

**The M.N. Mikheev Institute of Metal Physics, Urals Branch of RAS  
The Russian Federal Nuclear Center – Zababakhin All-Russian  
Scientific Research Institute of Technical Physics  
The Scientific Council on Radiation Physics of Solids, RAS**

**The Sixteenth International Ural Seminar**



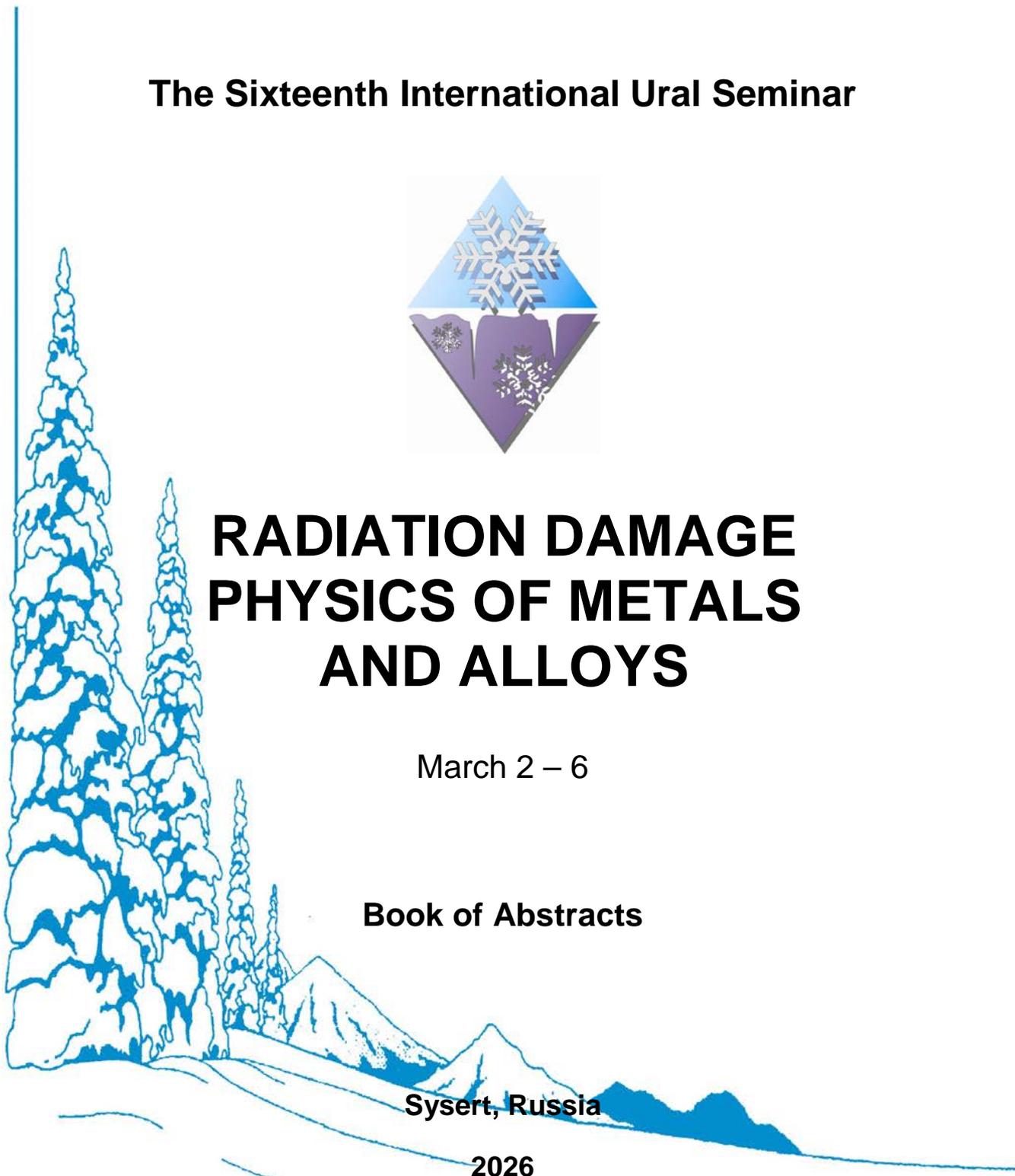
# **RADIATION DAMAGE PHYSICS OF METALS AND ALLOYS**

March 2 – 6

**Book of Abstracts**

**Sysert, Russia**

**2026**





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on  
RADIATION DAMAGE PHYSICS  
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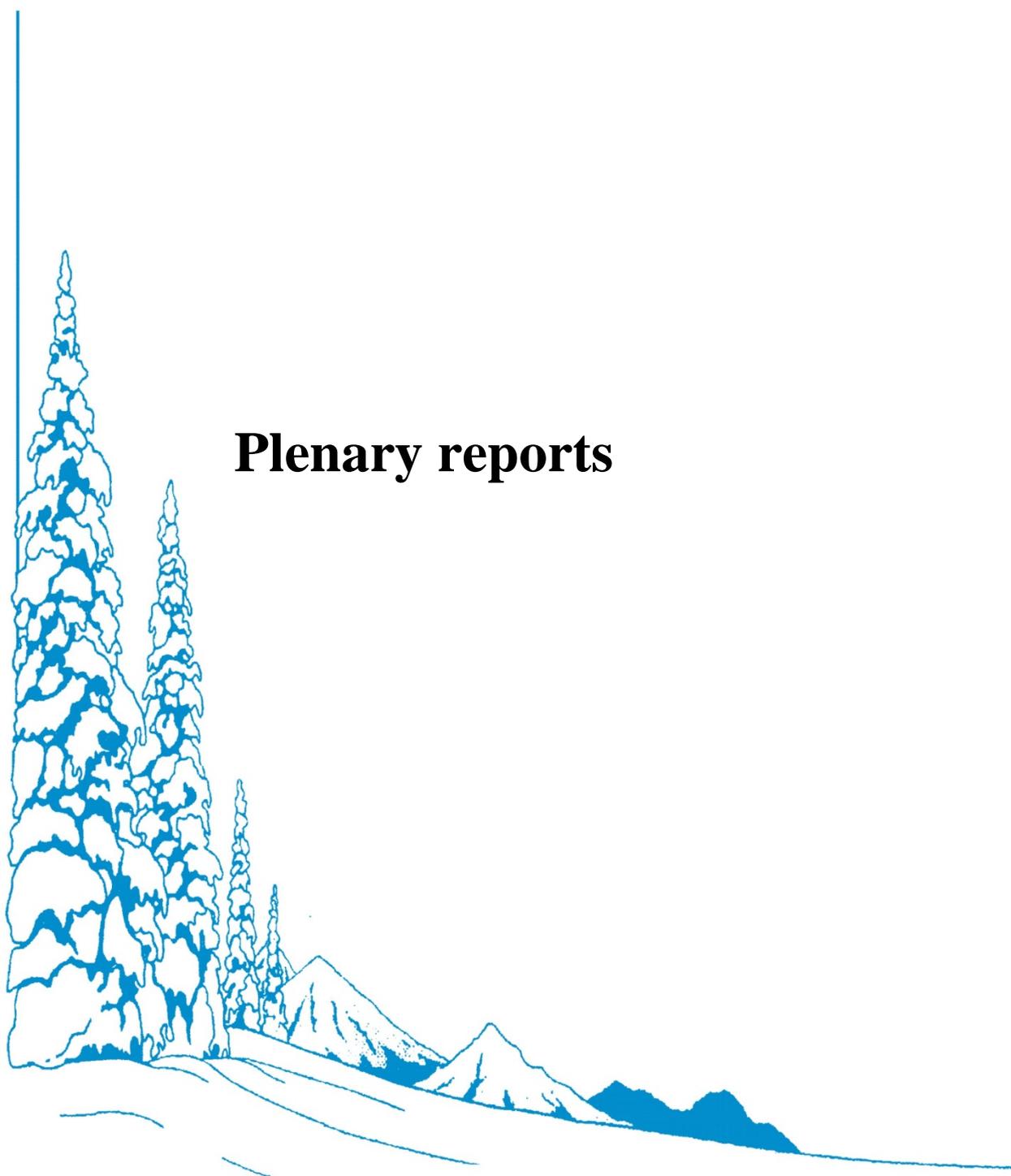
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# Plenary reports





## ACCELERATED TESTING OF STRUCTURAL REACTOR MATERIALS ON ION BEAMS. MODERN APPROACHES AND STATUS

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To design promising nuclear power plants, materials are required that can withstand doses of up to 200 displacements per atom (dpa) and higher, and in a wide temperature range of at least 350-700 ° C. A limiting factor in the development of new radiation-resistant materials is the need for long-term irradiation sessions to achieve maximum loads. The real way out of this situation is to carry out irradiation at increased rates of radiation damage dose set to assess radiation resistance under operating conditions.

To conduct a preliminary analysis of the radiation resistance of new materials, it is possible to use ion beams that can generate radiation damage 2-3 orders of magnitude faster than reactor irradiation. When irradiating materials with ions, the formation of radiation defects occurs heterogeneously along the direction of the ion path, therefore, in simulation experiments on ion beams, the area of radiation damage is analyzed by microscopic methods. Currently, the use of heavy ions with an energy of several MeV is considered the most acceptable in simulation experiments. When irradiating steels, Fe ions with an energy of ~5 MeV are used. These energies ensure, in a wide range of radiation damage doses, the presence of a depth range of the irradiated area of the material, where the influence of the surface and stresses arising in the ion embedding area can be ignored.

The main focus of such experiments is the irradiation of samples and subsequent investigation of the microstructure of damaged near-surface layers of the material using transmission electron microscopy (TEM) and atomic probe tomography (APT). This was facilitated by the development of precision sample preparation methods using focused ion beams for TEM and APT studies from ion-irradiated samples. To study changes in the mechanical properties of ion-irradiated samples, nanoindentation methods are used to analyze the effect of radiation damage on the hardening of the material.

This work presents a set of simulation experiments on heavy ion beams of the TIPr accelerator, implemented at the NRC "Kurchatov Institute" [1]. The use of heavy-ion irradiation has been tested in the analysis of the radiation resistance of a number of materials, such as Eurofer 97, EK-181 and ChS-139, titanium alloys, tungsten alloys. Extensive studies have been conducted to analyze the radiation resistance of dispersed oxide-hardened steels.

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## COMPOSITIONS, STRUCTURES, DEFECTS AND PROPERTIES OF LOW-ACTIVATION STRUCTURAL MATERIALS "BEFORE-DURING-AFTER" HIGH-DOZE IRRADIATION IN FAST AND THERMONUCLEAR REACTORS

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Structural materials (SM) determine the duration of fuel campaigns (FC) and the efficiency of the nuclear fuel cycle (NFC) for fast (FR) and thermonuclear (TNR) reactors. The designs of FR and TNR impose limit changes in the properties of SM (products) to ensure the duration and efficiency of FC. For the created FR (FR-III, open NFC) and the planned demonstration TNR (DEMO-TNR), the requirements for the FC durations (up to 3 years) and for the SM-III properties (100 dpa, heat resistance up to 700 °C) have been determined. The created SM-III (Fe-Cr-Ni-Nb-Mo steels) meet the requirements of FR-III and are highly long-lived radioactive after irradiation (millennia). Higher requirements have been defined for the new generation of FR (FR-IV, closed NFC). A full closed NFC, including the use of irradiated SM (products), is promising.

The compositions, structures, defects, and mechanisms of formation of the properties of SM for FR and TNR under the conditions of "before-during-after" high-dose (200+ dpa) irradiation are considered. Low-activation SM (LASM, time to use after irradiation less than 100 years) is promising for FR-IV and is the only alternative for DEMO-TNR and TNR. LASM should not be inferior (or superior) in terms of physical and mechanical properties to conventional (highly long-lived radioactive) SM, and should be superior in terms of nuclear and physical properties (lower parasitic neutron absorption, lower and rapidly decaying radioactivity). Created LASM-III (ferritic-martensitic steels Fe-(8-12)Cr-W, austenitic manganese steels Fe-Cr-Mn, alloys V-Ti-Cr) meet the requirements of FR-III and DEMO-TNR. The requirements for damage resistance of 200+ dpa and heat resistance up to 1000 °C have been defined for LASM-IV-TNR (FC duration of 5 years). The FR-IV and TNR require a new generation of LASM-IV. LASM-IV is being developed based on a modification of LASM-III and new multi-component refractory alloys.

The compositions, structures, defects, properties, and mechanisms of their formation in LASM-III-IV are considered. The type, energy, and mobility of atoms (matrix, alloying, and impurity atoms) and defects (point defects, clusters, dislocations, and pores) are crucial for the formation of microstructures, defects, and properties (strength, creep, cold brittleness, heat resistance, and swelling).  $\gamma$ -irradiation has a significant impact. Radiation creep occurring in LASM (cold-brittle "before-after" irradiation) "during" irradiation weakens the formation of cold-brittleness "during" irradiation.

The compositions, microstructures, defects, physical-mechanical and nuclear-physical properties of LASM-III-IV were studied "before – during -after" initial (<100 dpa, degradation of initial and formation of radiation defects, structures, and properties) and high-dose (>100 dpa evolution of radiation defects, structures and properties) irradiation. High-dose microstructures, defects, and properties are determined mainly by the composition and have little dependence on the initial microstructures and defects (thermal and mechanical regimes) and are different in FR and TNR irradiations. Promising LASM-IV are single-phase refractory multicomponent vanadium alloys.

## FORMATION AND EVOLUTION OF A DISPLACEMENTS CASCADE IN THE MATERIAL OF FUEL ELEMENT CLADDINGS MADE OF CR16-NI19 AUSTENITIC STEEL DURING OPERATION IN THE BN-600 REACTOR

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Currently, Cr16-Ni19 austenitic steel is used as the main material of the fuel element claddings of fast neutron reactors. The formation and evolution of displacement cascades in the steel under neutron irradiation is the first stage in the evolution of the microstructure that affects the fuel element's operating life.

The study describes the formation and evolution of displacements cascades in fuel element claddings made of Cr16-Ni19 austenitic steel during irradiation in a BN-600 reactor. In this case, the entire range of neutron energies is divided into intervals in which analytical expressions are obtained for the neutron flux density and for the cross sections of their elastic interaction with steel atoms as a function of the neutron energy. For this purpose, the neutron interaction cross section was averaged in selected energy ranges for the main steel components: Fe, Cr, and Ni.

The generation of point defects at the dynamic stage was calculated using the standard model [1]. Spontaneous processes were used to describe the evolution of cascades at the kinetic stage: recombination of vacancies and interstitial atoms and the formation of complexes of similar defects. A statistical model of defect migration was used to describe the thermodynamic stage [2]. Within the framework of this model, the output of defects from cascade regions into the crystal matrix was calculated. Due to the higher binding energy of interstitial atoms in interstitial complexes, compared with vacancies in vacancy complexes, the cascade efficiency of vacancies (the proportion remaining from those generated at the dynamic stage) is higher than that of interstitial atoms.

As a result, the rates of entry of point defects into the crystal matrix after the end of cascade formation were calculated, depending on the microstructure and characteristics of neutron irradiation. The obtained characteristics will subsequently be used to describe the evolution of the microstructure and material properties of the fuel element claddings made of Cr16-Ni19 austenitic steel during operation in the BN-600 reactor.

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## LOW-ACTIVATION AUSTENITIC STEELS: MICROSTRUCTURE, MECHANICAL PROPERTIES, THERMAL STABILITY

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Low-activation austenitic steels based on chromium-manganese were proposed as a replacement for heat-resistant and radiation-resistant chromium-nickel steels, which have been predominantly used as structural materials in the power industry to date [1]. Previously developed low-activation austenitic steels were inferior in austenite stability to highly activated chromium-nickel steels [2].

This paper summarizes the original results of the development and research [3-5] of new low-activation austenitic steels of the Fe–11Cr–26Mn–Ti–V–W system as promising structural materials for next-generation reactors and hybrid power plants. It is shown that a significant difference of the new steels is the increased stability of austenite with respect to transformations into  $\alpha'$ -martensite and ferrite. In the quenched and cold-formed state, flat dislocation pile-ups, stacking faults and deformation microtwins, as well as dispersed particles of MC (M – Ti, V, Ta, etc.) and  $M_{23}C_6$  (M – Cr, Mn, Fe) carbides are observed in the steels.

The strength properties of the new steels in the temperature range of 20–700°C in the quenched and cold-formed states are comparable to or exceed those of known analogs and chromium-nickel steels. The elongation at failure of the new steels is up to three times higher than that of their analogs.

The stability of the grain and microtwin structure is demonstrated during long-term (up to 1000 hours) annealing at 700°C. Under these conditions,  $M_{23}C_6$  carbides precipitate along grain boundaries and microtwins, as well as within grains, including as shells on MC particles. A tendency toward  $\sigma$ -phase precipitation was detected in one of the cold-formed compositions. The strength and ductility properties of the steels remain good after aging. The possibilities of modifying the elemental composition of the steels and the prospects for their use as low-activation structural materials for reactor systems are discussed.

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## LOW DIMENSIONAL MAGNETISM THEORY IN THE SPHERICALLY SYMMETRIC APPROACHES

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In low-dimensional magnetic systems, quantum fluctuations play a significant role. Frustration, another disorganizing factor, can lead to noteworthy effects that are often not intuitively obvious. For example, it can cause the formation of non-trivial spin configurations or the absence of spin long-range order even at zero temperature.

Frustration effects are especially strong in two-dimensional magnetic systems. It's not always possible to describe these effects via using traditional methods of magnetism theory. Therefore, there is a need for alternative approaches. One them is the spherically symmetric self-consistent method (rotation-invariant Green's function method in another notation) [1]-[3].

The report presents the main ideas and some of the most important results of the spherically symmetric self-consistent approach and several related theoretical algorithms received over recent decades [4].

A key feature of this class of methods, which sets it apart from usual spin-wave approaches, is that spin SU(2) and translation symmetry are preserved. This allows for the study of low-dimensional spin models, including frustrated, while strictly satisfying Mermin-Wagner and Marshall's theorems, as well as the spin constraint.

In this way, the difficulties that may arise in the traditional analysis of low-dimensional magnetic systems can be bypassed. The approach can be embedded in more complex constructions when considering spin models with free carriers, such as the basic and three-band Hubbard models, t-J and s-d models, and the Kondo lattice. This leads to non-trivial implementations of the spin polaron idea.

The algorithms of the method also work in the analysis of a low-dimensional spin-pseudospin model (Kugel-Khomskii model). In addition, in this case, it is possible to obtain not only standard thermodynamic characteristics, but also indications of the quantum entanglement of subsystems.

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## MODELING FOR IRRADIATION SWELLING OF STRUCTURAL STEELS IN ADVANCED NUCLEAR SYSTEMS

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The advanced nuclear systems provide promising energy resources due to their safety, efficiency, and economic advantages compared with the traditional nuclear systems. The materials in these advanced nuclear systems will stand extremely hard environments, especially high temperature, neutron irradiation, etc. The irradiation dose and temperature in the advanced nuclear systems are much higher than those in the traditional ones. Under the neutron conditions, there will be defect, microstructure evolution and property degradation in the materials. In fact, the neutron irradiation facilities which can provide the similar environment as that in the advanced nuclear systems are very precious, and the neutron irradiation experiments are expensive and time consuming. The ion irradiation experiments are often used to simulate the neutron-irradiation effects. To investigate the equivalence between the ion irradiation and neutron irradiation and predict the irradiation behaviors, the computational simulation modeling serve as important tools which are efficient, safe and economic.

The irradiation swelling of materials will become unacceptable under high dose irradiation in the advanced nuclear systems. The models for irradiation swelling have been developed for nuclear fuels, cladding and structural materials based on the methods of rate theory, phase field, etc. In the previous models, the nucleation of small defect clusters was modeled simply and roughly. The onset of irradiation swelling could not be predicted very well. The extrapolation of the model from low dose to high dose was not good enough. The recent development of advanced simulation and modeling approaches, as well as the rapid development of data-driven machine learning methods provide powerful and efficient tools for irradiation swelling modeling with high prediction accuracy.

This work presents the models for irradiation swelling based on the coupled model of machine learning and rate theory/cluster dynamics. The machine learning was introduced to predict the steady state irradiation swelling onset dose, while the improved rate theory was developed to simulate the swelling behavior after the incubation period. The cluster dynamics models were developed which are good at simulating the nucleation of small defect clusters. The prediction of irradiation swelling under high dose irradiation in the advanced nuclear systems were realized.

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## MULTI-SCALE HETEROGENEOUS DESIGN OF REFRACTORY HIGH ENTROPY ALLOYS FOR NUCLEAR APPLICATIONS

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The development of nuclear structural materials with exceptional comprehensive performance is a critical challenge in advanced nuclear energy systems. Refractory high entropy alloys (RHEAs), composed of multiple high melting-point elements, exhibit high strength, high hardness, and outstanding high-temperature mechanical properties, making them promising candidates as novel high temperature structural materials for fourth-generation nuclear power systems. However, their limited work-hardening capability and poor resistance to irradiation defects significantly hinder their practical applications. This study delves into the deformation behavior and irradiation performance of RHEAs based on the principles of multi-scale heterogeneous design. This study delves into the mechanisms by which multi-scale heterogeneous design influences the deformation behavior and irradiation performance of RHEAs. It was found that through large deformation cold rolling and short-term high-temperature recrystallization, a microstructure comprising micron-sized heterogeneous grains and nano-precipitates can be constructed. This structure enhances dislocation multiplication and interaction processes through microband induced plasticity, providing a continuous and stable steady-state plastic deformation process for the alloy. Additionally, based on the phenomenon of electronic and ion irradiation-induced disordering of nano-precipitates in RHEAs, a gradient structure of solute atoms and local lattice distortion gradient structure was designed, extending from the peak irradiation damage region to the unirradiated area. This promotes long-range downhill diffusion of solute atoms, and the additional downhill diffusion process increases the annihilation rate of solute atoms and voids, allowing the alloy to maintain zero swelling even at a damage level of 132 dpa.

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## NANOPRECIPITATE STRENGTHENING AND HELIUM ION IRRADIATION EFFECTS OF FACE-CENTERED CUBIC HIGH-ENTROPY ALLOYS

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Single-phase face-centered cubic (FCC) high-entropy alloys (HEAs) typically exhibit excellent ductility alongside functional properties like good irradiation resistance, but suffer from low strength. Nanoparticle strengthening is one effective method to enhance alloy strength; however, the increase in strength is invariably accompanied by a reduction in ductility. This paper systematically investigates the strengthening mechanisms and irradiation resistance of nanoparticle-strengthened HEAs. The influence of element content and type on nanoparticle formation was explored, revealing that chemical composition significantly affects the structural transformation of nanoparticles. With increasing pre-strain deformation, the precipitation time shortens, nanoparticle size decreases, and volume fraction increases. The effects of different nanoparticle characteristics on the magnitude and distribution of the matrix stacking fault energy (SFE) were systematically studied. The magnitude of the matrix SFE was found to depend on the volume fraction of precipitated nanoparticles, while the spacing between nanoparticles can regulate the distribution state of the matrix SFE. Finally, the impact of He<sup>2+</sup> ion irradiation at 500°C on the microstructural evolution of the newly designed HEAs was investigated. High-density nanoparticles can increase the surface area for adsorbing helium atoms during irradiation, enhancing helium dispersion and improving the ability to suppress helium bubble coarsening. Simultaneously, the reduction in matrix SFE induced by precipitation inhibits the transformation from stacking fault loops to perfect dislocation loops, prolonging the incubation period of dislocation loops and delaying their growth.

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**Pu 5f SHELL: ITINERANT OR CORRELATED ELECTRONS?**

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For several decades, the problem of quantum-mechanical ground state of metallic plutonium has remained one of the most significant in fundamental solid state physics. Much of the discussion has focused on the magnetic properties, reflecting the nature of the 5f electron states of Pu, which exhibit intermediate behavior between localized and itinerant regimes. Evidences in favor of possible effect of magnetism on thermal expansion and low temperature electrical resistivity were suggested already in early publications [1, 2]. The first successful theoretical descriptions of the Pu electronic structure also required the existence of magnetic moments on its atoms [3, 4]. However, efforts to detect magnetic moments experimentally have not been successful [5]. This contradiction between theory and experiment was resolving using an alternative approach based on the idea of valence-fluctuating (intermediate-valence) nature of the Pu 5f electron shell [6, 7]. This point of view was supported by the inelastic magnetic neutron scattering experiments performed by the US research team. They showed that  $\delta$ -Pu is an intermediate valence system with Kondo temperature 975 K [8]. By the other words, Pu 5f electrons turn out to be essentially localized but their magnetic moments are fully screened by the conduction band electrons resulting in nonmagnetic quantum-mechanical ground state. Thus, it could be considered that this result resolves the long-standing controversy between the experiment and theory concerning magnetism of the Pu metal. However, this conclusion was challenged by proponents of the density functional theory (DFT) description of the electronic structure, arguing for the itinerant nature of 5f electrons [9], as opposite to their treatment as strongly correlated electrons in terms of the approach based on dynamical mean field theory (DMFT) [8]. Here we discuss how these two concepts – treating Pu as either itinerant or correlated system - can explain the unusual thermal and elastic properties of metallic Pu [4,9,10], as well as new experimental studies showing that the problem of Pu electronic structure is far from resolved.

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## **RELATIONSHIP BETWEEN MICROSTRUCTURE PARAMETERS AND VARIOUS TYPES OF EMBRITTLEMENT OF SOME STRUCTURAL MATERIALS OF NUCLEAR POWER INSTALLATIONS**

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Nuclear power plants use various structural materials that differ in chemical composition. Such materials have different radiation-induced microstructures and mechanical properties that depend on them under different irradiation conditions, neutron fluence and irradiation temperature. The boundaries of test temperature intervals within which a decrease in the ductility characteristics (embrittlement) of these materials is observed are well known and recognized by all materials scientists.

These types of embrittlement are divided according to the temperature of irradiation and testing into low-temperature (at 300-450 °C) radiation embrittlement, medium-temperature (at 450-550 °C) radiation embrittlement or swelling-induced embrittlement and high-temperature (at 550-750 °C) radiation embrittlement. The temperature limits for the existence of these types of embrittlement are very approximate.

The mechanisms of the relationship between microstructure and hardening and embrittlement are, in general, known, but require clarification for specific structural materials and additional research, especially in relation to high-temperature radiation embrittlement.

Low-temperature radiation embrittlement is associated mainly with high concentrations of finely dispersed components of the microstructure, which leads to a decrease in the total average distance between defects and to a corresponding increase in strength and decrease in ductility.

Swelling-induced embrittlement is associated with the ratio of the average total distance between radiation defects inside the grain (pores, particles of second phases, their complexes and dislocation loops or dislocations) and the width of the defect-free zone near grain boundaries. If these parameters are comparable in value (and this occurs at swelling values greater than 5-7%), then a decrease in strength is observed with zero ductility during “quasi-ductile” fracture of the samples.

The relationship between microstructure and these types of embrittlement is confirmed by examples on structural materials irradiated with neutrons at various temperatures in various reactors.

## STRUCTURAL STABILITY OF HIGH-TEMPERATURE ALLOYS: ATOMISTIC MODELING

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The ability of materials to preserve their mechanical properties under exposure to radiation and temperatures above 0.3 of their melting point is determined by the rate of radiation- and temperature-stimulated processes that change their microstructure, for example, recrystallization, second phase precipitation in supersaturated dopant solutions, formation of dislocation loops etc.

The atomistic modeling of these processes in candidate steels requires the interatomic interaction models that (1) ensure high accuracy in the reproduction of energy and power characteristics from ab initio calculations on the micro-level, and (2) are as computationally effective as to allow the modeling to be done on high-performance computers. The state-of-the-art machine-learning potentials satisfy these requirements. Chromium (Cr) is most widely used as a dopant to make steels more heat resistant. In this work, for a Fe-Cr system we constructed a new-generation machine-learning potential of type mMTP (magnetic Moment Tensor Potential). The potential is based on the nonmagnetic MTP version [1] and includes the local magnetic moments on atoms.

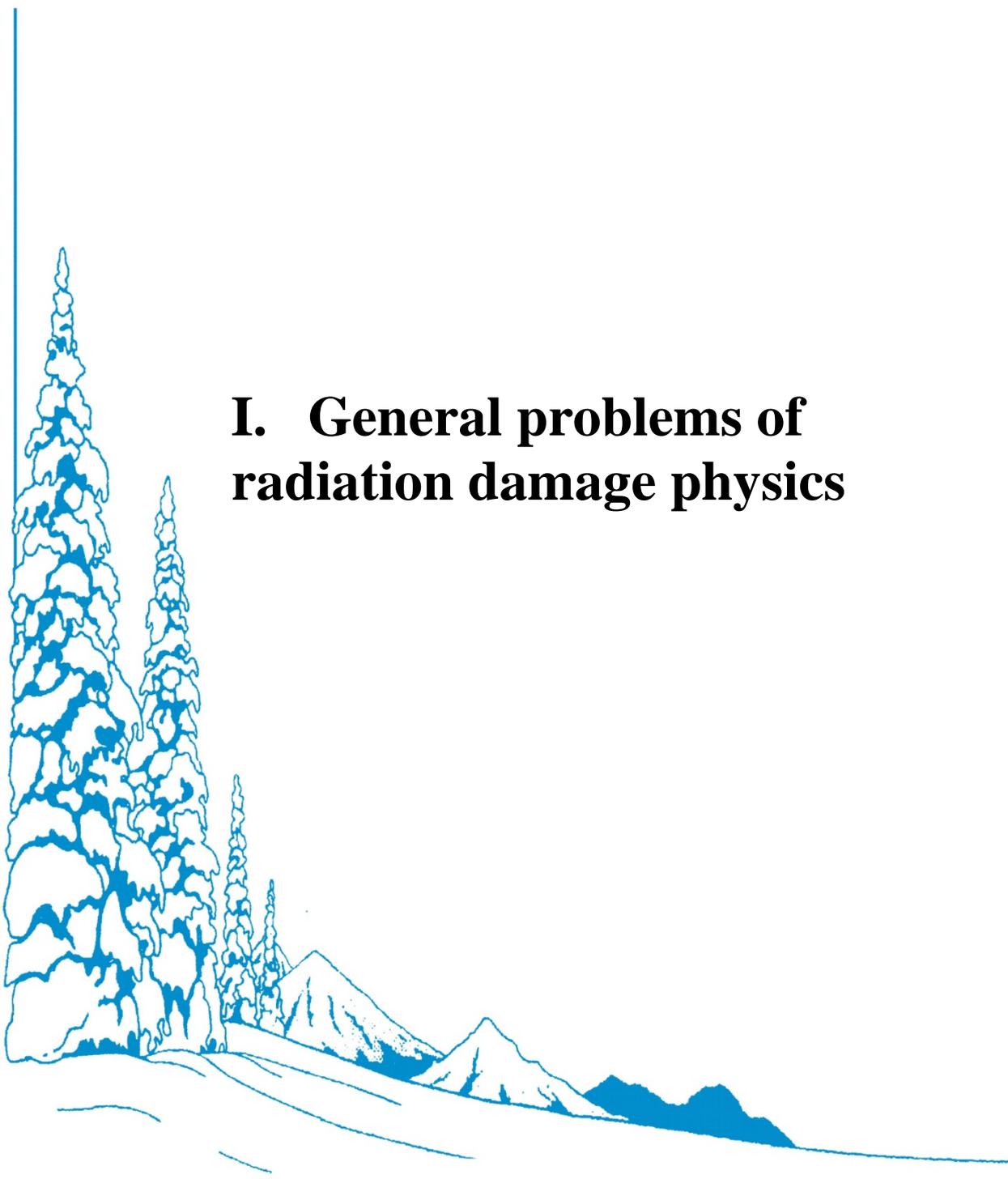
As a model system we used a Fe-Cr-Ni alloy that initially was in its BBC phase and included carbon (C) and phosphorus (P) as impurities. The effect of dopants and impurities on the recrystallization rate at high temperatures (>0.6 of the melting temperature) was studied. The technique used for the direct MD simulation of recrystallization was earlier developed and tested in [2]. Our direct atomistic simulations show that C and P migrating to grain boundaries retard recrystallization, whose rate is quantified from changes that occur with time in the total area of grain boundaries. The crystallization rate is estimated relative to pure iron. The highest retardation effect is observed in the samples, where along with carbon redistribution, chromium (whose initial concentration is higher than its solubility limit) is partly deposited in the form of nanometer precipitates that perform as effective barriers for the moving grain boundaries. Our calculations are done for a representative set of initial microstructures, dopant and impurity concentrations, and temperatures from 0.6 to 0.9 of the melting point.

*The work was done in Midi-science Laboratory 2 “Digital Clones of Industrial Objects and Numerical Materials Science”, National Physics and Mathematics Center.*

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# **I. General problems of radiation damage physics**



## **FRACTURE OF IRRADIATED Zr-2.5Nb ALLOY DAMAGED BY HYDRIDES**

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Zirconium alloys are widely used in the nuclear industry. They are the primary structural material for the cores of thermal water-moderated nuclear reactors. During operation, they interact with the coolant, altering the structure and properties of the structural materials.

The effects of low-temperature, prolonged neutron irradiation of a Zr-2.5Nb zirconium alloy in two structural states (annealed and repeatedly deformed with annealing) in contact with an aqueous coolant were studied.

The study included short-term mechanical tensile tests, fractographic, and structural studies.

It was found that the aqueous coolant causes hydrogenation of the alloy, forming hydrides that cluster into localized surface clusters in the form of "blisters." The most severe hydride damage was observed in the alloy with an annealed structure.

Failure during tensile testing begins with brittle cleavage along the blisters, with the formation of a lath-like relief caused by fracture along the hydride plates. This leads to a change in the loading pattern from plane-stress to wedging rupture.

The degree of degradation of strength properties and embrittlement depends on the degree of hydride damage, the alloy structure, and the damaging fast neutron fluence. The degree of hydride damage was determined by the proportion of brittle fracture based on fractographic studies.

*We express our gratitude to V.L. Panchenko for conducting transmission electron microscopic studies.*

## **INTERMETALLIC AGING OF A Fe-Ni-Al ALLOY DURING ANNEALING AND ELECTRON IRRADIATION**

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Using residual electrical resistivity measurements, the stages of formation of intermetallic nanoparticles, such as Ni<sub>3</sub>Al, and the behavior of vacancy defects in an FCC Fe-Ni-Al alloy containing 33.3 at.% Ni and 10.8 at.% Al were studied during annealing and electron irradiation (5 MeV). It was shown that in a Fe-Ni-Al alloy quenched from 1050 K, isochronous annealing at temperatures above 600 K leads to the formation of coherent particles, which increase the residual electrical resistivity. At temperatures above 700 K, these particles form nanoscale (~4.5 nm) intermetallic precipitates of Ni<sub>3</sub>Al composition, uniformly distributed throughout the alloy matrix. This growth leads to a decrease in residual electrical resistivity. This is due to the coarsening of the precipitates (their coalescence) and a decrease in the Al concentration in the solid solution.

Irradiation at room temperature leads to the accumulation of vacancy defects in the form of

vacancy complexes. Dissociation of these complexes at a temperature of approximately 400 K leads to the formation of freely migrating vacancies and, consequently, enhanced self-diffusion and the formation of coherent Ni<sub>3</sub>Al particles. With further temperature increases, the formation of intermetallic particles continues similarly to that observed during annealing of a quenched alloy. A similar dependence of the electrical resistivity of irradiated Fe-Ni-Ti alloy on the isochronous annealing temperature is known.

## RESISTIVITY RECOVERY, SHORT-RANGE ORDER FORMATION AND DEFECT MIGRATION IN Fe-11Cr AND Fe-16Cr ALLOYS IRRADIATED WITH 5 MEV ELECTRONS

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Data on resistivity recovery (RR,  $R(T) = \Delta\rho(T)/\Delta\rho_0$ , where  $\Delta\rho_0$  and  $\Delta\rho(T)$  are the initial and current residual electrical resistivity (RER) increments after irradiation and subsequent annealing at temperature  $T$ , respectively) in Fe-11Cr and Fe-16Cr alloys after low temperature (<77 K) irradiations are obtained and analyzed. RR is considered as consisted of two components (parts)  $R(T) = R_d(T) + R_{SRO}(T)$ , where  $R_d(T) = \Delta\rho_d(T)/\Delta\rho_0$  is the part induced by the defect contribution,  $\Delta\rho_d(T)$ , to RER while  $R_{SRO}(T) = \Delta\rho_{SRO}(T)/\Delta\rho_0$  is one caused by RER changes,  $\Delta\rho_{SRO}(T)$ , induced by radiation enhanced short-range order formation (SROF), i.e. SROF enhanced by long-range defect migration. RR spectra are also considered as consisted of two parts, i.e.  $dR(T)/dT = dR_d(T)/dT + dR_{SRO}(T)/dT$ . At low temperatures  $R_{SRO}(T) = 0$  and becomes non-vanishing only above the onset of long-range migration of defects.

RR plots of similar alloy samples, irradiated to different initial resistivity increments (i.e. different initial defect concentrations) diverge starting from 172 K (Fig. 1). This divergence is related to behavior of  $R_{SRO}(T)$  which increases in absolute value with the decrease of  $\Delta\rho_0$ . The manifestation of  $R_{SRO}(T) \neq 0$  and related to it the  $R(T)$  plots divergence indicates the onset of defect long-range migration at 172 K and this temperature value corresponds to the low temperature edge of the stage of long-range migration onset of fast Frenkel pair partner.

RR spectra are shown in Fig. 2. Three stage peaks are seen at the same temperatures as those found in the pioneer study [1] – 85-100 K, 180 K и 230 K (upper curves in Fig. 2). The difference in peak amplitudes at 230 K is due to 70 appm of impure N in our alloys. The observed RR spectra structure looks anomalous since the only peak at 230 K corresponds to two processes – the onsets of long-range migration of self-interstitial atoms (SIAs) and vacancies. The analysis has revealed that the stage of vacancy long-range migration onset is negligible in  $dR_d(T)/dT$  and observed only in  $dR_{SRO}(T)/dT$  around 200 K. Because of  $R_{SRO}(T)$  properties it is not traced in  $dR(T)/dT$  at high defect concentration (Fig. 2, upper curves). The appearance of appreciable vacancy stage in  $dR_{SRO}(T)/dT$  at lower defect concentrations looks in  $dR(T)/dT$  as the increase of a stage peak at 180K amplitude and shift of its position towards higher temperatures (Fig. 2, lower curves).

On the contrary, the stage observed around 230 K in  $dR(T)/dT$  (Fig. 2) is not seen in  $dR_{SRO}(T)/dT$ . This fact indicates the lower efficiency of migrating in the stage defects for

enhancement of SROF as compared to that of vacancies and allows interpreting this stage as the stage of long-range migration onset for SIAs.

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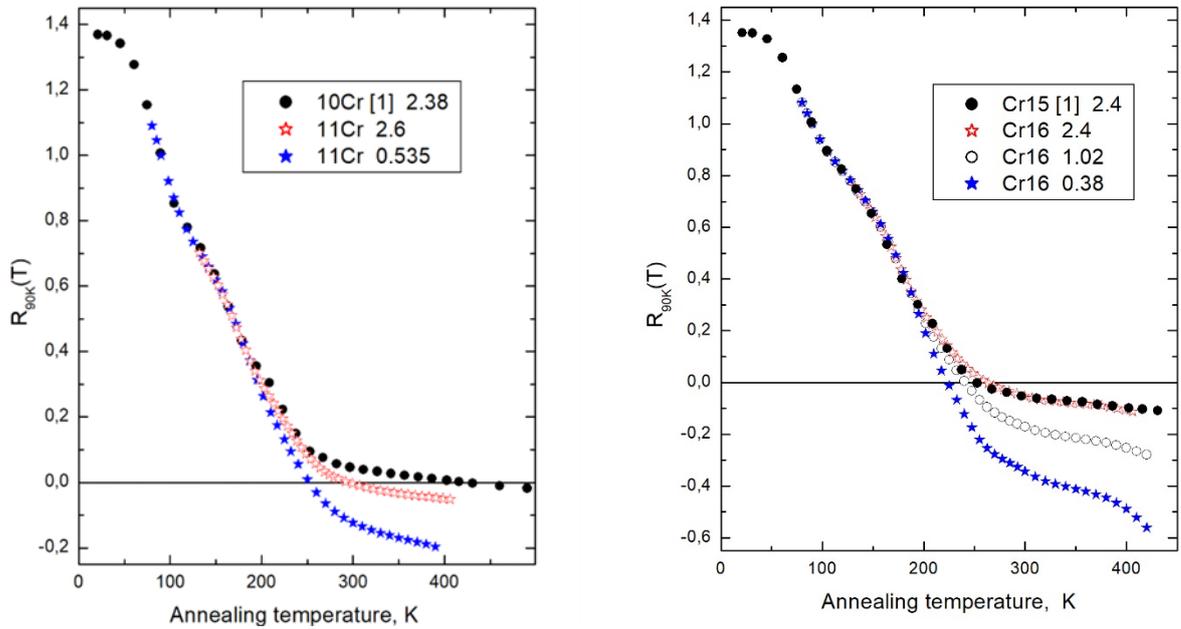


Fig. 1. RR plots of Fe-10Cr [1] and Fe-11Cr (left), Fe-15Cr [1] and Fe-16Cr (right) alloy samples irradiated to different initial resistivity increments. Figures in legends indicate the values of resistivity increments after annealing at 90 K in  $10^{-6} \Omega \text{ cm}$ .

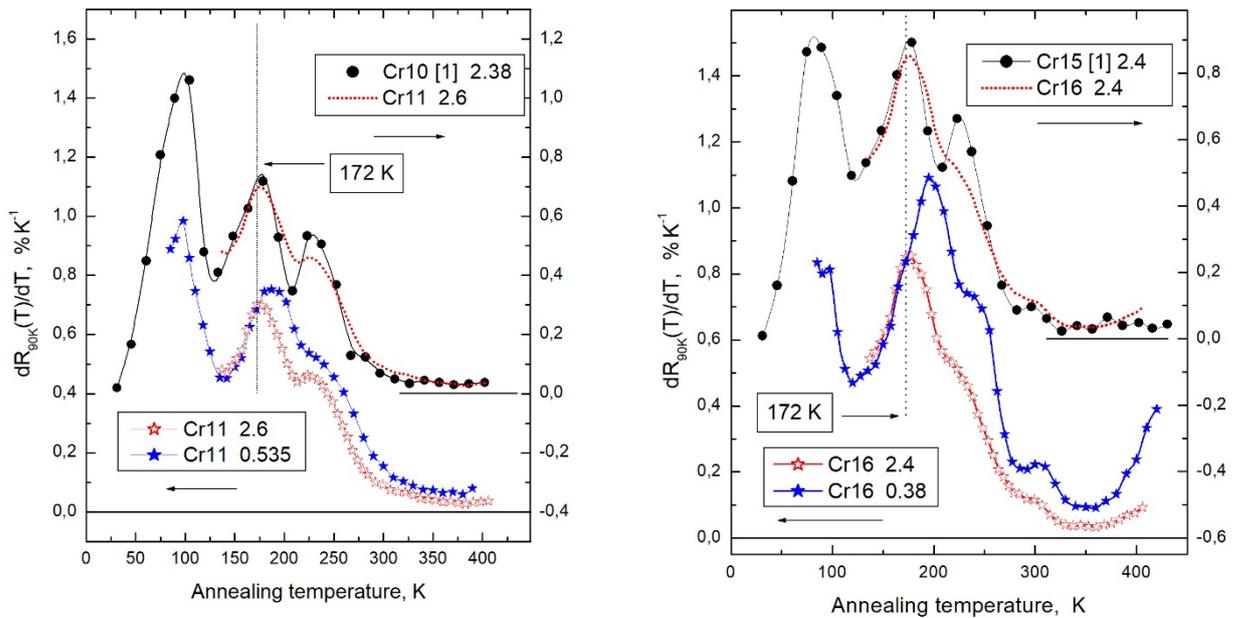


Fig. 2. RR spectra of Fe-10Cr [1] and Fe-11Cr (left), Fe-15Cr [1] and Fe-16Cr (right) alloy samples irradiated to different initial resistivity increments. Vertical line indicates the onset temperature of defect long-range migration.

## STRUCTURE AND PROPERTIES OF AUSTENITIC ALLOYS IRRADIATED WITH HELIUM AT APPM He/DPA > 1000

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In the present work, model austenitic steels EI847 (06C–Fe–16Cr–15Ni–3Mo–1Nb) and EP753 (18Cr–40Ni–5Mo–Mn–Nb) with different initial microstructures were studied. The samples were irradiated with 3 MeV He<sup>2+</sup> ions using the iThemba LABS (South Africa) in order to investigate radiation-induced processes under conditions of excess impurity of He concentration.

Structural examinations and measurements of radiation hardening were carried out within the region of uniform helium distribution. It was shown that irradiation led to a high density of radiation-induced defects in the damaged layer. To reveal the defect substructure, the samples were additionally annealed at 500 °C for 30 min. The microstructure contained dislocation loops with an average size of  $\approx 6$  nm, whose density in both steels increased linearly up to a dose of 0.1 dpa and then reached saturation. The linear dislocation density in EI847 steel was found to be slightly higher than in EP753.

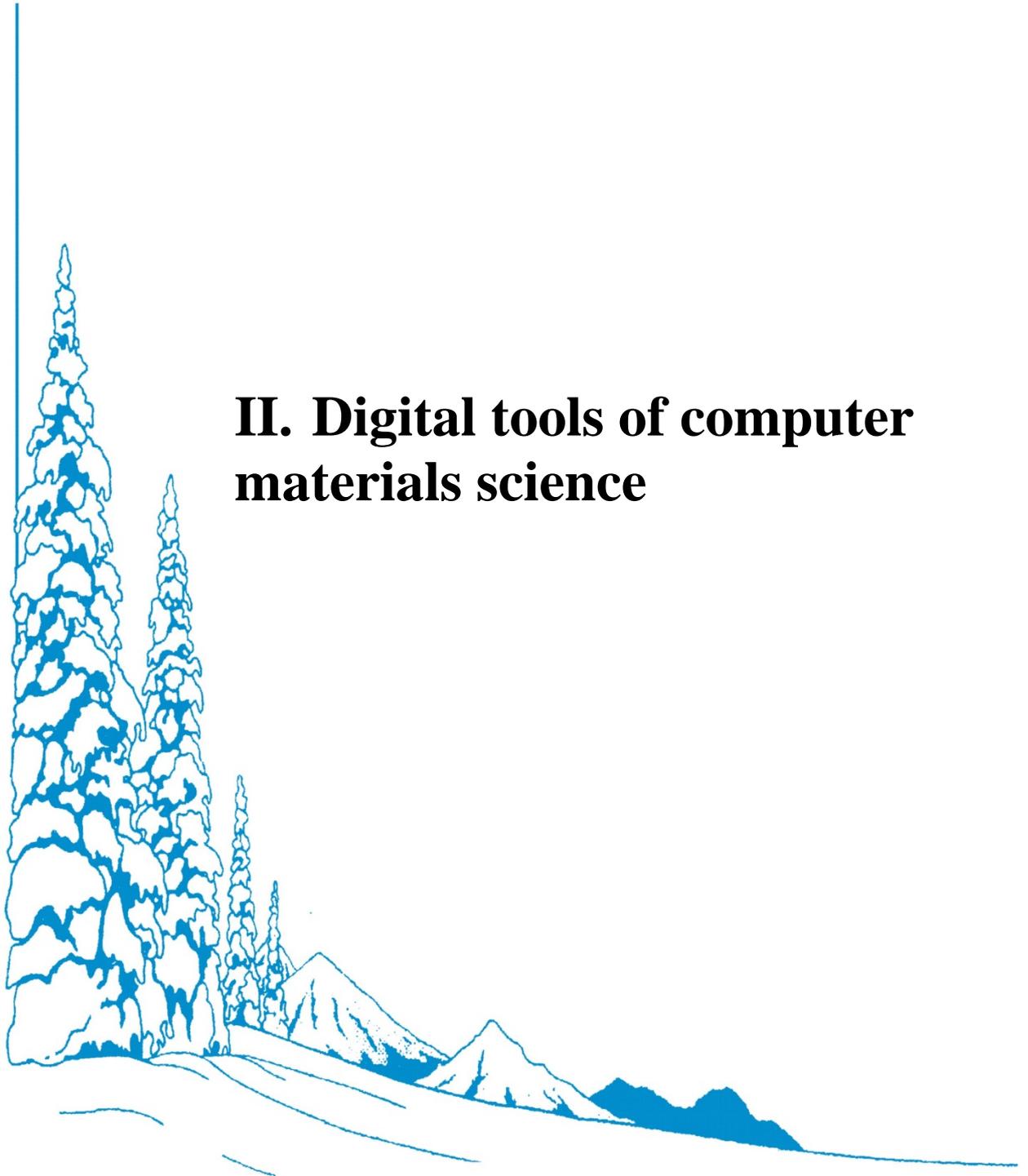
It was noted that the rate of defect accumulation under the given irradiation conditions significantly exceeds that observed for neutron and conventional ion irradiations [2, 3]. Nanoindentation measurements showed consistent behavior: the hardness increased up to a dose of 0.1 dpa and then saturated. The highest radiation hardening was observed in samples with a homogenized initial microstructure. A rough estimate of the strengthening coefficient  $\alpha$ , based on the dispersed barrier hardening (DBH) model, showed good agreement with literature data.

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## **II. Digital tools of computer materials science**





## APPLICATION OF MACHINE LEARNING FOR PREDICTING RADIATION HARDENING VIA STRUCTURAL PARAMETERS IN PRESSURIZED WATER REACTOR PRESSURE VESSEL STEELS

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Development of water-cooled water-moderated nuclear reactors (VVER, PWR) is moving towards improving operational efficiency and safety, and increasing the design service life. One of the necessary conditions for long-term operation is the preservation of the integrity of the reactor pressure vessel (RPV), which is the largest and, consequently, non-replaceable component of the reactor plant, determining its service life.

During long-term operation, under the influence of elevated temperatures (~300°C) and neutron irradiation, the properties of the RPV materials degrade. Operational impacts lead to microstructural changes, resulting in the degradation of the material's mechanical properties – a phenomenon known as radiation embrittlement. One mechanism of radiation embrittlement is a strengthening mechanism related to radiation hardening of the material, caused by the formation of radiation defects and radiation-induced solute atom clusters. The formation and growth of the density of radiation-induced clusters make a determining contribution to hardening and, consequently, to radiation embrittlement via the strengthening mechanism. Therefore, microstructural studies of cluster parameters make it possible to determine the value of radiation hardening with greater accuracy using the computational-experimental method. At the same time, long-term forecasting of radiation-induced structural changes is needed to increase the design service life of the reactor plant.

Radiation-induced clusters are characterized by sizes of 3–5 nm and densities of 10<sup>23</sup>–10<sup>24</sup> m<sup>-3</sup>, making atom probe tomography (APT) the most preferred and widely used investigation method. To date, the world has accumulated a large volume of results of APT studies of clusters in RPV steels of various chemical compositions in the range of Cu=(0.02–0.5) wt.%, Ni=(0.2–5.5) wt.%, Mn=(0.2–2.0) wt.% irradiated in power and research reactors with different fast neutron fluxes and fluences. Establishing patterns in such a wide range of data is a challenging task, making the use of machine learning methods a promising approach.

In this work, based on accumulated in-house and literature APT data on radiation-induced clusters in RPV steels, a machine learning regression model was developed. The architecture of the obtained model is based on the Cubist model architecture: the model combines decision trees and linear models by training a generalized linear model at each node of the tree. Additionally, the model performs linear smoothing, allowing it to consider not only the model trained at the leaf of the tree for prediction but also models located on the path from the leaf to the root. Using the chemical composition and irradiation conditions of the steels, the model predicted the parameters of radiation-induced clusters. Using the predicted cluster parameters in a barrier strengthening model, the dose dependencies of radiation hardening for VVER steels were obtained. These dependencies showed good agreement with experimental radiation hardening data that was not used during the model training.

# CALCULATION OF PHASE PRECIPITATION CHARACTERISTICS USING CALPHAD METHOD IN THE MODELING OF RADIATION-ENHANCED DIFFUSION IN MULTICOMPONENT SYSTEMS

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The kinetics of formation and growth of secondary phases in multicomponent systems under radiation exposure is considered using CALPHAD thermodynamic modeling with the Thermo-Calc software package [1]. The objects of the study are multicomponent systems based on pearlitic steel 15Kh2NMFA, ferritic-martensitic steel EP823, and austenitic steel EK164. The calculations accounted for the effects of radiation-enhanced diffusion, interstitial clusters, and ballistic mixing. Empirical parameters for the Thermo-Calc calculations (interphase boundary energy and additional Gibbs energy for the phases) were selected based on experimental data on the dependence of precipitation characteristics on irradiation dose for steels 15Kh2MFA, HT9, and HCM12A.

The obtained values of the volume concentration and average size of secondary-phase precipitates are consistent with published experimental data for the systems under consideration. It is shown that different types of irradiation (for example, ion and neutron irradiation) lead to different ratios between the number of ballistic and diffusive jumps. This has a strong impact on the dose dependence of the volume concentration and average precipitate size for different irradiation types.

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# ION-BEAM MODIFICATION OF ULTRATHIN BURIED OXIDES LAYERS

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Multilayer nanoscale systems incorporating buried ultrathin tunnel junctions, 2D materials, and solid electrolytes are crucial for next-generation logics, memory, quantum and neuro-inspired computing. Still, an ultrathin layer control at atomic scale is challenging for cutting-edge applications. In recent article [1] the scalable approach was introduced utilizing focused ion-beam irradiation for buried ultrathin layers engineering with angstrom-scale thickness control. It was experimentally demonstrated its performance on Josephson junction tuning in the resistance range of 2 to 37% with a standard deviation of 0.86% across 25×25 mm chip. Moreover, we showcase ±17 MHz frequency control (±0.172 Å tunnel barrier thickness) for superconducting transmon qubits with coherence times up to 500 μs, which is promising for useful fault-tolerant quantum computing. This work ensures ultrathin multilayer nanosystems engineering at the ultimate scale by depth-controlled crystal defects generation.

In this work, the mechanism of ion-beam modification of ultrathin buried oxides is discussed. Our molecular dynamics simulations of Ne<sup>+</sup> irradiation on Al/a-AlO<sub>x</sub>/Al structure confirms the pivotal role of ion generated crystal defects.

**Literature**

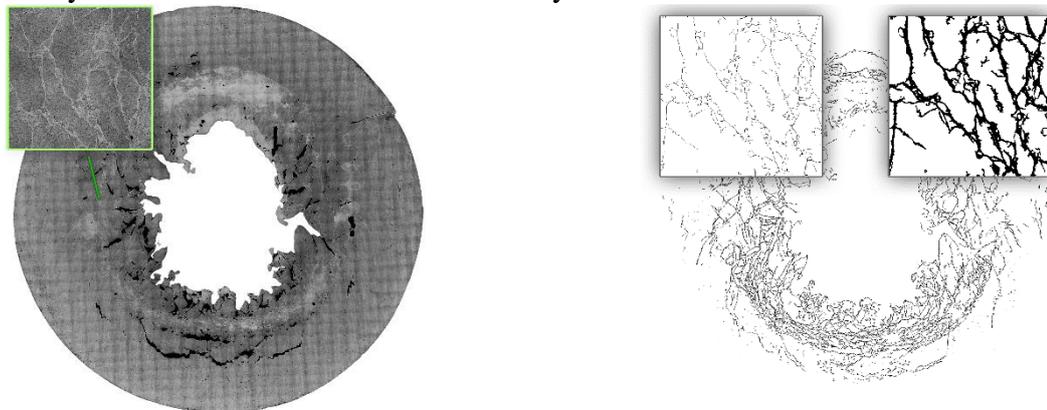
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**LOCALIZATION OF DEFORMATION IN U-Mo-Zr ALLOY UNDER SPHERICAL SYMMETRICAL EXPLOSIVE LOADING**

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A metallographic study of a shell recovered after explosive loading was conducted. The shell was made of uranium alloyed with molybdenum and zirconium. A sophisticated system of localized deformation was found in the meridional section of the shell [1].

A method to obtain quantitative characteristics of the revealed system of localized deformation was proposed and implemented to qualitatively describe the structure which used machine vision learning algorithms for semantic segmentation of images, integrated in advanced free software [2 — 5]. Statistic data on deformation localization in the shell section by segmented system skeleton was obtained and analyzed.



Meridional section of the shell recovered after explosive loading with a revealed system of localized deformation [1]

	Average	RMS	Median	Maximum
Average length of branches, μm	16.8	17.3	13.2	148.7
Maximum length of branches, μm	68.0	98.7	26.9	976.2
Largest shortest path, mm	0.38	1.22	0.029	23.9
Number of branches, pcs.	29.9	210.8	3	6756

The authors wish to thank Nina Iosifovna Taluts, Dr.Sc. (Phys.-Math.) from M.N. Mikheev Institute of Metal Physics, UB RAS, for fruitful discussions of metallographic analysis of the microstructure.

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## MOLECULAR DYNAMICS SIMULATION OF THE INFLUENCE OF CARBON ON THE STRENGTH OF FERRITIC STEELS

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The static strength properties of structural materials play an important role in analyzing the response of structures to various loads. Mechanical and engineering characteristics such as yield strength, ultimate tensile strength, and ductility are largely determined, unlike, for example, elastic moduli, by their microstructure (various defects present in the materials).

From the perspective of quantitative atomic-scale description of the mechanisms of elastic-plastic deformation, widely used in industry, ferritic and ferrite-martensitic steels are of practical interest. One of the factors that determines the mechanical properties of ferritic steels is carbon, specifically its amount and distribution within the material. At low concentrations, typical for steels, carbon is an interstitial impurity. It has sufficient mobility within the BCC (body-centered cubic) lattice of ferritic steels to model its dynamics through direct atomic-scale calculations.

Modeling the static strength properties of real materials is a non-trivial task because the typical time scales accessible for direct modeling within Classical Molecular Dynamics (CMD) do not exceed hundreds of nanoseconds in a reasonable timeframe. In this work, the CMD modeling method proposed and developed in [1–3] is used to determine the static strength characteristics of steels. The method is based on atomistic modeling of the relaxation of shear stress in specially constructed CMD samples with specific geometry and embedded dislocations. This allows for the evaluation of the stress at which dislocation motion stops, i.e., estimating the Peierls stress, and calculating the quasi-static yield point. The capabilities of the method, as well as its validation against extensive experimental data, have been demonstrated for various materials, such as pure metals [1], FCC alloys Pu-Ga [2–3], and austenitic Fe-Ni-Cr steels [4].

This work demonstrates the application of this stress limit calculation method using CMD modeling for ferritic steels, taking into account the real carbon content and distribution. The dynamics and influence of carbon on strength are considered. The study also touches on modeling secondary phase precipitation, which closely approximates the morphology observed in experiments.

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## TITANIUM-VANADIUM HYDRIDES STRUCTURE: ATOMISTIC SIMULATION BY MACHINE-LEARNING POTENTIALS

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Hydrogen embrittlement of structural materials, including under conditions of radiation exposure, represents a significant problem, primarily caused by the extremely high mobility of hydrogen atoms in the metal. Furthermore, titanium and its alloys with vanadium are considered promising materials for hydrogen storage. However, at present, fundamental knowledge about the physical properties of the Ti-V-H system is fragmented and limited to data on the phase diagram [1] at room temperature, as well as first-principles calculations at zero temperature within the framework of density functional theory (DFT) [2].

In this regard, this work performed molecular dynamics simulations for various crystalline phases of the  $Ti_{1-x}V_xH_y$  system. To achieve accuracy comparable to *ab initio* calculations, we propose an approach based on the use of machine learning interatomic potentials trained on DFT energies and forces. We use the Moment Tensor Potential (MTP) model for training Ti-V-H interatomic potential. Structures with hydrogen content ( $y < 1.0$ ) and Ti-V crystal lattices of the hcp ( $\alpha$ ) and the bcc ( $\beta$ ) cells were considered. The  $\delta$ -phase  $Ti_{1-x}V_xH_2$  was also considered for various vanadium contents. This phase has a fluorite-type crystal structure with the *Fm3m* space group, where metal atoms are arranged in a face-centered cubic (fcc) lattice, and hydrogen occupies tetrahedral interstitial sites. The potential was trained with a root-mean-square error compared to the training dataset for potential energy at the level of  $\sim 2.6$  meV/atom and 156 meV/Å for the forces acting on the atoms.

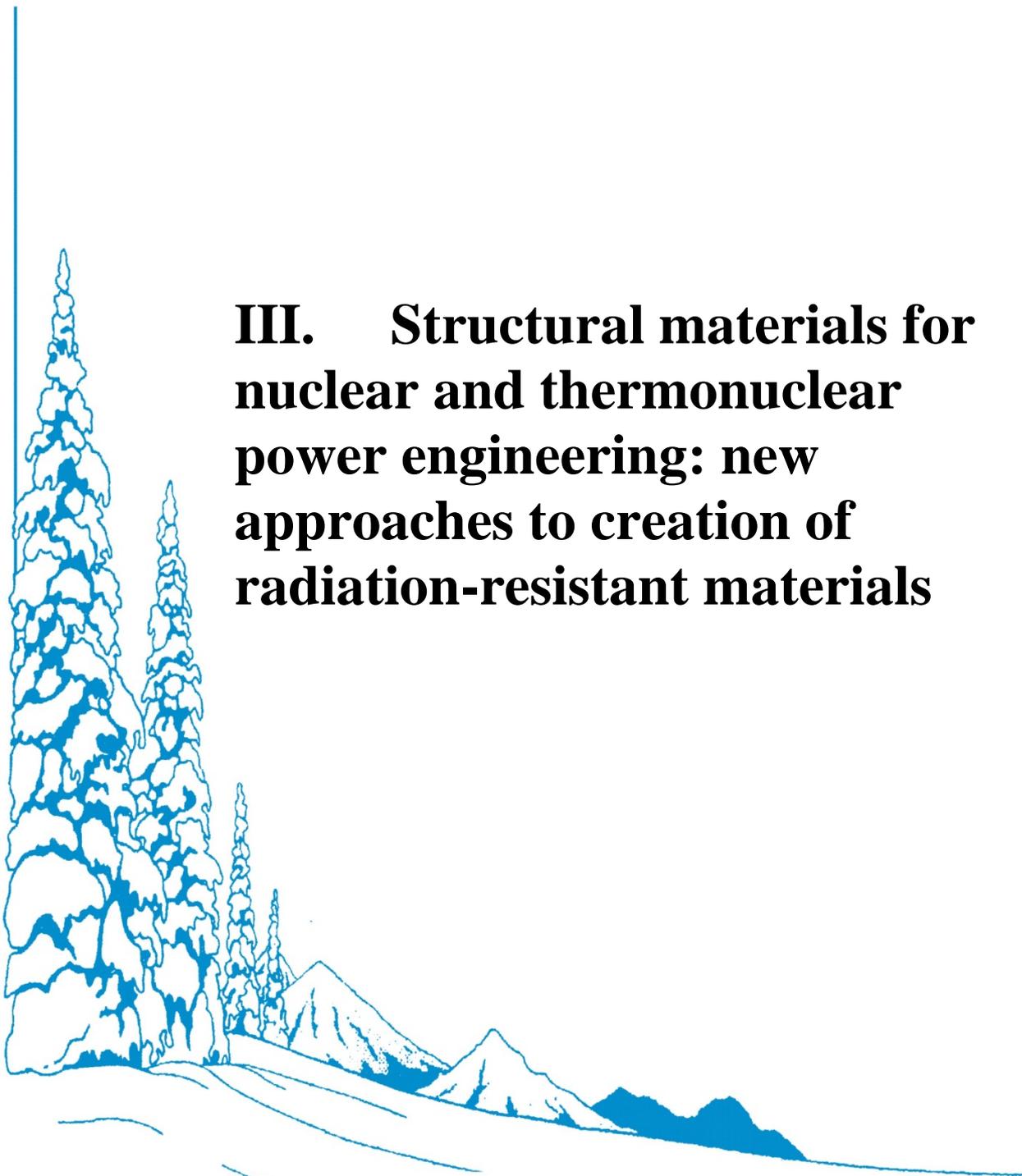
Using the constructed interatomic interaction potential, the values of the hydrogen diffusion coefficient in various phases were calculated for temperatures of 500-1000 K, from which the activation energy values for different vanadium contents in the alloy were obtained. The calculation of elastic moduli at finite temperatures was also performed.

*This work has received funding from the Russian Science Foundation (Project No. 25-22-20062).*

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### **III. Structural materials for nuclear and thermonuclear power engineering: new approaches to creation of radiation-resistant materials**



## DETERMINATION OF SAFE DRY STORAGE MODES FOR VVER-1000 FUEL ELEMENTS CONSIDERING STRUCTURAL CHANGES

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Currently, accumulation of spent nuclear fuel (SNF) at nuclear power plants (NPPs) significantly exceeds capacity for its radiochemical processing. As a result, significant portion of discharged fuel assemblies is sent to temporary storage sites. However, due to limited capacity of wet storage facilities and high capital costs, methods of dry fuel storage are being actively developed. This method of SNF storage is widely used abroad, having demonstrated its long-term safety and commercial advantages over wet storage, allowing SNF to be stored until transition to the closed nuclear fuel cycle or final disposal. Consequently, dry storage technology of SNF is included in projects of newly constructed foreign VVER-1000 units. Thus, implementation of dry storage for domestic reactors is necessary condition for maintaining competitiveness in the global nuclear energy market and is strategically important for transition to the closed nuclear fuel cycle.

At present, the thermomechanical code RTOP-SH (reactor fuel — dry storage) has been developed for improved assessment describing behavior of fuel elements during dry storage, verified with results of experiments simulating dry storage conditions conducted at NRC “Kurchatov Institute”.

This report presents experimental data on changes in structure and properties of E110 fuel cladding after operation in VVER-1000 reactor up to burnups of 64 MW·day/kg U and thermomechanical tests (TMT) simulating technological stages (drying and transportation) and subsequent dry storage over wide range of variable parameters. The most significant factors affecting reduction of mechanical properties of E110 alloy under such conditions have been identified. Comparative analysis was conducted between E110 alloy and materials of fuel claddings of foreign reactors, showing that domestic E110 alloy retains its plastic properties under expected operating and storage conditions, including emergency situations.

## EFFECT OF INITIAL NANOSTRUCTURE ON RADIATION RESISTANCE OF ODS STEELS AFTER ACCELERATED TESTS

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Oxide dispersion-strengthened (ODS) steels outperform conventional ferritic-martensitic steels in high-temperature strength due to the presence of a high density of uniformly distributed nanoscale oxide particles. These materials are being actively developed and are considered highly promising for applications in nuclear power engineering, including first-wall structures of fusion reactors, fuel cladding for fast-neutron reactors, and other critical components of Generation IV reactors [1, 2].

The operational potential of ODS steels includes service temperatures up to 750 °C and

resistance to radiation-induced swelling up to 200 displacements per atom (dpa) [3]. Their mechanical properties are largely determined by the nanostructure, specifically the size and spatial distribution of the dispersed inclusions. These characteristics, in turn, directly depend on the alloying element composition and the regimes of thermomechanical processing. Quantitative analysis of the oxide inclusions requires the combined use of microscopy techniques such as transmission electron microscopy (TEM) and atom probe tomography (APT).

Given that the superior performance properties of ODS steels are directly linked to the stability of the oxide nanoparticles and clusters in matrix, particular attention is devoted to studying the evolution of their nanostructure under irradiation conditions [3, 4].

The aim of the present work is a systematic and comprehensive study of radiation-induced changes in ODS steels of various classes (9Cr ODS, 10Cr ODS, 13Cr ODS, EP450 ODS, EP823 ODS) that exhibit significant differences in their initial microstructure. The investigation was carried out after simulated irradiation to a dose of 30 dpa at a temperature of 350 °C, which corresponds to the low-temperature radiation embrittlement range.

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## **EFFECT OF NEUTRON IRRADIATION ON MICROSTRESSES IN Cr16-Ni19 AND Cr16-Ni15 TYPE AUSTENITIC STEEL**

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Austenitic steels of the Cr16-Ni19 and Cr16-Ni15 types are used as fuel cladding for fast neutron reactors. The main factors limiting the use of this class of steel are: their susceptibility to corrosion damage, radiation creep, reduced strength, embrittlement, and radiation swelling [1]. Changes in the physical and mechanical properties of the material, and distortion of the shapes and sizes of fuel elements under the influence of irradiation affect the safety of the reactor.

The structural factors that inhibit swelling are [2]: increased stability of the solid solution and stability of the dislocation structure, obtained by cold deformation of ~ 20% at the final stage of processing of shell tubes.

The dislocation structure formed during cold deformation is the main reason for the occurrence of microstresses in the material, causing microdeformation of the crystal lattice. Under irradiation, the dislocation structure is transformed and radiation defects of the crystal structure are formed [3], such as clusters, dislocation loops and pores, as a result of which the level of microstresses changes.

The change in the structure's state under irradiation depends on both the irradiation temperature and the rate of accumulation of the damaging dose, as well as the initial degree of cold deformation. Separating the contributions of irradiation and the initial state is possible by tracking the change in microstresses after fuel rod cladding operation.

Microstresses are assessed using X-ray diffraction based on the broadening and position of diffraction maxima.

This paper presents the results of X-ray structural studies of the effect of neutron irradiation in a fast-neutron reactor on the microstresses in fuel rod cladding. A regression method was used to evaluate the contribution of various factors, such as irradiation temperature and damaging radiation dose, to the microstresses in pipes made of Cr16-Ni19 and Cr16-Ni15 steels.

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## **FEATURES OF THE INFLUENCE OF PROTECTIVE CHROMIUM COATING ON THE HYDROGEN AND RADIATION RESISTANCE OF ZIRCONIUM E110 ALLOY**

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There are numerous studies aimed at determining the mechanisms of defect formation in zirconium alloys due to hydrogen impact, as well as the evolution of the defect structure in structural materials of modern nuclear power under the influence of radiation exposure. However, there is a notable lack of work focused on investigating the synergistic effects of these factors. This is partly due to the necessity of a whole range of expensive experimental equipment, but the main reason lies in the high complexity of conducting such research because of the induced radioactivity in materials after neutron irradiation. One solution to this problem is irradiation with other high-energy particles, as employed in this work—krypton (Kr) ions with an energy of 145 MeV, which are products of uranium decay.

The authors of the work conducted comprehensive studies aimed at investigating the specific changes in the structural and phase composition of E110 alloy with a Cr-coating under high-temperature hydrogenation and irradiation with Kr ions. The mechanisms of formation and evolution of the defect structure in the studied material were also determined. It was established that as a result of hydrogenation, the sample without a Cr-coating forms phases of two hydrides: ZrH<sub>2</sub> and ZrH. The sample with a Cr-coating transforms into ZrH<sub>2</sub>. Furthermore, the Cr-coating reduces the thickness of the Kr radiation damage zone by 15–20% and decreases the density of radiation-induced defects compared to the E110 alloy without the protective coating. It is worth noting that the samples with a Cr-coating are characterized by a more uniform distribution of hydrogen. According to first-principles calculations and positron annihilation spectroscopy data, dislocations not containing hydrogen predominate in the Cr-coated E110 alloy after hydrogenation and irradiation. These results confirm the effectiveness of

depositing Cr coatings on zirconium alloys to reduce the degree of radiation damage and enhance the hydrogen resistance of materials in modern nuclear power.

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## **HYDRIDE MEMORY EFFECT IN FUEL CLADDING MADE OF E110 ALLOY DURING DRY STORAGE OF SPENT FUEL ASSEMBLIES**

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At present the nuclear industry in developed countries faces the challenge of long-term operation and subsequent disposal of spent fuel assemblies. The expansion of nuclear power plant capacity worldwide, and in Russia particularly, coupled with the lack of cost-effective spent fuel assemblies reprocessing technology, requires an increase in the number of storage facilities, which significantly increases operating costs and the final cost of nuclear energy, making it less competitive. One solution to this problem is the development of dry storage technology, which significantly reduces the capital and operating costs of spent fuel assembly storage.

During operation of VVER-1000 nuclear reactors, fuel rod cladding made of E110 alloy is exposed to coolant at operating temperatures, leading to hydrogen accumulation due to an oxidative reaction. The amount of hydrogen accumulated in the material during operation can be a determining factor in justifying the safety of dry storage of spent fuel assemblies. For example, the formation of a radially oriented hydride structure leads to a significant reduction in mechanical properties. Various studies have shown that the formation of the hydride structure is influenced by many factors, one of them is the hydride memory effect, which consists of the preferential formation of hydrides at sites of their previous dissolution. This is due to the presence of dislocation defects formed during stress relaxation during hydride precipitation due to the difference in the specific volumes of the Zr-matrix and zirconium hydride. The study of the influence of the memory effect on the behavior of hydrides has been widely carried out in foreign zirconium alloys; however, these effects for domestic alloys, in which the hydrogen content in the fuel element cladding after normal operation is significantly lower, have not been sufficiently studied.

This paper presents microstructural studies, as well as differential scanning calorimetry (DSC) studies of unirradiated E110 alloy fuel claddings after hydrogenation to hydrogen concentrations of 75, 115, and 200 wppm. The temperature dependence of hydride dissolution on the hydrogen content in the fuel cladding was determined using in-situ TEM with electron energy loss spectroscopy, and the data were compared with the results of similar DSC studies. The annealing temperatures for dislocation structures remaining at hydride dissolution sites, at which memory effect suppression is observed, were determined. Annealing of varying durations were performed directly in the transmission electron microscope column to assess the possibility of memory effect suppression at various temperatures, up to the maximum permissible temperature in the event of emergency situations under dry storage conditions.

## MICROSTRUCTURE AND DEFECTS IN FUNCTIONALLY GRADED NB/ZR NANOLAMINATES AFTER HELIUM ION IRRADIATION

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Helium accumulation is a critical factor in material degradation in fusion reactors. Functionally graded nanolaminates (FGN) Nb/Zr with a high density of interfaces are considered promising materials for protecting components made of E110 alloy due to their potential to effectively absorb radiation-induced defects and helium atoms, thereby suppressing bubble formation and embrittlement [1]. The aim of this work is to experimentally study the microstructural stability and defect structure in gradient Nb/Zr nanolaminates upon helium ion implantation. The coating architecture consisted of an adhesive Zr layer (~8 μm), a nanolaminate of alternating Zr and Nb layers (individual layer thickness ~60-80 nm, total ~1.4 μm), and a corrosion-resistant Nb layer (~3.2 μm). The FGN Nb/Zr were deposited onto an E110 alloy substrate by magnetron sputtering. Irradiation was performed with helium ions at an energy of 2 MeV and room temperature to fluences of  $3.4 \times 10^{14}$  ions/cm<sup>2</sup>.

Microstructure was analyzed by transmission electron microscopy (TEM) and X-ray diffraction (XRD). To study the defect structure, positron annihilation spectroscopy (PAS) was employed, including variable-energy Doppler broadening spectroscopy (DBS) for the near-surface layer (~1 μm) and positron annihilation lifetime spectroscopy (PALS) measurements for bulk analysis (~150 μm). TEM analysis showed complete preservation of the layered coating architecture after irradiation across the entire fluence range. No phase transformations were observed. A trend towards a slight reduction in internal stresses and smoothing of the layer relief was noted at the maximum fluence. High-resolution TEM recorded a minor decrease in the interplanar distance in the Zr nanolayer at the interface with Nb ( $d_{Zr}(100) = 0.269$  nm) after maximum irradiation, while the Nb lattice parameters remained unchanged. Diffractograms revealed no formation of new phases or significant changes in the lattice parameters of  $\alpha$ -Zr ( $a = 3.22$  Å,  $c = 5.11$  Å) and  $\beta$ -Nb ( $a = 3.30$  Å). PAS data indicate an extremely low level of radiation defect accumulation. PALS spectra of all samples contained three characteristic components:  $\tau_F = 163 \pm 1$  ps (delocalized positrons in Zr),  $\tau_A = 182 \pm 1$  ps (dislocations or incoherent interfaces), and  $\tau_B = 514 \pm 2$  ps (large vacancy complexes). Increasing the fluence to  $6 \times 10^{14}$  ions/cm<sup>2</sup>

changes in the average positron lifetime. The only statistically noticeable effect was a slight increase in the intensity of the long-lived component  $I_B$  from  $(2.5 \pm 0.2)\%$  to  $(4.2 \pm 0.4)\%$ , indicating very limited formation of nanoscale vacancy clusters, possibly containing helium. This is consistent with the coincidence Doppler broadening spectroscopy (CDBS) data: at the maximum fluence, the S parameter increased slightly from 0.6006 to 0.6018, while the W parameter decreased from 0.01022 to 0.01008. Such minor changes confirm the absence of large-scale defect accumulation and the constancy of the chemical environment at the annihilation sites, which remained typical for zirconium.

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## MODIFICATION OF THE STRUCTURE AND CREEP CHARACTERISTICS OF EP 823 FERRITIC-MARTENSITIC STEEL, INCLUDING ODS MODIFICATION

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Nowadays, EP 823 ferrite-martensitic steel is one of the promising materials for nuclear power plants with lead-bismuth coolant. The goal of the current study was investigation of structural phase stability in terms of long-lasting creep and long-term strength testing of the EP 823 steel.

In the work, long-term creep strength tests of EP 823-ESR (electroslag remelting EP 823) steel microsamples were carried out after processing according to VSQ and ATON modes at temperatures of 500–600 °C and loads of 100–300 MPa. Higher efficiency of ATON processing is shown. In particular, at 600 °C and load of 200 MPa, EP 823 ATON steel samples withstand more than 1200 hours without rupture, while EP 823 VSQ samples can withstand only about 30 hours. Electron microscopic studies of the structure of various EP 823-ESR reactor steel samples were performed (tubes Ø 9.7×0.5 mm after VSQ heat treatment; tubes Ø 9.7×0.5 mm after ATON heat treatment; tubes Ø 10.5×0.5 mm after ATON heat treatment; tubes Ø 12.2×0.5 mm after quenching and high tempering at 700–720 °C). All of the studied samples contain a small number of ferritic grains and mainly consist of high-temper lath martensite, which has undergone a return, partial polygonization and retained an increased density of dislocations. Me<sub>23</sub>C<sub>6</sub> carbides with a size of 50–200 nm are located along the boundaries of the martensitic laths, and dispersed carbides of the VC type with a size of ~ 5 nm are located in the crystal volume. High temperature creep tests cause additional development of return processes, polygonization and partial recrystallization in martensitic laths.

The creep characteristics and structural changes of transverse samples made of Ø 6.9×0.4 mm fuel rods of reactor steels EP 823-ESR, EP 823 and EP 823-ODS (oxide dispersion strengthened EP 823) at loads of 60–100 MPa and temperatures of 650 °C and 670 °C were determined. At 650 °C and load of 100 MPa, EP 823-ESR steel withstood 1882 hours, while EP 823 steel withstood only 258 hours. At a temperature of 670 °C and load of 100 MPa, the rupture time of EP 823-ESR and EP 823 steels is 371 hours and 74 hours, respectively. This indicates the advantage (in terms of creep resistance) of electroslag remelting steel EP 823-Sh. It is shown that the EP 823-ODS steel samples containing strengthening Y-Ti oxides (cut from the plate) have the highest long-term strength at 650 °C and 670 °C. The samples of the same steel made from the presented tubes (fuel-element claddings) have significantly lower long-term strength. The structure and high-temperature creep resistance of EP 823 steel samples, including ODS modification, were analyzed in comparison with other Russian BCC steels (EP 900, EK 181, ChS 139, EP 450, EP 450-ODS). Among the "oxide-free" steels, EP 823 steel has the lowest resistance to high-temperature creep.

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## RADIATION DEFECTS AND DEUTERIUM RETENTION IN STRUCTURAL MATERIALS FOR NUCLEAR AND THERMONUCLEAR ENERGY

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The energy crisis and the enormous potential of thermonuclear energy encourage us to make great efforts to develop thermonuclear fusion. The final application of thermonuclear energy mainly depends on the development of key materials for a thermonuclear reactor. On the other hand, materials for advanced nuclear and hybrid fission-fusion reactors are also being developed. Due to the high melting point, good thermal conductivity, low erosion, low permeability and accumulation of hydrogen isotopes, tungsten-based materials are reference materials in contact with plasma. Ferritic-martensitic steels with low activation, RAFM, such as Eurofer, and oxide dispersion hardening (ODS) steels with the addition of Y<sub>2</sub>O<sub>3</sub> particles are promising structural materials for thermonuclear reactors, as fuel cell shells in fast neutron reactors, and for a number of designs of generation IV reactors. However, the stability of the properties of these materials under both neutron and deuterium irradiation has been poorly studied, especially at high temperatures. The stability of material properties under neutron irradiation and hydrogen embrittlement in nuclear, thermonuclear and hybrid reactors are important factors that determine the applicability of the material and can lead to a reduction in the life-time of reactor components. In addition, for reasons of safety, cost and recycling, the total tritium retention in materials should not exceed an acceptable level. Thus, it is necessary to be able to predict the amount of radioactive tritium retained in materials and develop procedures for its removal. For this reason, the stability of the structure and properties of materials under irradiation and the retention of deuterium (D) in radiation defects in promising materials are investigated in this work. To simulate radiation defects, the materials were irradiated with Fe<sup>2+</sup> ions with an energy of 5.6 MeV in the temperature range of 250-500°C and dose range of 3-50 dpa. Radiation defects were investigated using transmission electron microscopy, energy dispersive X-ray spectrometry, and atomic probe tomography. To decorate radiation-induced defects, low energy D was implanted into damaged materials. The retention of D was studied by thermal desorption spectroscopy (TDS). It was found that (i) radiation-induced defects in the W-Cr-Y alloy are mainly vacancy-type defects, and (ii) radiation-induced Cr clusters suppress the formation of both vacancy and dislocation-type defects in the W-Cr-Y alloy. On the contrary, the formation of radiation-induced Cr-Mn clusters in Eurofer only slightly influence the development of dislocation loops. Both the hardening of the material and the accumulation of D in radiation defects correlate with the formation of (i) vacancy clusters in W, (ii) Cr clusters in W-Cr-Y alloy, and (iii) dislocation loops, Cr-Mn clusters, and vacancy clusters in Eurofer. It has been shown that certain alloying elements inhibit the development of pores and, consequently, the accumulation of deuterium during irradiation. The binding energies of deuterium with various types of radiation defects in promising materials were calculated.

## RADIATION-INDUCED PHASE FORMATION IN STRUCTURAL MATERIALS OF LIGHT-WATER REACTORS

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The key role in addressing current challenges of nuclear energy lies with structural materials that must endure increasingly severe loads both during the extended operation of existing reactors and to meet stricter requirements for new designs. Long-term exposure within a reactor environment which combines intense neutron fluxes, high temperatures, and stresses significantly impacts material degradation at microstructural levels and the mechanical properties of structural materials as a result. This can potentially lead to unacceptable premature failure of critical components.

For light-water reactors, crucial elements with limited replacement options due to technical complexity and prohibitive costs include the reactor pressure vessel (RPV) and components of reactor vessel internals (RVI). The structural materials used for RPVs are low-alloy pearlitic steels with tempered bainitic structure and bcc lattice, while RVIs employ austenitic stainless steels with fcc.

Neutron irradiation continuously generates excess concentrations of point defects – vacancies and interstitial atoms. These point defects migrate towards various sinks, carrying dissolved atoms along their paths. This process underlies a wide variety of interrelated phenomena specific to irradiated materials, leading to microstructural changes and chemical element redistribution and ultimately affecting properties of reactor-grade materials during operation.

Therefore, to substantiate the performance of RPV and RVI materials, in addition to mechanical characteristics, a deep understanding of radiation damage processes and reliable quantitative information on microstructural changes are required. Despite significant differences in the composition, type, structure, and operating conditions of RPV and RVI steel, a common consequence of irradiation for them is the formation of nanoscale precipitates with typical average sizes (2–5) nm and number densities of  $10^{22}$ – $10^{24}$  m<sup>-3</sup>. Atomic probe tomography (APT) is the most suitable research method for quantitative determining the parameters of such precipitates.

This study integrates APT data on parameters of precipitates in RPV and RVI steels used in VVER and PWR reactors after irradiation in commercial and research reactors across multiple studies by different laboratories. This allowed to summarize the trends in phase formation depending on steel composition (precipitate-forming element content) and irradiation conditions (dose level, dose rate, temperature). Additionally, theoretical models and simulations have been incorporated to better understand the phase formation mechanisms and their relationship with other radiation damage processes contributing to structural degradation.

Overall, these findings enhance reliability and accuracy in predicting performance characteristics of structural reactor materials throughout different stages of service life, particularly when extending operational lifetimes beyond the initial design limits.

## STUDY OF THE NANOSTRUCTURE OF OXIDE DISPERSION-STRENGTHENED STEELS BY ATOM PROBE TOMOGRAPHY, TRANSMISSION ELECTRON MICROSCOPY AND SMALL-ANGLE NEUTRON SCATTERING

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In advanced nuclear and fusion reactors, core materials should have high radiation resistance and heat resistance at temperatures up to 650 °C and doses of up to 200 dpa (displacements per atom). Promising materials that can meet these requirements are oxide dispersion-strengthened (ODS) steels containing homogeneously distributed thermally stable nanoscale oxides in their matrix.

In this work, the nanostructure of ODS steels was studied by small-angle neutron scattering (SANS), transmission electron microscopy (TEM), and atom probe tomography (APT) [1-3]. The studied steels differ in the content of Cr, V, Ti, Al, and Zr. Methods of local analysis of TEM and APT revealed a significant number of nanosized oxide particles and clusters. Their sizes, number densities and compositions have been determined.

The use of SANS made it possible to identify the presence of magnetic and non-magnetic inclusions of various sizes in the materials under study. It is shown that the use of magnetic fields makes it possible to better identify diffuse nanoscale clusters detected by atom probe tomography.

*The work was carried out on the equipment of the KAMIKS Center for Shared Use (<http://kamiks.itep.ru>) of the National Research Center "Kurchatov Institute".*

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## STUDY OF THE STABILITY OF OXIDE PARTICLES IN OXIDE DISPERSION STRENGTHENED STEELS AFTER THERMAL AGING

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Oxide dispersion strengthened (ODS) steels are promising materials for the future generation of nuclear power plants. These materials must have increased radiation resistance (up to 200 displacements per atom) and withstand high exploitation temperatures (up to 650°C). The special properties of the material are provided by the introduction of oxide particles into the ferrite matrix. [1]. The aim of this work is to investigate changes in oxide particles caused by prolonged

exposure to high temperatures.

The three steels with different chemical composition were selected for atom probe tomography study [2]: Eurofer ODS, 10Cr ODS и KP-3 ODS. The research was conducted in initial state and after thermal aging at a temperature of 650 °C for 500 and 1000 hours.

The number density of clusters increases (average size increases or is maintained) after aging for 500 h. However, the number density decreases after aging for 1000 h. The observations are described by a model containing the stage of conception, growth and subsequent coalescence.

*The work was carried out on the equipment of the Collective Use Center KAMIKS (<http://kamiks.itep.ru>) of the NRC "Kurchatov Institute".*

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## VOID CHARACTERISTICS CHANGES IN NEUTRON IRRADIATED STEEL CR16-NI19 TYPE DEPENDING ON IRRADIATION TEMPERATURE

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Neutron irradiation in BN-type reactors leads to significant changes in the structure of material of the fuel cladding element, which also entails changes in the physical and mechanical properties of the fuel cladding element. Different sections of the fuel cladding element are exposed to different irradiation conditions during operation, such as temperature and dose rate, resulting in different accumulated doses over different irradiation times. Over the past ten years, a large data volume has been accumulated on changes in the microstructure of cold-processed steel Cr16-Ni19 type, currently used as the primary material of the fuel cladding element for BN reactors. The aim of this study was to systematize this data and identify the dominant factors influencing microstructural changes in steel Cr16-Ni19 type under neutron irradiation.

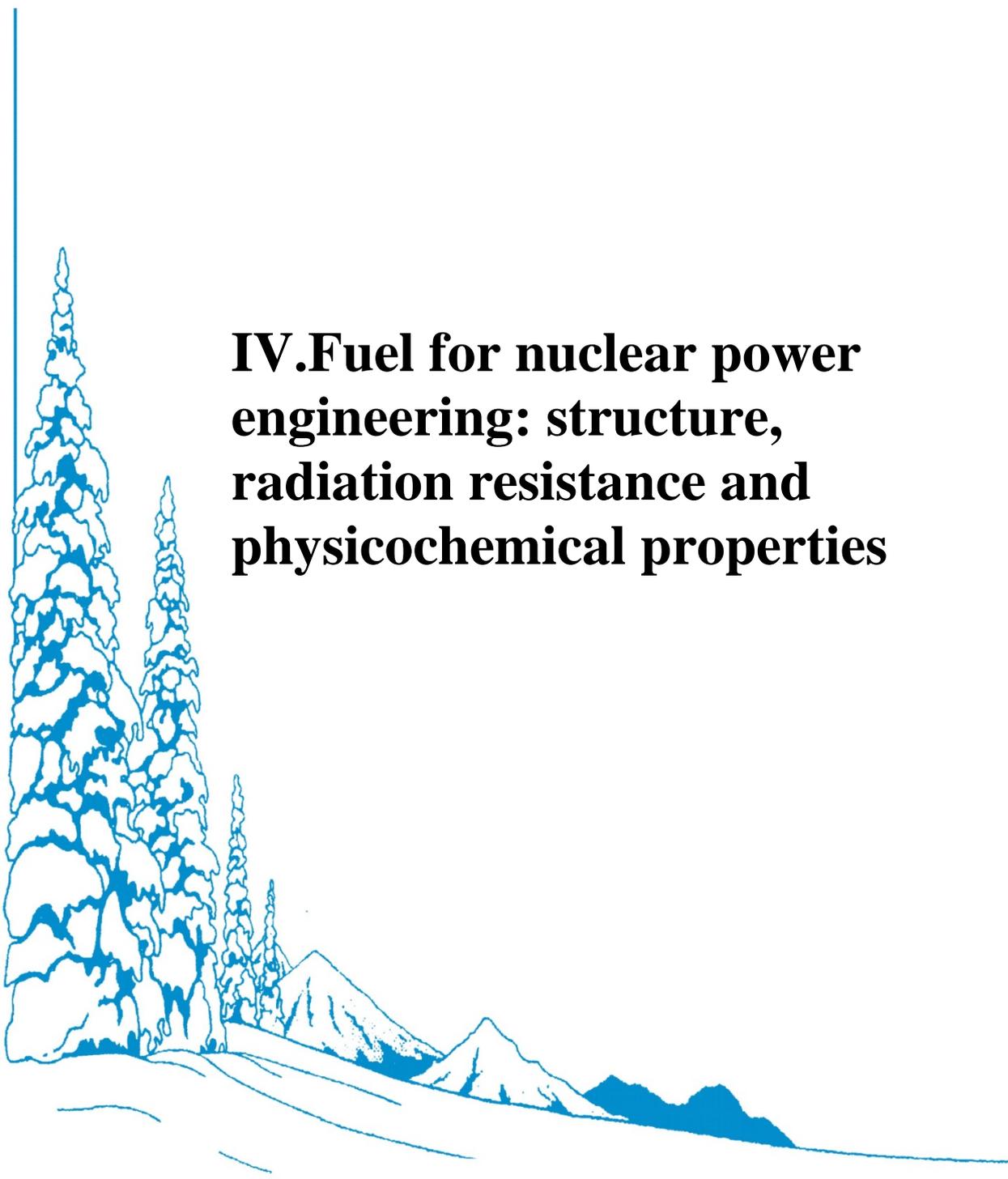
Comparative studies were conducted on the characteristics of the porosity formed in steel Cr16-Ni19 type after operation in the BN-600 reactor in zones with different enrichment levels for varying periods. Different enrichment zones have different neutron spectra, which not only leads to differences in the rate of damaging dose accumulation in the material but also to differences in damageability due to these spectral differences.

Changes in microstructural elements were studied: dislocation structure – its qualitative description; the precipitate of second phases was assessed qualitatively (type, composition, lattice, and interactions with other elements), and the porosity characteristics were analyzed (qualitatively, interactions with other elements; quantitatively, void size distribution histograms). Three void types were identified: "small" voids, which are gas-vacancy void nuclei, "medium-sized" and "large" voids. To determine the influence of irradiation temperature on the changes in the void characteristics formed in steel Cr16-Ni19 type, the dependences of the average size and concentration of "large" and "medium-sized" voids on the irradiation temperature were analyzed

for samples of all studied fuel cladding elements from fuel assemblies in various enrichment zones with different operating times, separated into narrow intervals based on the rate of damaging dose accumulation (no more than  $0.2 \times 10^{-6}$  dpa/s).

It was shown that, in all intervals of damaging dose accumulation rates, an increase in the average size of "large" voids with increasing irradiation temperature was observed. The concentration of "large" voids increases sharply with increasing irradiation temperature from  $\sim 420^\circ\text{C}$  to  $\sim 430^\circ\text{C}$ . Further increases in irradiation temperature lead to a sharp decrease in the concentration of "large" voids across all ranges of damaging dose accumulation rates. The average size of "medium-sized" voids changes slightly with increasing irradiation temperature, generally remaining in the range of 10 to 15 nm across the entire studied range of irradiation temperatures and damaging dose accumulation rates. The concentrations of "medium-sized" voids, depending on irradiation temperature, exhibit ambiguous behavior in samples of different fuel elements from different fuel assemblies. The specific surface area of voids and porosity were also plotted and analyzed as functions of irradiation temperature across various ranges of damaging dose accumulation rates.





## **IV. Fuel for nuclear power engineering: structure, radiation resistance and physicochemical properties**



## SIMULATION OF THERMONUCLEAR BURNING OF TRADITIONAL FUEL IN MAGLIF DEVICES UNDER CERTAIN CONDITIONS

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Promising Magnetised Liner Inertial Fusion (MagLIF) based thermonuclear reactors will require provision of specific conditions to ignite and confine the fusion fuel. The right combination of electrical and magnetic fields should be realized which will allow to achieve extreme values of the temperatures and densities corresponding to fusion reactions [1, 2].

In this report, we consider the process of plasma's thermonuclear burning under extreme conditions, most typical for MagLIF devices, where they are expected to be provided. The temperature range is taken as about tens of *keV* and higher. The densities of matter are taken with an order of solid-state densities [1, 2]. Analysis of the reactivity curves of the main thermonuclear reactions shows that at lower temperatures, the *D+T* interaction reactivity has relatively higher values, and with an increase in the burning temperature, the rate of the *D+<sup>3</sup>He* interaction increases more rapidly and starts to prevail over other interactions.

Considering the temperature enhancement of burning region due to the energy release from the corresponding main fusion reactions, as well as taking into account the main types of radiation losses, the kinetics pattern of thermonuclear burning is evaluated.

In the result it was obtained that, considering all initially set certain conditions, the burning of different types of fuel has a completely different character. When burning *DD* fuel, all energy release is compensated by radiation losses. The burning of *DT* and *D<sup>3</sup>He* fuels has a rapid temperature enhancement at the initial stages. Calculations led us to conclude that their burning is self-sustaining, and these fuel types are promising. Moreover, the *D<sup>3</sup>He* fuel is relatively neutron-free which can be an important argument for this fuel type choice. We calculated the energy release due to charged particles to be 10-15 times greater than that of neutrons.

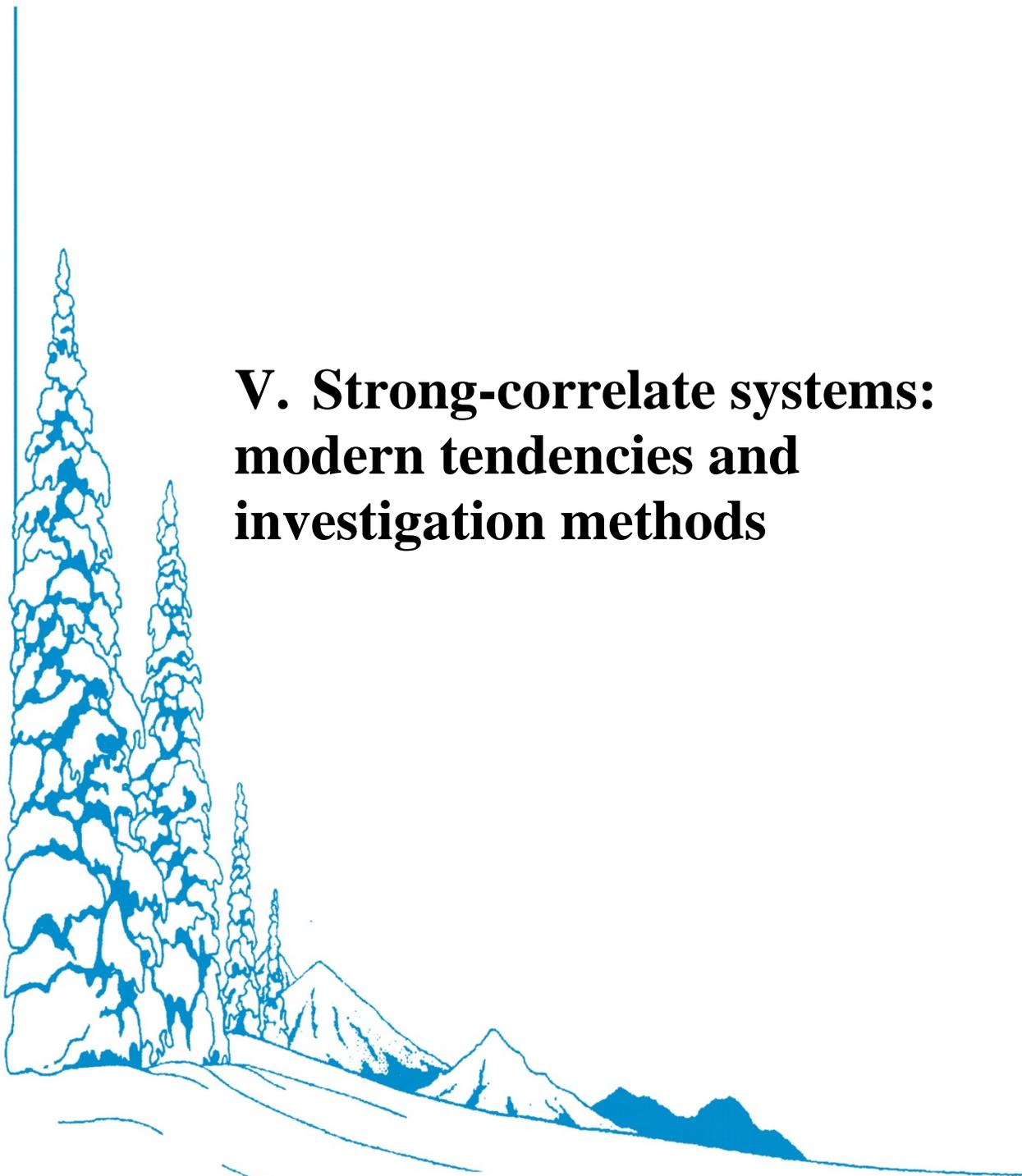
During the burning of all fuel types, there will be the main component concentration decreasing with the production of secondary products. Evidently, for longer plasma confinement, there should mainly *D-T-<sup>3</sup>He* mixture burning observed later.

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## **V. Strong-correlate systems: modern tendencies and investigation methods**



**MECHANISM OF UNCOMMON MAGNETISM IN INTERMEDIATE-VALENCE EU INTERMETALLICS**P.S. Savchenkov<sup>1,2</sup>, P.A. Alekseev<sup>1,2</sup><sup>1</sup>*NRC Kurchatov Institute, Moscow, Russia (savch92@gmail.com)*<sup>2</sup>*NRNU MEPhI, Moscow, Russia*

The physics of strongly correlated electron systems (SCES) remains one of the most pressing areas of modern condensed matter physics. Interest in them stems from the diversity of exotic phases—from high-temperature superconductivity to non-Fermi-liquid behavior—that often arise near the quantum critical point, where interaction competition reaches its maximum. Europium-based compounds, exhibiting a uniform intermediate valence, occupy a special place among SCES. The uniqueness of such systems, in particular the  $\text{EuT}_2\text{X}_2$  family (where T is a 3d/4d metal and X is Si/Ge), lies in the formation of a quantum-mechanically mixed ground state. It arises from the strong hybridization of localized 4f electrons with the conduction band and competition between the magnetic configuration of  $\text{Eu}^{2+}$  ( $J = 7/2$ ) and the nonmagnetic singlet of  $\text{Eu}^{3+}$  ( $J = 0$ ). Contrary to theoretical expectations of complete suppression of magnetic correlations by fast valence fluctuations, a key feature of a number of these systems is the anomalous coexistence of long-range magnetic order and a stable state of uniform intermediate valence.

The key unresolved question for  $\text{EuT}_2\text{X}_2$  systems remains the microscopic nature of this magnetism. Experimental data indicate that at low temperatures, these systems realize a nonmagnetic singlet ground state, separated from the excited states by a spin gap. This makes the situation similar to Van Vleck paramagnets or PrNi-type systems, where magnetic order arises not through the reorientation of existing moments, but through the polarization of the singlet ground state—the mechanism of induced magnetism. However, for systems with intermediate valence Eu, the dynamics of this transition and the stability of the magnetic phase remain open. Standard theoretical models (e.g., the Anderson impurity model) do not provide a complete description of the coexistence of valence fluctuations and long-range magnetic order.

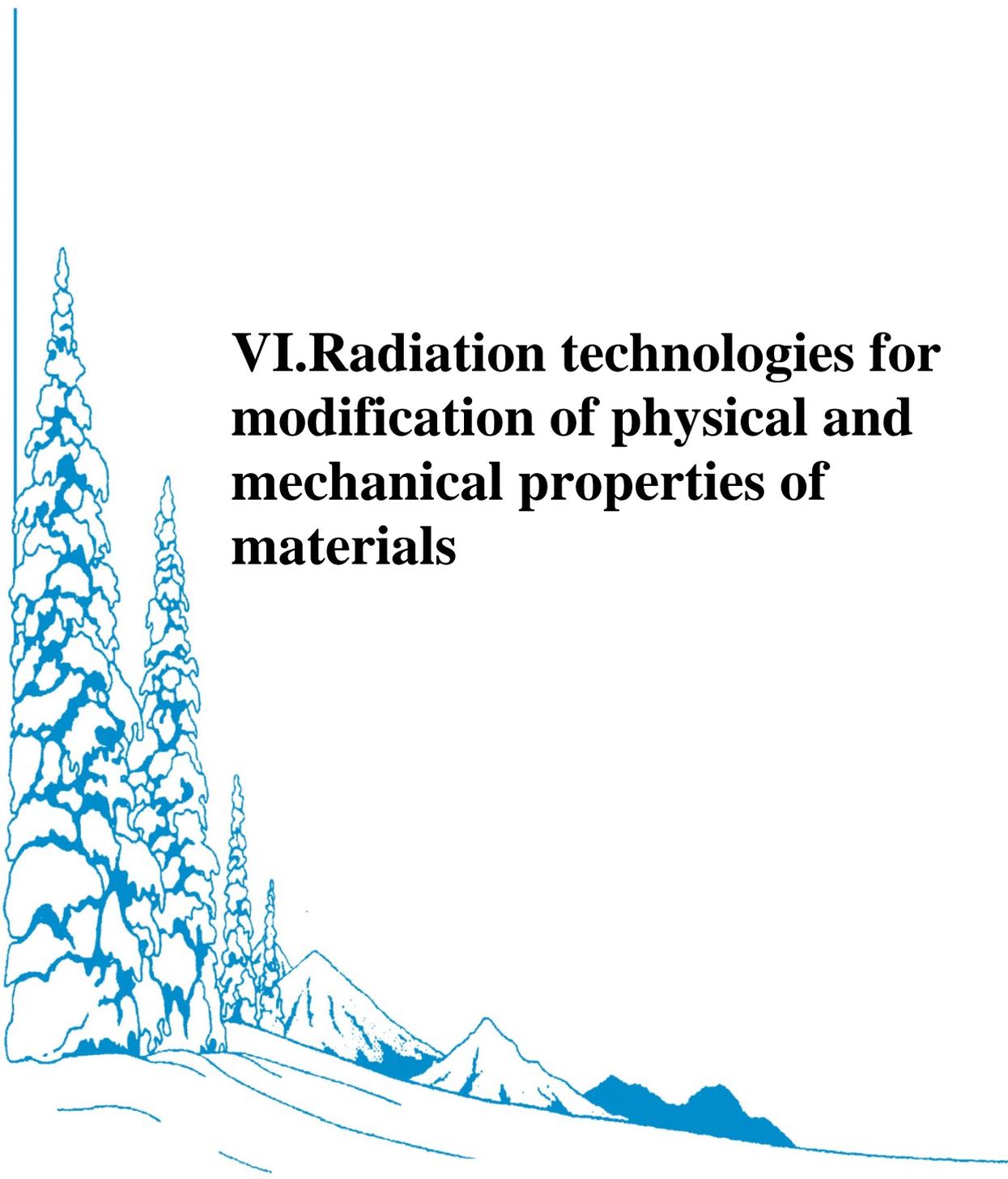
This paper presents the results of a comprehensive study, the key element of which was inelastic neutron scattering. The use of neutron spectroscopy allowed us to directly study the spin dynamics and evolution of magnetic excitations during the transition to an ordered magnetic state. It will be shown that the formation of long-range magnetic order in  $\text{EuT}_2\text{X}_2$  systems occurs according to the induced magnetism scenario.

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## **VI. Radiation technologies for modification of physical and mechanical properties of materials**



## EFFECT OF ION PLASMA NITRIDING ON THE FORMATION OF SURFACE LAYERS OF TITANIUM ALLOY Ti-6Al-4V

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Titanium alloys are widely used in various fields of technology due to their high strength, ductility and low biotoxicity. The development of technologies for surface modification of titanium alloys to increase their hardness, wear resistance, corrosion resistance and biocompatibility is relevant [1, 2].

The paper investigates the formation of the surface morphology, the elemental and phase composition of the surface layers, the microstructure, and the microhardness of the VT6 titanium alloy under conditions of nitriding in the plasma of a glow discharge of  $N^+$  ions at a temperature of 800 °C. Nitrogen was injected into the chamber at a rate of 165 ml/min. The processing time is 1 hour.

The microstructure of the initial sample is mainly represented by grains of the  $\alpha$ -Ti phase with a small fraction of the  $\beta$ -Ti phase along the grain boundaries with an average grain size area of about 6  $\mu m^2$ .

After ion plasma treatment, the surface layers have a band structure: I - a zone of small crystals of titanium nitrides TiN, Ti<sub>2</sub>N and grains of  $\alpha$ -Ti; II - a diffusion zone of large crystals of solid nitrogen solution in  $\alpha$ -Ti (grain size increases to 101  $\mu m^2$ ); III - duplex structure of plates of  $\alpha$ -Ti and  $\beta$ -Ti.

Atomic force microscopy studies indicate a 7-fold increase in the surface roughness parameter Ra of the treated samples, which is due to the phase formation of titanium nitrides TiN and Ti<sub>2</sub>N over the entire surface.

The formation of titanium nitrides, the diffusion zone of the solid solution and the mixed duplex structure cause an increase in the microhardness of the samples by 2.7 times.

*The work was performed within the framework of the State Assignment of the Ministry of Science and Higher Education of the Russian Federation No. GZ124021900017-1 and with the support of the Ministry of Science and Higher Education of the Russian Federation under Agreement No. 075-15-2025-455 dated 05.26.2025 regarding the conduct of scanning electron microscopy research. The research was performed using the equipment of the Center for Physical and Physico-Chemical Methods of Analysis, Investigation of Surface Properties and Characteristics, Nanostructures, Materials and Products of the UdmFIC Ural Branch of the Russian Academy of Sciences.*

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# EFFECT OF NITROGEN ION IRRADIATION DOSE ON CHANGES IN SURFACE MORPHOLOGY, CHEMICAL COMPOSITION, AND PHYSICO-MECHANICAL PROPERTIES OF MULTILAYER NI/AL NANOCRYSTALLINE FILMS

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Methods of ion-beam and ion-plasma treatment, having a number of fundamental advantages over traditional methods of chemical-thermal treatment, have been actively developed in the field of modification of surface layers of metals and alloys in order to increase their strength properties [1-3]. In addition to the classic advantages of ion treatment (the possibility of exceeding the solubility limit, control of the depth of impurity distribution, the possibility of selective processing of parts, etc.), in the last decade, it has been possible to add completely new methods of influencing the surface layers of materials. In particular, by forming on the surface of the target, one or several layers of other materials of a nanometer thickness range, and their subsequent ion treatment with high-energy particles, it was possible to form new compounds and phases in the surface layers [4, 5].

In this work, X-ray photoelectron spectroscopy, atomic force microscopy, scanning electron microscopy, and microhardness measurements were used to study surface morphology, chemical composition formation, and changes in the physico-mechanical characteristics of surface layers of multilayer nanocrystalline Ni/Al films on the surface of VT1-00 titanium depending on the dose of nitrogen ion irradiation ( $10^{16}$ - $10^{18}$  ion/cm<sup>2</sup>).

*The work was carried out within State Task of the Ministry of Science and Higher Education of Russian Federation (No. 124021900017-1). The work was performed with the equipment of the Centre for Shared Usage "Center of physical and physical-chemical methods of analysis and research of properties and characteristics of surfaces, nanostructures, materials, and samples" of the UdmFRC UB RAS.*

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## IMPLANTATION OF IONS IN PREHEATED METAL MATERIALS

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The work is devoted to the study of metallic materials preheated and irradiated with ions of gases: argon, nitrogen, oxygen. As is known, ion implantation, being an energetic effect, can significantly change the physico-chemical properties of materials. During ion irradiation, the surface of the treated material receives a significant amount of energy, which, dissipating deep into the material, leads to heating of the material. The heating temperature depends on the ion current density, ion energy, and thermophysical characteristics of the target material. In some cases, the temperature in the area of thermal peaks can reach several thousand degrees. Of course, heating materials to such temperatures leads to a number of effects, such as structural and phase transformations, accelerated diffusion, etc. In experiments investigating the effect of ion implantation in metallic materials, attempts are made to reduce the effect of the temperature factor by additional cooling of the target, increasing the heat sink, reducing the ion beam power, etc. At the same time, most of the metal materials exposed to ion irradiation (as well as other types of energy exposure) are always in a heated state – this is true both for research facilities and for parts in operation, for example, reactor parts. In this case, the approach to planning an experiment to study the effect of ion implantation is changing – the effect of implantation into a heated metal target is being investigated.

The paper examines samples of metal alloys of iron, alloys based on copper-nickel alloy, aluminum-based alloys. The samples are heated in an induction furnace located directly in the vacuum chamber of the ion source. The temperature of the sample is controlled both during heating and during irradiation. The irradiated samples were studied by X-ray photoelectron spectroscopy, structural analysis, microhardness measurement, and atomic force microscopy. Based on the results of the work carried out, it was determined that ion irradiation of preheated samples leads to an increase in the depth of the modified layer and a change in the microhardness of the surface. In this case, the degree of preheating of the target before irradiation is important.

## MOLECULAR – DYNAMICS STUDY OF THE COMPLEX SYSTEMS UNDER ION IRRADIATION

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In modern materials science, thin-film systems are the most rapidly developing area. The sequential combination of substances with different physical properties allows for the formation of structures and systems with controlled functional properties. When developing and studying such systems, structural studies are essential. This includes studying the processes of self-organization, interdiffusion of elements, and the nature of interfaces.

Several computer simulation methods can be used for structural studies of systems. Monte Carlo simulations use random numbers.

The molecular dynamics method takes into account the interaction of an incident particle or

recoil atom with all neighboring atoms. A weakness of this method is the multiparticle interaction potential, which must be selected based on the given problem.

In this study, molecular dynamics simulations were performed using the LAMMPS software package [1]. The interaction between atoms was described by the embedded atom potential. This potential demonstrates sufficient accuracy in describing the interatomic interactions of Fe-C. It also describes the interaction of pure iron. This potential is widely used to study the properties of the Fe-C system. The equations of motion were integrated using the Verlet method with a time step of  $5 \cdot 10^{-18}$  s. A two-component model consisting of ~50 thousand atoms was constructed. The calculation was carried out for 1 ps. The initial energy of the incident  $\text{Ar}^+$  ions was 30 keV.

The simulation results showed that after  $\text{Ar}^+$  ions pass through the interface, a complex configuration is formed. A mixture of atoms occurs in this region. The crystal lattice at the interface is disrupted. A cascade of atomic collisions is also formed, which is detected in the region of the iron atoms.

The proposed computer model is a test system for studying the main patterns of formation of structural inhomogeneities in two-component samples.

The work was carried out within the framework of the state assignment of the Ministry of Science and Higher Education of the Russian Federation №124021900017-1.

**Literature:**

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**STUDY OF THE ION IRRADIATION IMPACT ON THE Fe-Mn, Fe-Cr,  
AND Fe-Si ALLOYS ATOMIC STRUCTURE**

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This work is devoted to studies of the processes of various types of short- and long-range atomic order formation, as well as the formation of phases in binary alloys based on iron under the influence of irradiation with continuous beams of argon ions ( $E = 10 - 15$  keV at temperatures below the threshold of the onset of intensive thermally activated processes.

It has been shown that in a number of Fe-based alloys in a metastable state, under the influence of continuous beams of  $\text{Ar}^+$  ions ( $E = 10 - 15$  keV), it is possible to obtain states that are not observed during conventional thermal heating at temperatures used in experiments (below thermal activation). Thus, in the model two-component Fe – 6.29 at. % Mn alloy after cold plastic deformation, short-term irradiation ( $t = 4$  s) with heating up to temperatures of 300 – 450 °C causes an  $\alpha \rightarrow \gamma$  phase transformation with the formation of Mn-enriched austenite (from 23.8 to 38.0 at. %). After SPD, the  $\alpha \rightarrow \gamma$  transformation process in the Fe – 7.25 at. % Mn alloy occurs already during irradiation at a maximum temperature of 280 °C. With similar thermal heating, the alloys remain single-phase.

In the Fe – 6.25 at. % Si alloy after cold plastic deformation, which destroys the atomic order in the sample, nevertheless, an observed degree of long-range atomic order is not zero ( $\eta = 0.42 \pm 0.02$ ), which is due to the high tendency of ferrosilicon alloys to ordering. After irradiating a sample of a cold-formed alloy with argon ions for 4 seconds with heating during irradiation up to ~ 300 °C, it was possible to achieve an increase in the degree of the long-range order to  $\eta = 0.52$ . After heating in the furnace in similar modes, the degree of long-range order increased slightly:  $\eta$

= 0.45. In the Fe – 6.25 at. % of Si alloy exposed to SPD ( $\eta = 0.21$ ) was irradiated for 6 s at  $T = 200$  °C. A long-range atomic order was formed, namely the Fe<sub>15</sub>Si superstructure of the 3rd rank (the best description of the Mossbauer spectrum in the Fe<sub>16</sub>-kSi<sub>k</sub> model is achieved at  $k = 1$ ). The range parameter reaches a high value ( $\eta = 0.70$ ). When heated without irradiation, the  $\eta$  values decrease by 20-30%.

In the Fe – 15 at. % Cr alloy after SPD, as a result of irradiation ( $t = 1$  s,  $T = 300$  °C), the formation of a short-range atomic order with a sufficiently high  $\alpha$  parameter equal to 0.41 is observed. For a sample after SPD annealed at 300 °C for 1 hour,  $\alpha = 0.34$ . When trained at  $T < 200$  °C for 1 – 5 seconds,  $\alpha = 0.24$ .

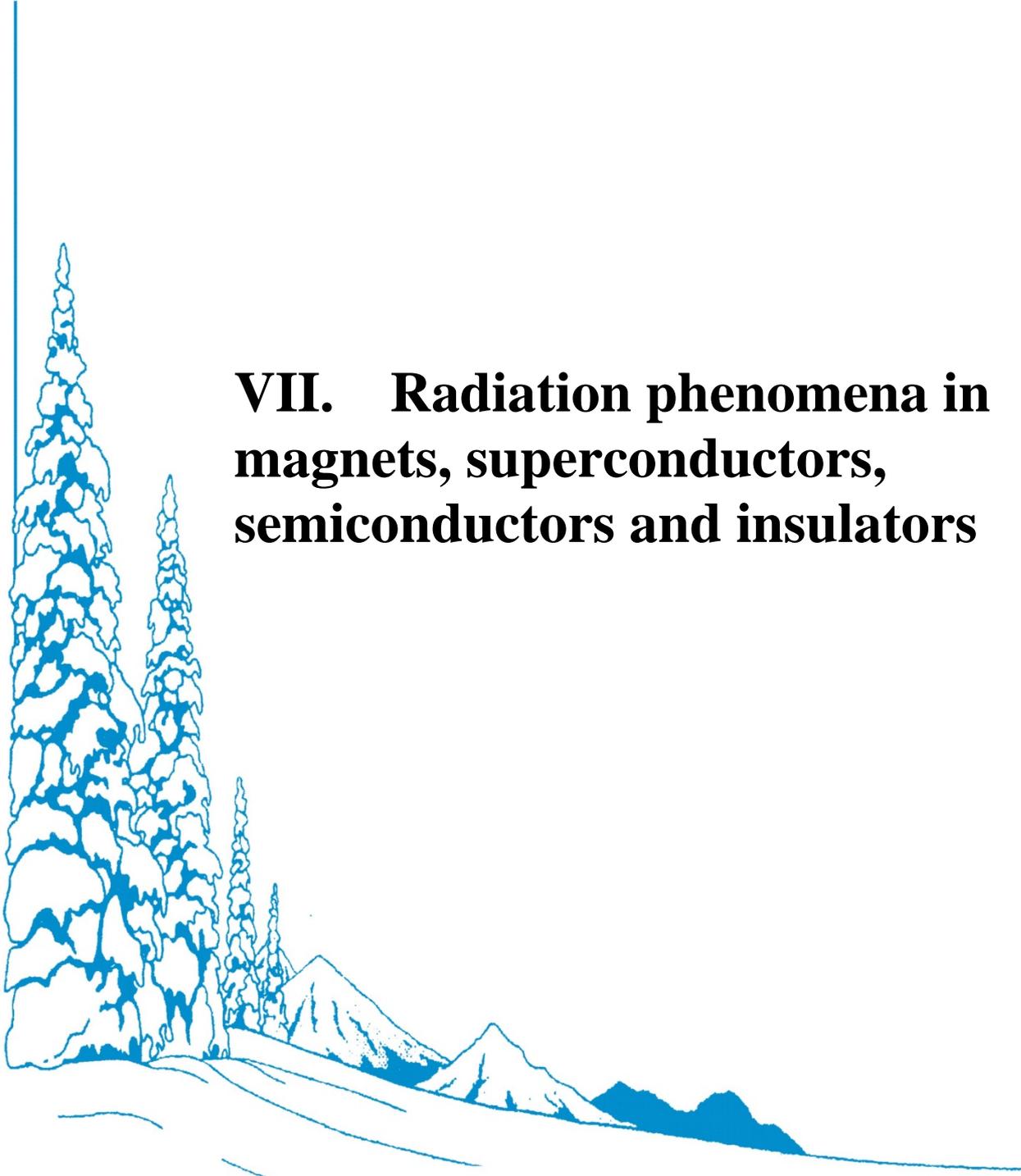
All of these processes occur over the entire thickness of 25 microns of the studied samples at an average projected ion range of up to 10 – 12 nm, at low temperatures at which diffusion is inhibited in these alloys, and in short times (seconds and tens of seconds of irradiation). The established patterns indirectly confirm the fact of a gigantic increase in the mobility of atoms as a result of radiation shaking of the medium by post-cascade shock waves [1 – 3].

The research was carried out with the financial support of the Russian Science Foundation (project No. 19-79-20173).

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## **VII. Radiation phenomena in magnets, superconductors, semiconductors and insulators**



## FEATURES OF INJECTION-ENHANCED ANNEALING OF QUANTUM-WELL A<sup>III</sup>B<sup>V</sup> HETEROSTRUCTURES

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Optoelectronic devices based on AIII BV (GaAs/GaN/InGaP) are an important part of the state-of-the-art equipment of space vehicles, aircraft, and nuclear power plants. Among these devices, one can particularly note light-emitting diodes, optrons, laser diodes, as well as quantum-well and quantum-dot photodetectors. Their implementation significantly improves the interference immunity and weight dimension characteristics of the equipment and increases the data processing scope and rate. The latter is of special importance for the development of the advanced automated systems with real-time machine vision and artificial intelligence.

However, the methods used nowadays for radiation tests of up-to-date devices were developed for and verified against traditional homostructure devices. By now, there is still no clear understanding of the specific nature of radiation-induced effects in the devices with quantum-sized heterostructures.

The present work is aimed to continue our study [1] that demonstrates such special aspect of radiation-induced effects in quantum-sized heterostructures as significantly higher importance of injection-enhanced annealing, compared to homostructures. Injection-enhanced annealing is observed when injection current passes through an irradiated p-n junction and restores its characteristics. Unlike thermal annealing, the recovery is caused by the minority carriers injected into the material. Change in the charge state of defects and local energy release across the defects due to nonradiative carrier capture [2] are considered as possible mechanisms of this phenomenon.

The work experimentally studied the effect of fission spectrum neutrons, 8 MeV electrons and <sup>60</sup>Co gamma-quanta on the photovoltaic and light-emitting properties of quantum-well GaAs/GaN/InGaP heterostructures. Injection-enhanced annealing of the photovoltaic and light-emitting properties was under investigation. The density of the electric current that induced the annealing varied in a wide range from 10–4 to 102 A/cm<sup>2</sup>.

The obtained results demonstrate that after the injection-enhanced annealing, the change in light-emitting properties of the test samples is six times higher than that in their photovoltaic properties. According to available research data, this difference is about 15% in case of homostructures [3]. The obtained results are explained by one of the main aspects of quantum-sized heterostructures, namely, the limited region of the injected carrier distribution. Due to this fact, injection-enhanced annealing is also limited by the quantum-well region.

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## FEATURES OF PHOTO-INDUCED ANNEALING OF OPTICAL FIBERS UNDER PULSED IONIZING RADIATION

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Despite numerous studies on investigation of ionizing radiation (IR) effect on optical fiber characteristics, e.g. [1, 2], there is a lack of attention to radiation-induced effects in optical fibers with a length significantly exceeding the quantity  $1/\Delta\alpha$ , where  $\Delta\alpha$  is the radiation-induced absorption coefficient. In this case, the system response will be determined by the propagation of the photobleaching front from the photon source along the irradiated fiber. Knowledge about such processes is important, for example, in designing high-power laser systems as well as in developing optical systems that require high synchronization of optical signals transmitted through fiber lines.

The work [3] describes the annealing of radiation color centers in the optical fiber using optical radiation under static irradiation of the fiber at a dose rate of  $\approx 100$  R/s. The samples were irradiated at liquid nitrogen temperatures that allowed preserving the unstable radiation color centers. Such centers completely absorbed the optical signal that resulted in movement of the antireflection radiation front in the optical fiber under photo-induced annealing. The dependencies of the propagation velocity and the length of the photobleaching front on the IR dose and probing source parameters, namely, power and wavelength of the optical radiation, were obtained.

The study of the features of photo-stimulated annealing in the extended optical fibers under pulsed IR is a continuation of the work [3]. In the current work the optical fiber was irradiated at IR pulse duration of order of  $10^{-8}$  s. Such times are insufficient for unstable radiation color centers to be annealed even at room temperature that allows observing photobleaching front movement within the fiber with duration of microsecond order.

The standard telecommunication fiber Corning SMF-28 and the radiation-hardened fiber manufactured by the PNPPK company were selected as extended optical environment. The samples were irradiated using an electron accelerator in the bremsstrahlung output mode. The exposure dose rate in sample irradiation was  $\sim 10^{10}$  R/s. Depending on the experimental conditions, the sample temperature was varied from  $-196$  to  $20$  °C, the absorbed dose in the sample was varied 100 to 600 R, the length of the irradiated fiber part was varied from 3 to 30 m, and the power of optical radiation transmitted through the optical fiber was varied from 0.01 to 1 mW.

The dependencies of the recovery time of the probing radiation and the front parameters of photo-induced annealing of the optical fiber on the absorbed dose in the fiber, temperature and the length of the irradiated fiber part as well as on the probing optical power under pulsed IR were obtained.

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## IN-SITU OPTICAL SPECTROSCOPY OF $\text{Al}_2\text{O}_3$ CRYSTALS WITH SWIFT HEAVY ION BEAMS

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Single crystalline corundum  $\alpha\text{-Al}_2\text{O}_3$ , is one of the most radiation-resistant dielectrics and widely used as an optical material and electrical insulator for working in radiating fields. Most of the information about defects in these crystals was obtained using optical spectroscopy techniques in post-radiation experiments. Much less studies have been devoted to the kinetics of accumulation of structural disorder in  $\alpha\text{-Al}_2\text{O}_3$  immediately during irradiation, especially in the process of swift heavy ion impact. This report presents an overview of the results of "in-situ" studies of high-density ionization effects in the formation of a defect structure in corundum irradiated with heavy ions with energies above 1 MeV/nucleon. The first part discusses real-time measurements of mechanical stress field parameters, depending on the value of electron stopping power and ion fluence. The dose dependence of the stress tensor components was determined using a method based on the use of the piezospectroscopic effect, which relates changes in the ionoluminescence spectra to the magnitude of mechanical stresses. It has been found that at fluences corresponding to beginning of overlap of track regions, determined from the results of microstructural analysis and modeling using molecular dynamics methods [1,2], stress relaxation is observed in the irradiated layer of the crystal.

In the second part of the report, the dependence of the spectral content of ionoluminescence on the specific ionization energy losses is discussed and the decay kinetics of the luminescence of  $\text{Al}_2\text{O}_3$  single crystals generated by single high-energy heavy ions is analysed.

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## ION IRRADIATION FOR OBTAINING AND MODIFICATION OF METALLIC NANOWIRES

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In this paper, the features of ion irradiation in the production of metallic one-dimensional

nanostructures -metallic nanowires (NWs) are considered. NWs are created by template synthesis based on matrices - polymer track membranes (TM). In the production of magnetic NPS, ion irradiation can be used at the initial stage (obtaining matrices) and at the "finishing" stage - processing the obtained arrays of NPS.

**MATRIXES.** It is known that irradiation with heavy high-energy ions is used to produce the TM themselves. Subsequent chemical treatment leads to the formation of through channels-pores. TM production in our country is carried out at JINR (Dubna). The main application of TM is fine filtration (medicine, food industry). Template synthesis is an alternative field of application. The requirements for membranes for filtration and for matrix synthesis differ markedly. In the second case, membranes with uniformly oriented pores and low density are usually required. Obtaining matrices with such parameters can be achieved by changing the conditions of ion irradiation, which is performed at JINR.

**MATRIX SYNTHESIS** is a process in which the pores in TM are filled with the required substance; it is usually electroplating process. Arrays of metallic NWs obtained by this method are of interest in various directions-emitters, catalysts, and electronics devices. One of the directions is the creation of micromagnets, where specific features (first of all, a high aspect ratio) can play a role in changing magnetic properties.

**ION IRRADIATION.** In this work, the possibilities of changing the magnetic properties of NWs due to ion irradiation were investigated. NWs arrays made of nickel and an iron-nickel alloy were irradiated with Ar and Xe ions with an energy of 20 keV: when a certain dose was reached, the NW shape changed – bending and subsequent "melting", the occurrence of which has a threshold character. It is concluded that thermalized regions of dense cascades of atomic displacements (thermal spikes, nanoscale zones with high energy release density) are formed during irradiation, which play the main role in changing the structure. At the next stage, NWs samples from nickel and cobalt (of two types-cubic and hexagonal) were irradiated with Ar ions with an energy of 15 keV. The fluences ranged from  $10^{11}$  to  $10^{15}$ . A SEM study of the irradiated samples showed that starting from doses of  $10^{13}$ , there is a noticeable change in the shape of the tips of the NW- bending and recrystallization (the tips of the hexagonal cobalt NW acquire a hexagonal shape, while other samples acquire a cubic shape). Hexagonal cobalt alloys undergo the strongest changes, despite the fact that their melting point is noticeably higher than that of nickel. Magnetic measurements (vibrational magnetometry) have shown that for these samples, a non-monotonic change in magnetic properties occurs- up to a dose of  $10^{13}$ , there is a significant increase in saturation magnetization and coercive force (by a factor of 2-3), with an increase in dose, these parameters decrease slightly. The reason for this may be the accumulation of defects at the first stage and their subsequent annihilation with an increase in the radiation dose. The study of the described effects is important both for assessing radiation stability and for finding ways to produce magnetically rigid materials from 3-d metals without using rare earth metals.

**ION IRRADIATION.** In this work, the effect of ion irradiation on the structure and magnetic properties of NWs was studied. NWs arrays made of Ni and  $\text{Fe}_{0.56}\text{Ni}_{0.44}$  alloy were irradiated with  $\text{Ar}^+$  and  $\text{Xe}^+$  ions ( $E = 20$  keV,  $F = 10^{16} - 10^{18}$   $\text{cm}^{-2}$ ). After irradiation, the presence of nanoscale melting zones on their surface is observed, as well as significant curvature and destruction of individual NW. At the next stage, NW samples from Ni and Co (of two types, cubic and hexagonal) were irradiated with  $\text{Ar}^+$  ions ( $E = 15$  keV,  $F = 8.6 \times 10^{11} - 6.3 \times 10^{15}$   $\text{cm}^{-2}$ ). The SEM study showed that starting from the  $6.3 \times 10^{13}$   $\text{cm}^{-2}$  fluence, there is a noticeable change in the shape of the tips of the NW from bending and recrystallization (some tips of NW acquire a hexagonal shape, others a cubic one). Magnetic measurements have shown that a non-monotonic change in magnetic properties occurs for these samples: up to a fluence of  $6.3 \times 10^{13}$   $\text{cm}^{-2}$ , there is a significant increase in saturation magnetization and coercive force (by a factor of 2-3), with a further increase in fluence, these parameters decrease somewhat. The reason for this may be the accumulation of defects at the first stage and their subsequent annihilation with an increase in ion

fluence. The study of the described effects is important both for assessing radiation stability and for finding ways to produce magnetically rigid materials from 3-d metals without using rare earth metals.

*The samples and their SEM tests were done within the State Assignment of the NRC "KI". The authors would like to thank P.Yu. Apel (JINR) for providing samples of various types of TM.*

## IRRADIATION-INDUCED AMORPHIZATION ACCELERATED BY ELEMENTAL MIGRATION NEAR THE SURFACE OF FLUORAPATITE

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The free surface, acting as a sink, invariably exerts an impact on the evolution of irradiation damage in the near-surface region, though its mechanism in multi-component compounds remains unclear. This study investigates fluorapatite, a potential nuclear waste form, through ex-situ and in-situ irradiation experiments, and MD simulations. Results show that the near-surface region tends to be amorphous preferentially due to the unbalanced elements diffusion, with effects extending over 400 nm at 493 K. Directional irradiation induces displacement atoms inward, increasing surface vacancy accumulation. Higher defect concentrations enhance element diffusion coefficients. Once amorphized, defects diffuse rapidly and are pinned by sinks, such as the free surface and numerous vacancy-type defects. Studying the amorphization of the near-surface region is helpful for grasping the weaknesses of irradiation resistance, and is crucial for evaluating the long-term service performance of nuclear waste forms.

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## **RESPONSE OF UP-TO-DATE LIGHT-EMITTING STRUCTURES TO PULSED IONIZING RADIATION**

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To date, one of the promising areas in electronics is the development of quantum-sized

heterostructures. Heterostructures are the basis of modern semiconductor devices in microwave electronics and optoelectronics. Structurally, they are complex multi-layered systems [1] consisting of various materials.

The paper presents the results of a study of the response of up-to-date quantum-sized heterostructures to a pulsed electron beam. Non-irradiated and pre-irradiated samples were studied. The samples were irradiated with fission-spectrum neutrons and gamma-quanta ( $\text{Co}^{60}$ ). LEDs and laser diodes based on GaAs and GaN were used as light-emitting structures.

The sample's response to ionization is a flash of light (Fig. 1), and its emission spectrum differs significantly from the one in normal LED operation. The observed difference is due to the recombination of charge carriers that takes place not only in the quantum well (QW), but also in the barrier layers and the substrate. Notably, the intensity of the flash in the QW is much higher than that in the barrier layers, which can be attributed to the compression of charge carriers in the QW. Using up-to-date methods of numerical simulation, we show the compression of charge carriers in the QW during the bulk ionization of the samples under study.

We also demonstrate that radiation defects affect the emission characteristics, reducing the amplitude of the flash that occurs when a sample is exposed to an electron beam, both in the QW and in barrier layers. Additionally, the annealing of radiation defects observed during electron beam exposure was investigated.

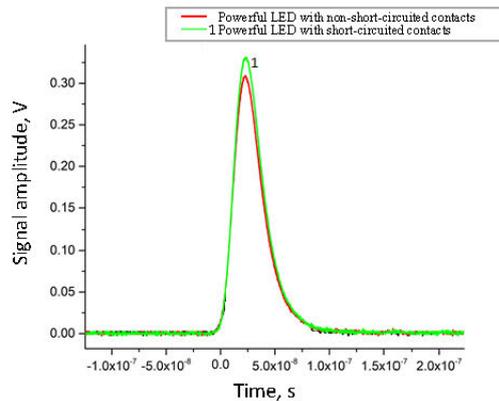


Figure 1. A typical oscillogram of the LED response for different connection schemes

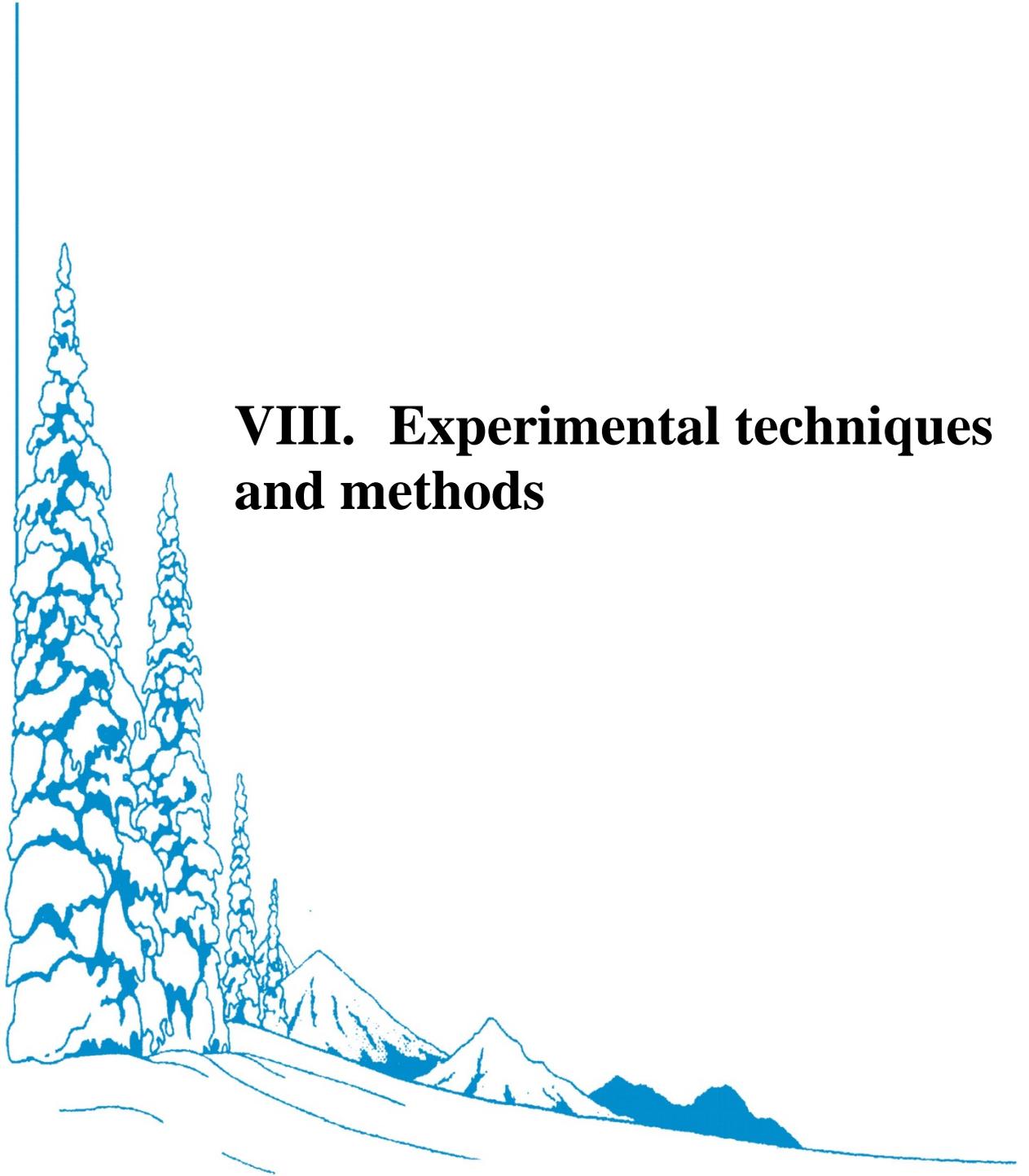
The results of the study can be used to develop a detector of ionizing radiation based on a quantum-sized heterostructure, characterized by a higher conversion rate as compared to the currently used scintillators and a possibility to set a specific wavelength.

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## **VIII. Experimental techniques and methods**





## A METHOD TO MEASURE NEUTRON FLUENCE AND ABSORBED GAMMA-QUANTA DOSE IN MIXED GAMMA-NEUTRON FIELDS

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Technological development and reduction in size in manufacture of integrated circuits have resulted in significantly increased radiation-induced effects associated with local ionization caused, among others, by individual neutrons. For example, references [1-5] imply that probability of single radiation-induced effects caused by neutrons in chips with a size less than 1  $\mu\text{m}$  is extremely high. The effects can appear at representative neutron fluence of  $\sim 10^9$  particles/cm<sup>2</sup>. However, when using standard methods in radiation experiments, measured neutron fluence range is typically  $10^{12}$ - $10^{15}$  particles/cm<sup>2</sup>.

Numerical simulation estimations show the possibility of extending the recorded neutron fluence range using standard detectors, conventionally applied for the purposes of photon dosimetry. However, this approach is challenging since the absorbed dose in detectors is conditioned not only by neutrons but also by the accompanying gamma-radiation.

To diagnose radiation in mixed gamma-neutron fields, the present work suggests using existing dosimetry techniques, which include application of detectors made of materials with different sensitivities to neutron and gamma-radiation. The use of two photon radiation detectors with different sensitivities simultaneously during the measurement allows separating and, then, estimating gamma and neutron contributions to the total dose.

To verify the offered method, two photon detectors used in qualified techniques of dosimetric radiation hardness tests were selected: thermal luminescence glass-plate detectors [6] and alanine detectors based on electron paramagnetic resonance [7]. A neutron generator and reactors with solution and metal cores were used as a radiation source.

The experimental and numerical simulation results revealed that the detector readings are determined by the absorbed dose contributed by both neutrons and gamma-radiation. The use of a set of two detectors also provides the opportunity to identify the contribution of each radiation to the total absorbed dose within the error of the technique used (20 %). The described approach allows recording neutron fluence in the range of  $10^9$ - $10^{14}$  particles/cm<sup>2</sup>.

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## **DETERMINATION OF DEFECT FORMATION MECHANISMS IN MAGNESIUM-BASED COMPOSITES USING POSITRON ANNIHILATION SPECTROSCOPY**

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Magnesium-based composite materials modified with various additives remain relevant in hydrogen energy research due to their promising properties for reversible hydrogen storage. Alloying elements can improve the properties of pure magnesium, for example, by reducing the activation energy of hydrogen diffusion and dissociation/recombination of H<sub>2</sub> molecules on the surface, and by weakening Mg–H bonds in the hydride, which lowers the hydrogen desorption temperature. Thus, to effectively improve the properties of magnesium-based composites, it is necessary to understand the mechanisms of defect structure formation and evolution throughout the sorption-desorption cycle, which is successfully addressed using positron annihilation spectroscopy (PAS) methods.

To study the evolution of defects in Mg/MgH<sub>2</sub> composites containing single-walled carbon nanotubes (SWCNTs), MIL-101(Cr) metal–organic framework compounds (MOFs), and nanosized nickel (nanoNi) and aluminum (nanoAl) powders using in situ Doppler annihilation line broadening spectroscopy (DUAL), the authors used a specialized PAS system, which integrates several key components, including an automated gas reactor, spectrometric modules, and a vacuum chamber. During the study, a methodology was developed for analyzing DUAL spectra by assessing the patterns of change in the S and W parameters under controlled thermal and hydrogen exposure. Analysis of the obtained data revealed a significant effect of each additive on the defect structure, hydrogen sorption and desorption kinetics, and thermodynamic properties. This paper highlights the utility of in situ HAS for identifying patterns underlying the mechanisms that contribute to the improvement of magnesium-based composite properties and provides recommendations for the development of highly efficient advanced hydrogen storage materials.

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## DETERMINATION OF LOWER WEIGHT LIMIT OF HIGH-DENSITY SAMPLES IN MEASURING DENSITY BY HYDROSTATIC METHOD

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An important characteristic of high-density, mostly radioactive metals is density which can vary due to accumulation of radiation-induced defects and decay products in long-term storage and due to any physical impacts.

Hydrostatic weighing method is the most common and feasible one among all other methods to measure density.

The work was aimed at experimental study of the influence of a supplemental liquid (distilled water, isopropyl alcohol, tetrachloride carbon) on accuracy in measuring density of miniature metal samples by hydrostatic weighing method in glove-box condition.

In the study, tungsten samples of a mass ~200 mg to ~6 g were used simulating high-density materials, i.e. uranium and plutonium. The use of distilled water was found to result in the highest error in measuring density of miniature metal samples. Isopropyl alcohol or tetrachloride carbon were shown to be the most adequate supplementing liquids to ensure the error of less than 0.09 g/cm<sup>3</sup> in measuring density of the samples. At that, the weight of a sample should be not less than 2 g. As a result, the recommended liquid type and sample weight are used in the work of RFNC-VNIITF material science laboratory.

## DETERMINING THE STRUCTURE OF THIN FILMS USING ELECTRON CHARACTERISTIC LOSS SPECTRUM ANALYSIS

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Intensive experimental and theoretical research conducted in recent years has led to significant advances in thin-film formation technologies. However, due to the rapid evolution of information in this field, it is necessary to regularly review current technological approaches and their characteristics. One of the most important tasks in this area remains the study of film characteristics, particularly their mass density, since this allows us to assess the physicochemical properties of the material [1].

Mass density is directly related to characteristics such as mechanical strength, thermal conductivity, electrical conductivity, and optical properties. Moreover, it serves as an important criterion for assessing the quality of coatings in microelectronics, optics, sensors, and other areas where the operational characteristics of devices depend on the stability and homogeneity of the material [2]. Such approaches are particularly relevant for studying nanometer-scale films deposited on sensitive or non-standard substrates. X-ray photoelectron spectroscopy remains a key analytical method, allowing not only to determine the elemental composition of the surface but also to assess the chemical state of the elements and, indirectly, the structure and density of the film. For example, the presence of satellite peaks in the spectra of elements such as Cu and

Co allows us to draw conclusions about the phase state and electron density.

This paper focuses on determining the mass density of thin films of carbon, cobalt, and copper deposited on metal substrates using magnetron sputtering technology. It is demonstrated that XPS can be used not only to determine the elemental composition and chemical states but also for semiquantitatively assessing the density of thin films. Satellite peaks proved particularly important, allowing for precise determination of the state of copper and cobalt.

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## DEVICE AND METHODS FOR SEPARATION OF FINE POWDER MATERIALS

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It is known that many nanodispersed powder materials, including those used to create alloys and composite materials (for example, boron-based materials for nuclear power), are produced using plasma methods, which results in a wide dispersion (size spread). When producing a powder material with particles of a specific size (or size range), it is important to have an appropriate separation method. Existing methods do not always produce the desired result, as the particles tend to aggregate into large conglomerates.

The paper presents devices and methods designed for the separation of finely dispersed powder materials. One method (method I) is based on plasma technologies (in argon plasma), the other (method II) is based on the use of mechanical separation principles (from a suspension in a specially designed device [1]). Using method I, boron particles of 100–1000 nm, intended for introduction into aluminum during the production of boron-aluminum alloys, were separated into particles of 4–11 nm (Fig. 1a) [2], and using method II, FeNi/C particles were separated into particles of 40–50 nm and 6–15 nm (Fig. 1b) [3].

*The research was carried out within the state assignment of Kirensky Institute of Physics, Federal Research Center KSC SB RAS; The research was carried out at the expense of a grant Russian Science Foundation No. 25-29-00794, <https://rscf.ru/project/25-29-00794> (in terms of plasma processing of boron particles).*

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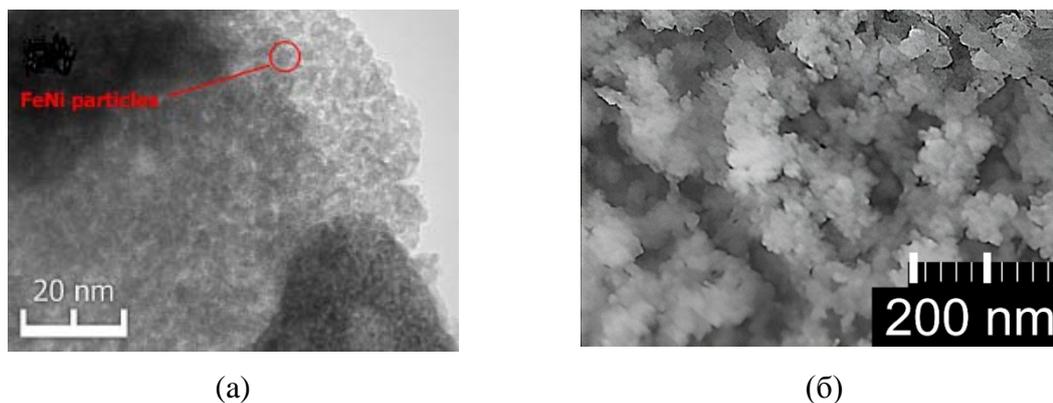


Figure 1. Powder with FeNi/C particles processed in the device [1] (a); boron powder processed by plasma (b). Images were obtained in mapping mode.

## EQUIPMENT AND METHODS FOR X-RAY STRUCTURAL RESEARCH OF ACTIVE MATERIALS

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X-ray diffraction analysis is one of the most common physical methods for studying and controlling materials and components in research institutes and laboratories.

Using various X-ray diffraction analysis techniques, it is possible to determine the phase composition of materials, the composition of solid solutions, the size and shape of crystals, internal stresses, preferred crystal orientations (textures), and other parameters.

Since 2023, JSC INM has been using a laboratory diffractometer for various research of materials and samples with activity up to  $1 \times 10^8 \text{Bq}$ , equipped with a standard sample holder, a thermal chamber, and an Euler attachment.

The thermal chamber allows for research to be carried out in a temperature range from room temperature to  $1600^\circ\text{C}$ , using a system for pumping air out of the chamber, which allows for achieving a vacuum of approximately  $5.5 \cdot 10^{-3} \text{ mbar}$ .

The Euler attachment is used to perform the following tasks: determining stresses of the first and second kind, namely stresses in the entire volume of the sample, as well as stresses in individual grains created due to dislocations and other defects. In addition to these functions, the Euler prefix allows one to determine the preferred orientation of grains in the structure of materials (texture).

The report presents methodological approaches developed at JSC INM for diffraction studies of nuclear reactor core materials, which have found application in substantiating their performance and predicting their properties.

## GENERATION OF PICOSECOND DURATION ELECTRON BEAMS WITH PEAK POWER OF 50 GW

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Generation of high-power pulsed electron beams with durations of less than 1 ns is of interest in radiation physics and chemistry, for obtaining short X-ray flashes, calibration of ionizing radiation detectors, and for generation of high-power microwave pulses [1]. To obtain the shortest and most powerful electron beams traditionally direct-action accelerators are used, the main element of which is a high voltage accelerating pulse generator.

High voltage subnanosecond devices using spark-gap-based switches allow obtaining accelerating voltage pulses with duration of about 100 ps at a voltage up to 1 MV and peak power on the order of 10 GW [2]. Recently a new approach to generating extremely high-power pulses of subnanosecond and picosecond duration has been developed based on nonlinear transformation of the wave travelling in coaxial lines filled with ferrite. Such an approach does not require the use of switching elements and allows obtaining pulses with peak power of about 100 GW at pulse duration of 100 ps [3]. In the present work we describe the use of such a pulse for obtaining picosecond electron beams with peak power of tens of GW in a sealed vacuum diode IMA3-150E with beam extraction into the atmosphere and in a magnetically-insulated coaxial diode (MICD).

To transmit the accelerating pulse to each of the diodes the constructions of transmission lines and feedthrough insulators were developed, providing the best matching of the feeder line. For the measurement of electron energy aluminum filters of varying thicknesses were used, and to register the beam current waveform a collector sensor based on a coaxial transmission line was used. To analyze cross-sectional profiles of the beams, dosimetry film TsVID was used.

Using the IMA3-150E diode an electron beam of round cross section with the following parameters was obtained: maximum energy of 3.2 MeV, peak current of 12 kA, peak power of about 40 GW, pulse duration of about 80 ps, beam diameter of 20 mm. It was found that due to short duration of accelerating pulse the diode can withstand the gradient of 500 MeV/m in the accelerating gap without breakdown. In the design using MICD the beam had the following parameters: maximum energy of about 2 MeV, peak current of about 30 kA, peak power of about 50 GW, and current pulse duration of about 90 ps. The cross section of the beam comprised a ring with the mean diameter of 20 mm and the width of 2 mm.

*The presented research was supported by the Russian Science Foundation, grant No. 24-19-00407, <https://rscf.ru/project/24-19-00407/>.*

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## MULTIPURPOSE CYCLOTRON COMPLEX DC-140 FOR APPLIED RESEARCH.

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The main activity of the Flerov Laboratory of Nuclear Reactions is focused on fundamental science, but considerable efforts are also directed towards applying the accumulated experience in practical fields. Currently, the primary areas of applied science at the FLNR are development of track membrane production methods; ion implantation technologies and radiation materials science; testing on-board electronics (avionics and space) for radiation hardness.

Based on its long-term experience and aiming to enhance the productivity of applied research, the FLNR has developed and implemented a project for a new multipurpose accelerator complex for applied research. Due to user requirements, ease of operation, and pricing policy, the main parameters of the future machine and experimental setups have been defined. DC140 will provide accelerated ion beams with energies of 2.1 and 4.8 MeV per nucleon, up to bismuth.

The multipurpose cyclotron complex includes the specialized compact heavy-ion accelerator DC140 and a complex of dedicated research channels. This report will present the status of the project, the technological parameters of the cyclotron and its experimental infrastructure. The complex is expected to welcome its first users in 2026.

## POSITRON ANNIHILATION STUDIES OF PRECIPITATION IN COLD-WORKED AGING Fe–35.2 at.%Ni–2.9 at.%Ti ALLOY

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The introduction of edge dislocations and interfaces between second-phase precipitates and the matrix in steel reduces swelling in austenitic steels, because dislocations and precipitates act as sinks for point defects formed during irradiation. The nucleation of precipitate particles at dislocations arouses particular interest. In this case, the particles not only act as sinks for point defects but can also influence the efficiency of dislocation-defect interactions and stabilize the dislocation structure [1-2]. However, a complex defect structure is formed in steels and alloys during deformation. Preliminary plastic deformation significantly influences the formation of second-phase precipitates during thermal annealing [3]. Therefore, knowledge of cold-formed aging steels and alloys original microstructure is necessary for correct interpretation the results of their irradiation.

Transmission electron microscopy is the most common direct method for studying the structure of steels and alloys. It reliably identifies the dislocation structure, but cannot detect small vacancy defects and second-phase precipitates smaller than one nm in size. Thus, methods that are highly sensitive to defects both visible and invisible in TEM is necessary to study the deformed alloys.

Positron annihilation spectroscopy (PAS) and residual electrical resistivity (RR) measurements are among such methods. PAS and RR are highly sensitive to point and linear

defects in the crystal lattice. Furthermore, RR is sensitive to atomic redistribution processes in the solid solution. Combining PAS and RR enables for accurate identification of processes that occur during deformation and annealing.

In this study, PAS and RR measurements were used to study the microstructure evolution of a cold-worked, aging Fe-35.2 at.% Ni-2.9 at.% Ti alloy during isochronous annealing. It was found that nanoparticles of the intermetallic  $\gamma'$ -phase Ni<sub>3</sub>Ti formed at dislocations during annealing of vacancy defects reduce the efficiency of positron capture by dislocations. Moreover, this effect depends on the degree of deformation. In particular, the magnitude of the positron capture blocking effect is determined by the ratio of the number of deep positron traps to the number of precipitate particles present at dislocations.

*The work was carried out within the framework of the state assignment of the Ministry of Science and Higher Education of the Russian Federation for the IMP UB RAS with using the equipment of the Collaborative Access Center «Testing Center of Nanotechnology and Advanced Materials» of the IMP UB RAS.*

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## **SYNTHESIS OF BORON-CONTAINING MATERIALS BASED ON ALUMINUM AND MAGNESIUM AND DETERMINATION OF THE QUANTITATIVE CONTENT OF BORON IN THEM**

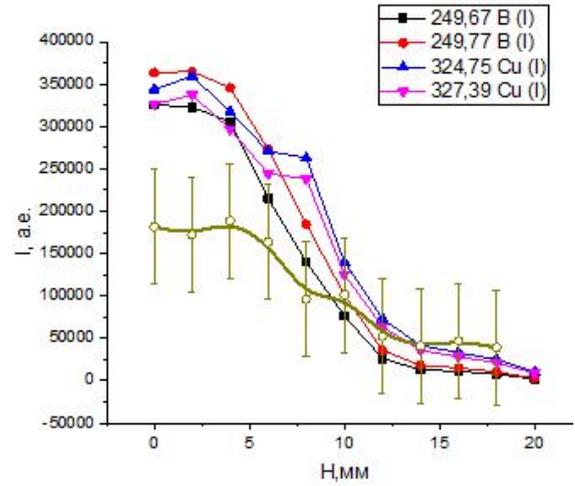
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This paper describes a method and light source for the quantitative analysis of boron content in aluminum and magnesium boron-containing alloys, based on optical spectral analysis. Studies on the production of boron-containing aluminum alloys have shown that their mechanical properties depend significantly on the type of interaction between Al and B [1]. In one case, alloys are obtained in which aluminum and boron do not dissolve in each other and do not react chemically (eutectics), i.e., two phases are formed. In the other case, alloys are obtained in which boron and aluminum form chemical compounds (AlB<sub>2</sub>). The type of alloy depends on the specified synthesis parameters and the amount of introduced elements. Moreover, quantitative determination of the stoichiometry of the resulting substance is a complex task, especially for light elements. Therefore, a method for determining the quantitative content of boron in an aluminum or magnesium matrix is required. To address this issue, we developed a method based on atomic emission spectral analysis using a dual-jet plasma torch as a light source [2], enabling highly accurate quantitative determination of boron content in aluminum and magnesium boron-containing alloys. We use the dual-jet plasma torch as a light source and to control the amount of boron added to the matrix in the boron-containing alloy synthesis setup. To address both issues,

we conducted plasma studies using the dual-jet plasma torch (Fig. 1).



(a)



(b)

Figure 1. Photograph of a two-jet plasma torch (a); pattern of distribution of the radiation intensity of boron and copper lines along the discharge height (b).

The research was carried out at the expense of a grant Russian Science Foundation No. 25-29-00794, <https://rscf.ru/project/25-29-00794>.

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