genetic effects arising from irradiation by heavy charged particles is cluster damage of DNA resulting from high local energy deposition in genetic structures. DNA break repair mechanisms are ineffective against this kind of damage. Among the most poorly studied problems of biologic effect of heavy charged parties are problems of their effect on cellular membranes, which, together with DNA, are now considered to be a critical target of radiation effect.

Radioecological investigations, ultrapure radioisotopes for nuclear medicine and biomedicine

These investigations are carried out to improve radiation monitoring of the environment and safety measures at nuclear installations as new radioactive material processing procedures are being developed. Methods for production of highly pure isotopes ^{67}Cu, ^{73}As, ^{88}Zr, ^{99}Mo(^{99}Tc), ^{97}Ru, ^{149}Tb,^{178}W(^{178}Ta), ^{186}Re, ^{188}Re, ^{211}At, ^{225}Ac, ^{237}U, ^{236}Pu, ^{237}Pu are developed. They are used in nuclear medicine for diagnostics and therapy. Particular attention will be paid to production of radionuclides in (α, xn) reactions at the U200 cyclotron and in photonuclear reactions at the MT25 microtron.

3. New materials.

Theoretical studies.

Recent years have seen unprecedented progress in production of high-quality samples and high-precision instrumentation, which allowed first-rate results in studies of thermodynamic, transport, and spectroscopic properties of **new complex materials** exhibiting strong electronic and magnetic correlations. Among them there are such materials as layered cuprates in the normal and superconducting states, oxides of transition metals, in particular manganites with enormous magnetic impedance and geometrically frustrated antiferromagnetic spinels, fullerene clusters and lattices. Studies of these materials are of great interest both from the point of view of fundamental physics and in connection with their possible uses in technology.

In the proposed long-term programme the emphasis will be placed on theoretical analysis of the above-mentioned systems with strong electron correlation, which implies studies of new co-operative phenomena, new forms of ordering, magnetism in low-dimension systems, and quantum critical phenomena.

Considerable experimental study of these materials using neutron scattering, which is carried out at the Frank Laboratory of Neutron Physics, JINR, also stimulates development of theoretical studies in this field.

The main goal of the planned investigations **for the nearest 10 years** is to carry out "realistic" calculations of various experimentally measured physical quantities by new effective methods, which may shed light on rather complicated interrelation of the electron structure, magnetic and transport properties of these complex systems. These calculations may show ways to production of new materials and development of **innovation projects**.

Neutron investigations of new materials

In the past two decades it has become possible to synthesize new oxide materials with some unusual properties, such as high-temperature superconductivity, enormous magnetic impedance, coexistence of magnetism and ferroelectricity. The microscopic basis for the unusual physical properties of these compounds is some features of their crystalline and magnetic structure manifesting themselves, for example, in occurrence of various types of ordering—magnetic, charge, orbital one. Specific features of interaction of neutron radiation with a material and presence of the magnetic moment in neutrons allow neutron scattering methods to be successfully used for precise determination of characteristics of the atomic structure of nanosystems and materials with light atoms, first of all hydrides and oxides, and their magnetic structure. The common objective of the investigations associated with Section 4 is to study correlations of the features of the atomic and magnetic structure of crystals with their physical properties. One of the properties governing the behaviour of the oxides of transition metals is their trend to form inhomogeneous states at various length scales from nanodimensions (~20 Å) to mesoscopic dimensions (~2000 Å). The study of fundamental causes for this trend is also one of the currently central topics. This section also involves the study of transition processes, including oxidation-reduction processes, in new materials for battery electrodes.

Modification of properties of materials using heavy ions

Ion-matter interaction mechanisms, structure evolution, and variation in microscopic and macroscopic properties are to be studied. These fundamental studies offer considerable scope for applied uses, mainly for formation of nanosize structures in materials. The main lines of research, both under way and projected, are as follows:

- Study of formation of radiation defects in crystalline and amorphous metals, alloys, semiconductors, and dielectrics exposed to heavy-ion beams of energy $E > 1$ MeV/nucleon.
- Study of surface modification and formation of nanosize defects in materials caused by single ions under the conditions of electron deceleration.
- Elaboration of the main principles of heavy-ion implantation technology.

Accelerated heavy ions are known to be a unique tool for investigations in radiation solid-state physics. An important point in the use of heavy ions is a possibility of modifying macroscopic properties of materials and formation of nanosize structures in them. Another advantage of accelerated heavy ions is their high defect-inducing capability, which makes it possible to produce in short time the radiation defect density in materials which is comparable with the density produced by neutron irradiation for several years. Beams of heavy ions whose cross section of interaction with lattice atoms is many orders of magnitude larger than that of neutrons allow faster accumulation of radiation defects. High atom displacement rates (10^{-2}–10^{-3} dpa/s) at ion irradiation allow a large dose (~150 dpa) to be obtained in a relatively short time. It is also possible to simulate various radiation defects caused by neutron irradiation. The U400 and Its100 heavy-ion accelerators operating at JINR offer vast opportunities for experimental investigations in the energy range 1–20 MeV/nucleon for ions from boron to xenon.

4. Dynamic systems, Earth sciences, engineering studies.

Theoretical studies of chaos, integrability, and self-organization.

In theoretical physics, the last decade of the past century was marked by increasing interest in strongly non-equilibrium phenomena and non-linear problems. Our goal for the nearest future is to develop mathematical approaches for adequate description of avalanche dynamics, signal propagation in unstable and non-linear media, and non-equilibrium processes which are described by continuous and discrete models. Methods of the theory of integrable systems, such as the Bethe ansatz, inverse problem, matrix product ansatz, Grassmann variables, will be used to solve non-linear equations and multiparticle systems occurring in a wide range of non-equilibrium and non-linear phenomena.

Neutron investigations of rocks and structural materials.

Studies of materials of construction and rocks are planned to involve experiments on measurement of internal stresses in bulk engineering products, composite and gradient ceramic materials, determination of the atomic structure and dynamics of liquid-metal heat-transfer agents, investigation of crystallographic textures of rocks and their relation to physical properties. The advantages of neutron diffraction over other methods of engineering diagnostics are so great that special diffractometers for the investigation of internal stresses and textures have been built in practically all modern neutron centres within the past 10 years. As applied to reactor materials technology, the neutron diffraction method is important for investigating bimetallic joints, austenite surfacing of ferrite steels, behaviour of welds and reactor parts under irradiation and loads. Rock texture experiments make it possible to reveal relations between the kinetics of phase transitions in minerals and rocks and the nature of seismicity, to advance in scientific justification of the use of some rocks for long-term burial of nuclear wastes.

III. Experimental and methodological basis.

Neutron research.

- The research is mainly carried out at the IBR-2 reactor, a JINR basic facility with world-level parameters, the only one of this kind in the JINR Member States.
- Research with spectrometers at the IBR-2 reactor involves a users' programme based on requests from the JINR Member States.
- The IBR-2 upgrading programme is being successfully implemented, which opens up possibilities of its effective use within the coming 25 years.
- A detailed programme has been elaborated for development of the spectrometer complex at the IBR-2 reactor.

As the IBR-2 reactor has been shut down for another stage of conversion, the research activities are shifted to the related research centres in Russia and abroad, while the activities at the IBR-2 has been focused on the upgrading of the spectrometers. After the upgrading is accomplished and the IBR-2M reactor is put into operation, it will become the main basic facility of JINR for the studies of condensed matter properties. In the coming four years neutron scattering experiments will be carried out at the reactors of the Kurchatov Institute (Moscow), PINP (Gatchina), and IMP (Yekatirinburg). The work under the programme will be carried out at European neutron sources (BNC, BENSC, PSI, LLB, ILL, RAL, etc) within the framework of the accepted proposals for experiments. Experiments with synchrotron radiation will be carried out at the Kurchatov Institute and at the European sources (DESY, BESSY, ESRF, SLS).

Heavy ion accelerators.

The planned investigations are carried out with special experimental facilities for irradiation of various materials and samples at the U400 and ITs-100heavy ion accelerators and the MT-25 microtron.

The instrumentation used includes JSM-840 and LEO1530 scanning electron microscopes (Poland), Tenzatron for implantation of various ions (Czech Republic), a superconducting ECR source of heavy ions for production of low-energy beams, setups for chemical etching of irradiated polymers.

To extend investigations, it is planned to build a new beam line at the MTs-400 accelerator, to construct the DC-60 accelerator, and to purchase a new scanning filed-emission microscope.

Experimental basis for radiobiology.

The main experimental facilities for studies of biological effect of heavy charged particles are the JINR accelerators Nuclotron and U400M. Some of the experiments are planned to be carried out with the therapeutic proton beam from the Phasotron and in the gamma-ray field of the Rokus-M facility. A necessary condition for success in the planned studies is the possibility of having two–three runs at the Nuclotron and three–four runs at the U400M. To advance radiobiology studies, it is utterly important to increase the mass of ions accelerated at the Nuclotron at least to iron and to ensure stable extraction of nuclear beams with decreased energy (to 300 MeV/nucleon).

A stationary automated setup Genom is installed on the U400M accelerator channel. Unfortunately, there is no special channel for radiobiological experiments at the Nuclotron. C channel like this may only be built within the framework of Med-Nuclotron project.

In 2007 it is planned to get a confocal CARS microscope, which will allow a new field to be opened in intravital studies of human cells and diverse cytological and molecular-biological studies to be carried out. It is also planned to develop a multisphere technique for measurement for neutron spectra in a wide energy range, to improve beam dosimetry methods, and to implement new programmes of radiation transport in substances.

IV. Innovation and technological potential of the research.

Use of nanostructures.

Methods for fabrication of asymmetrical nanopores which can be used in resistive pulse technology have been developed in co-operation with foreign partners. Now this idea attracts considerable attention in connection with the possibility of detecting biologically important molecules and reading out genetic information as DNA molecules are translocated through the pore sensor. Asymmetrical track nanopores filled with an electrolyte exhibit some interesting properties, e.g. rectification of electric current. These properties are being studied in connection with development of a research field called microfluidics. Among other promising applications of profiled nanopores is, for example, focusing of atomic beams first employed in co-operation with the Institute of Spectroscopy (Troitsk) in 2006. Further improvement of the method may result in a new nanoimaging technique.

In addition to the already adopted materials (polyester and polycarbonate) it is planned to use new promising materials for track membranes, which can serve as X-ray filters, imitators of biological cells, high-quality ultrafiltration membranes, etc. More traditional lines of research are microfiltration and ultrafiltration track membranes. Work on improvement of structural and performance properties of track membranes will continue.

Applied aspects of radiobiological studies.

An important applied aspect of these studies is related to the ambitious international project of the manned flight to Mars. The success of the mission will much depend upon the reliable estimation of the biological hazard of high-energy heavy ions appearing in the galactic cosmic radiation. Exposure of cosmonauts to high-energy heavy nuclei may cause various mutations in cells, development of tumours in distant post-exposure periods, structure damages of central nervous system and retina, development of cataract. Estimation of the radiation risk will provide a basis for elaboration of radiation safety measured of spaceship crews.

Another important applied aspect of studies of the biological effect of heavy charged particles is related to beam treatment of human tumours. It is necessary to continue comparative studies of efficiency of proton and carbon beams in treatment of various kinds of tumours and their effect on normal tissues. In addition, the studies may help to solve other important problems: estimation of the risk for occurrence of chronic myeloid leukaemia in people exposed to low radiation doses, development of biological dosimetry methods (biosensors), elaboration of methods for detection of hidden damages in biological membranes induced by heavy charged particles.

Innovation proposals based on the prior development activities are put forward, including the proposal for production of an Ac-211-based radiopharmaceutical for target therapy of melanoma. Another interesting project is establishment, with the participation of JINR, of the Polymerase Chain Reaction Laboratory for early diagnostics of tumours and viral infections which is now under way. It is planned to carry out research and development in biological nanotechnology: investigation of magnetic bacteria (production and study of magnetosomes for target drug therapy), investigation of rhodopsin as a biological trigger prototype.

Construction of accelerator complexes for condensed matter physics and nuclear medicine studies.

The work on development of dedicated accelerator complexes for condensed matter physics and nuclear medicine studies will continue. As regards condensed matter physics, emphasis will be placed on development of compact, low-power-consumption heavy-ion accelerators of energy 1–3 MeV/nucleon. The cyclotrons DC-60 (Astana, Kazakhstan) and ITs-100 (JINR) were constructed and commissioned in 2006. Development of nuclear medicine studies requires construction of multipurpose accelerators with proton and heavy ion beam parameters allowing both production of isotopes for diagnostics and treatment and radiotherapy (proton therapy, boron-neutron-capture therapy). The first of these accelerators DC-72 will be constructed at the Cyclotron Centre of the Republic of Slovakia in 2007.

Applied research using neutron scattering.

Applied research partially financed from external funds includes: studies of internal stresses and texture in bulk parts of engineering devices and materials, investigation of new materials for fuel rods, investigation of geological materials, neutron-dynamics studies of liquid metals with various impurities. Proposals for further development of this research with indication of possible innovation aspects are summarized in the form of an analytical note on establishment of an engineering services centre in Dubna.

V. Manpower and resources.

Highly skilled scientists, engineers, and technicians, including a lot of young scientists from the JINR Member States and other countries, are drawn into implementation of the above research programme. Many research directions are supported by national and international funds, grants of Plenipotentiaries of the JINR Member States or funding within their programmes, which points to their great interest in and support of further development of this field. In general, it is realistic to gain the planned goals with the funds allocated to this field from the JINR budget. At the same time the available funds are obviously not enough to rise to a fundamentally new level of research and take a leading position in the world. Thus it is necessary to concentrate resources on the minimum number of the projects that promise considerable advances in the nearest years.