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

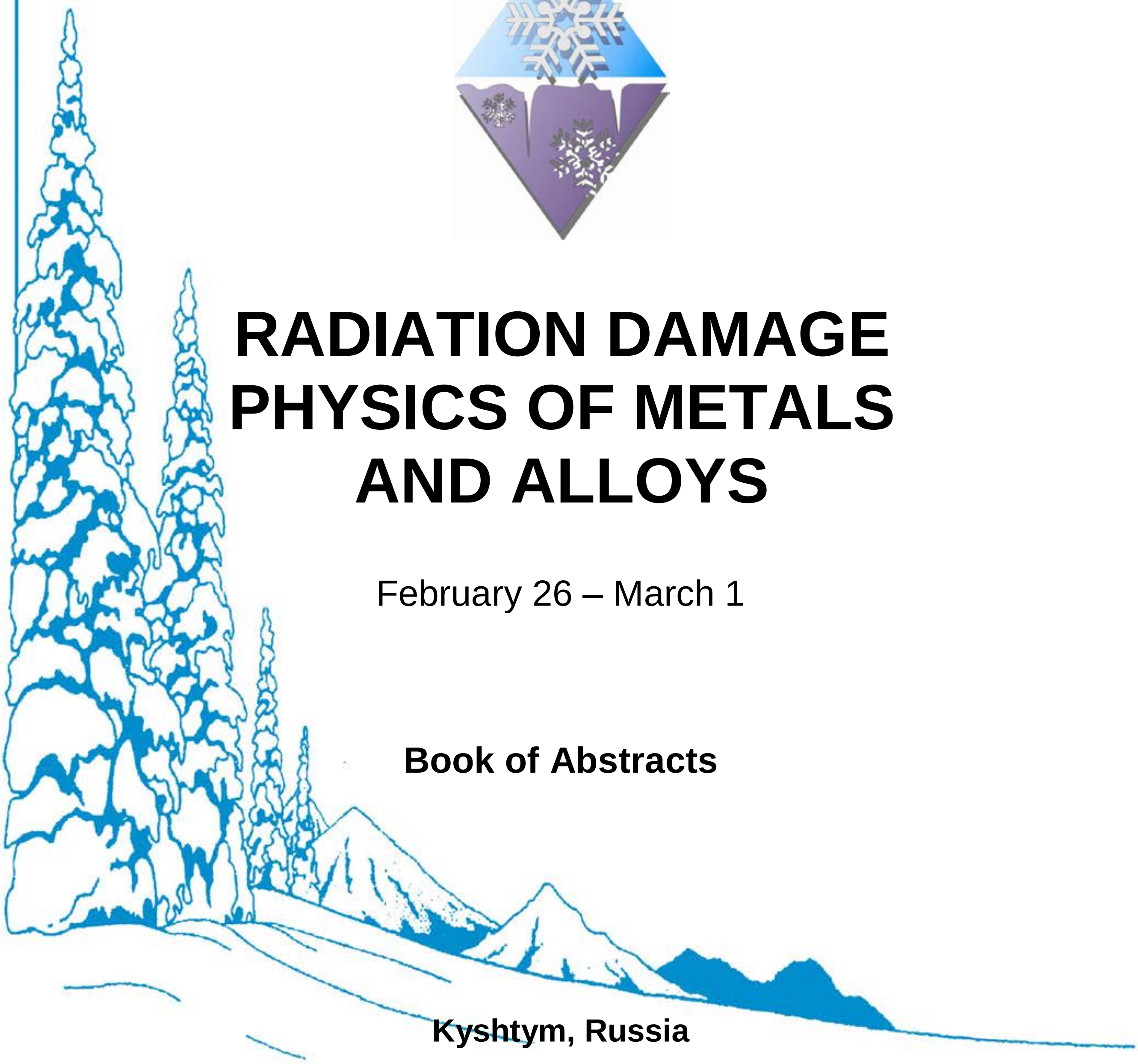
The Scientific Council on Radiation Physics of Solids, RAS

The Fifteenth International Ural Seminar

RADIATION DAMAGE PHYSICS OF METALS AND ALLOYS

February 26 – March 1

Book of Abstracts



Kyshtym, Russia

2024

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The Organizing Committee cordially thanks all Sponsors for their support to the Russian science. We hope that our meeting in Snezhinsk will serve to promote and expand further scientific contacts.

Compiled by
Denis Perminov

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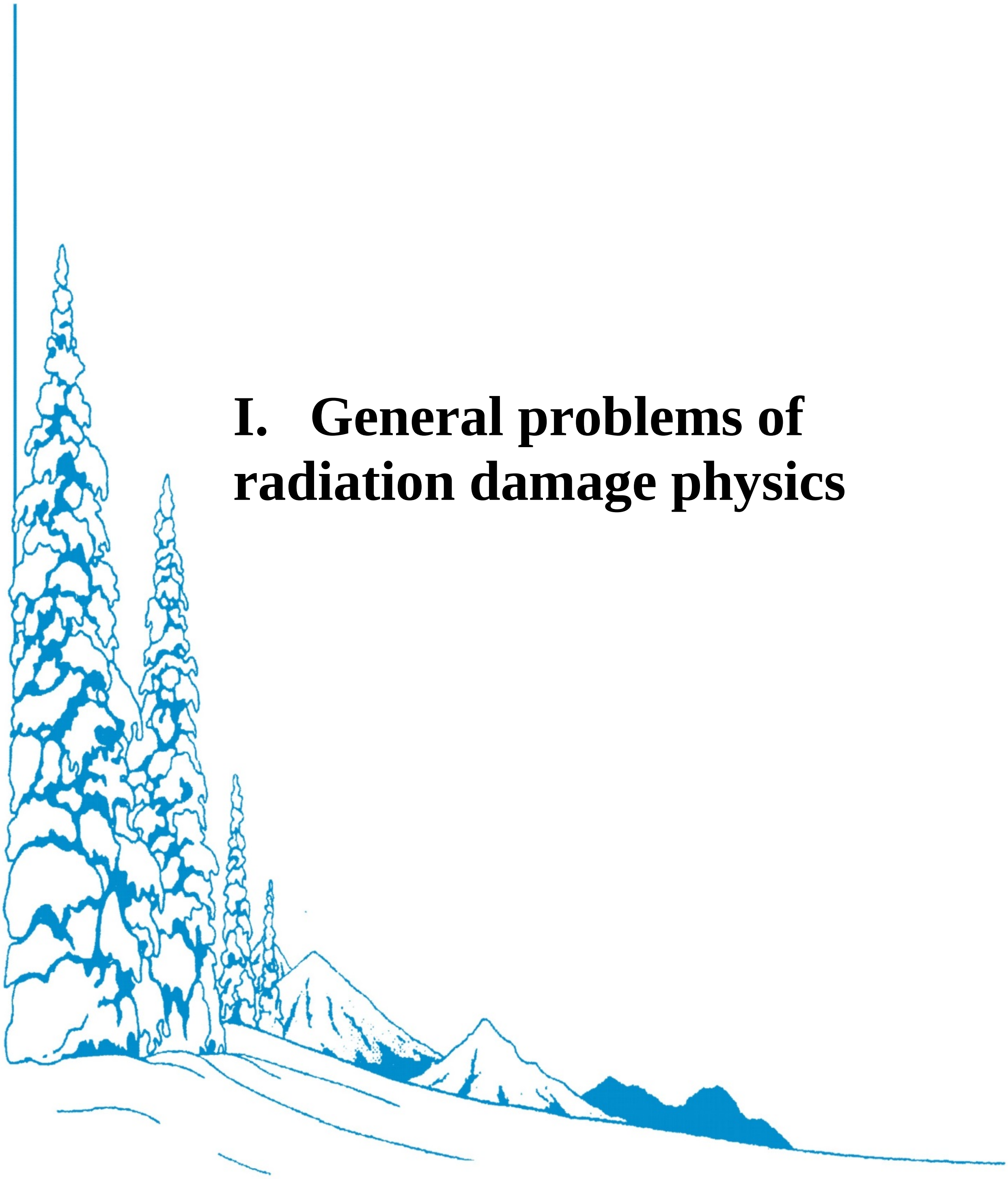

I. General problems of radiation damage physics

CHANGES IN MAGNETIC PROPERTIES DURING POST-IRRADIATION ISOCHRONOUS ANNEALING OF AUSTENITIC STEELS 12Cr18Ni10Ti AND 08Cr16Ni11Mo3 IRRADIATED IN BN-350 AND VVR-K REACTORS

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Neutron irradiation of metastable austenitic steels causes the formation of atomistic and microstructural defects, radiation induced segregation, and transmutation [1]. All these often lead to negative effects as swelling, hardening and embrittlement, and irradiation-induced formation of new phases in the austenitic matrix, for example, α-ferrite enriched in Cr and Fe [2]. Recovery annealing may ameliorate these issues, in which the reactor vessel and internal devices are annealed at high temperatures for several days. In this work, changes in the magnetization of austenitic steels irradiated in the VVR-K and BN-350 reactors (maximum damaging dose 57.6 dpa) during isochronous annealing were investigated and correlated to the reduction in deleterious, irradiation-induced ferrite via changing magnetization measurements.

Samples of steels 08Cr16Ni11Mo3 and 12Cr18Ni10Ti were cut from non-irradiated and irradiated hexagonal casing tubes of fuel assemblies from the BN-350 fast neutron reactor, subjected to preliminary thermomechanical treatment - cold deformation of 20% followed by tempering at 800°C for one hour. Before starting the experiments, the samples were subjected to mechanical grinding and electrolytic polishing in order to remove corrosion products, as the materials were stored in a spent fuel pool for decades. Post-irradiation isochronous annealing was performed in a Nabertherm B-130 furnace in an evacuated tube (<1 Pa) from 150–850°C in increments of 50°C; the holding time at temperature was 30 minutes. The samples were then cooled in an evacuated tube in water at room temperature. After each annealing, electrolytic polishing was repeated to remove the surface layer depleted in alloying elements. The amount of ferromagnetic α'-phase in the samples was measured using a ferroprobe "Feritscope MP-30," pre-calibrated to factory standards. The final result was obtained by averaging of 10–15 measurements.

In this presentation, we present diagrams of changes in the volume percentage of the ferromagnetic α'-phase vs. annealing temperature in °C. It has been determined that annealing of the martensitic α'-phase begins at a temperature of 450-500°C, while the annealing of α-ferrite begins at a temperature of 600°C. Both chemical composition and irradiation parameters such as irradiation temperature and dose rate affect the extent of annealing of these two phases. These results have specific implications for the design of annealing heat treatments to recover beneficial properties of reactor pressure vessels and internals.

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CONSTRUCTION OF A SET OF FUNDAMENTAL PHYSICAL CONSTANTS OF UNIT AND ZERO DIMENSIONS

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A method for obtaining an exhaustive set of multiplicative equations of relationship between the elements of an arbitrary set of the tested physical constants C_j in the form of their products in integer powers m_j ranging from $-N$ to N is proposed and used (calculations were performed for $N = 2$ and 4). A formal application of the proposed procedure reveals the minimum quanta of charge, mass, time, and distance and also a number of the relations describing the most general physical laws. It is shown that it is possible to construct a system of fundamental physical constants l_e, t_e, e_e, m_e, α, and β (α is the fine-structure constant) with the simplest (m, s, kg, C) and zero dimensions to describe electromagnetic and gravitational interactions, as well as with the addition of Boltzmann's constant (*k*), to describe the laws of thermal radiation. Planck's constant (*h*), the speed of light in vacuum (*c*), electric (ε0), magnetic (μ0) and gravitational (*G*) constants are expressed through the revealed minimum quanta of length, time, charge, mass, and dimensionless constants.

DEFORMATION AND DESTRUCTION OF AUSTENITIC STEEL UNDER INFLUENCE OF NEUTRON IRRADIATION

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High-alloy corrosion steels, which include austenitic stainless steels (ANS), are widely used as a structural material for elements of the cores of nuclear power plants, including fuel rod claddings. Work continues to improve and create new materials and methods of processing them in order to increase their performance and durability under irradiation conditions. To do this, it is important to understand the mechanisms of deformation and possible destruction under the influence of loads and neutron irradiation.

Based on cartograms by Forst and Ashby [1, 2] the existing mechanisms of deformation and destruction of ANS, which relate to FCC materials, were analyzed depending on stress and temperature.

The features of plastic flow in the near-surface and internal layers, as well as the nature of destruction of a number of ANS (Х18Н20, Х16Н15М3Б, Х17Н15М3) were studied. It has been established that at temperatures of 400-700 °C in the surface layers, the controlling mechanism of deformation is grain-boundary sliding, and accommodation occurs due to the formation of cracks along the grain boundaries. The internal layers of the material remain continuous, and the contribution to the deformation of various mechanisms (intragranular sliding, grain boundary sliding, diffusion creep) is different and depends on the material and test conditions. The fracture is mixed, predominantly transcrystalline cup-like with a small proportion of intercrystalline.

Irradiation facilitates the formation of surface cracks, reduces deformation before failure, and increases the proportion of intercrystalline fracture in the fracture.

The strength properties of grain boundaries and the matrix of Х16Н15М3Б steel in the initial state and after irradiation to a neutron fluence of $2\cdot10^{21}$ cm^{-2} were assessed. It has been established that after irradiation, the material matrix is strengthened, and the border regions at temperatures above 300 °C are softened. When irradiated samples are deformed, grain boundary sliding occurs with the formation of intercrystalline cracks in the surface layers.

Based on the results obtained, the determining role of grain boundaries in the processes of deformation and destruction of ANS under the influence of loads and neutron irradiation is shown.

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EFFECT OF IRRADIATION WITH FAST NEUTRONS ON THE STRUCTURAL STATE OF NIOBIUM OXIDE

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Niobium monoxide (NbO) is known for its high metallic conductivity [1], due to which it is widely used as a porous anode material in electrolytic capacitors; it has better combustion resistance compared to pure, tantalum and niobium, metals and exhibits more effective self-healing properties at the same morphology [2]. The crystal structure of NbO is ordered into the Nb_3O_3 cubic phase (sp. gr. *Pm*-3*m*), in which Nb ions occupy the 3*c* position with coordinates (0, ½, ½) and O ions – 3*d*: (½, 0, 0), with lattice parameter a = (0.4211±0.0005) nm [3]. In this NbO structure, ordering of 25 % of niobium and oxygen vacancies can be observed at sites 1*a*: (0, 0, 0) and 1*b*: (½, ½, ½), respectively [4], the replacement of which at high pressures (over 70 GPa) induce a transition to the Nb_4O_4 phase [2].

We irradiated a polycrystalline NbO sample with fast neutrons to fluences of $1\cdot10^{18}$ n/cm^2 and $1\cdot10^{20}$ n/cm^2. Niobium monoxide was irradiated in an aluminum container in the vertical channel of the IVV-2M nuclear research facility. Neutron diffraction measurements of NbO before and after irradiation were carried out using the method of elastic coherent neutron scattering on a high-resolution diffractometer D-7a installed on the horizontal channel of the IVV-2M (Department of works in a nuclear reactor (A separate institute subdivision IMP UB RAS in Zarechny). The neutron wavelength was 0.15321 nm. From the calculation of neutron diffraction patterns, it follows that the crystal structure of the initial NbO corresponds to the cubic structure of Nb_3O_3 with a crystal lattice period (0.42110±0.00002) nm. Irradiation of NbO with fast neutrons to a fluence of $1\cdot10^{18}$ n/cm^2 doesn't cause disordering of the crystal structure, only an increase in the lattice parameter up to (0.42137±0.00002) nm is observed, however, a significant background is visible in the neutron diffraction pattern at large angles, which indicates an increase in ion vibrations in structure. Irradiation NbO sample with fast neutrons up to $1{\cdot}10^{20}$ n/cm^2 induces an order-disorder phase transition (*Pm*-3*m* – *Fm*-3*m*) and causes a significant increase in the lattice parameter (*a*) up to (0.42665±0.00002) nm. In Nb_4O_4 phase (sp. gr. *Fm*-3*m*) Nb ions occupy position 4*a* with coordinates (0, 0, 0) and O ions – 4*b*: (½, ½, ½).

This work was supported by the Russian Science Foundation (project 19-73-20012-П, https://rscf.ru/en/project/19-73-20012/) and was performed at the Institute of Solid State Chemistry UB RAS, using Physics Technological Infrastructural Complex of the Institute of Metal Physics UB RAS.

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EFFECT OF RADIATION DEFECTS DIFFUSION MECHANISM ON DISLOCATIONS SINK STRENGTHS IN BCC Fe AND V METALS

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The diffusion of radiation defects (RD) to sinks (dislocations, grain boundaries, subgrains, phase interfaces, etc.) and their absorption lead to the evolution of the microstructure of structural materials for fusion and fission reactors and, as a result, to changes in their physical and mechanical properties (radiation-enhanced creep, radiation embrittlement, and radiation-induced swelling of materials). In order to build physical models of property changes in materials under radiation, mechanical, and thermal loads, it is necessary to know the characteristics of RD, which are parameters of such models. An important characteristic of RD that influences the change in material properties is its diffusion mechanism.

RD such as clusters of self-interstitial atoms (SIA) have a mixed 1D/3D diffusion mechanism: the defect moves along one crystallographic direction with relatively rare changes in the direction of movement. It is known [1, 2] that the length of the one-dimensional displacement of RD can have a significant influence on the sink strengths of various microstructure elements (dislocations, pores, grain boundaries) for these RD.

The presence of non-uniform elastic fields created by microstructure elements (ME) in the case of a 1D/3D diffusion mechanism changes the energies of formation of saddle configurations of RD for processes of its migration or change of diffusion direction (reorientations). This leads to changes in the frequencies of diffusion jumps and reorientations of RD and, accordingly, to changes in the sink strengths of ME.

In this work, using the kinetic Monte Carlo method, the sink strengths of dislocations of various types for di-interstitials (clusters of SIA consisting of two SIAs) in the temperature range of 300-1000 K for BCC Fe were calculated. A comparison of the sink strengths of dislocations for di-interstitials, calculated taking into account the 1D/3D diffusion mechanism and using a previously developed approach [3-5], in which the diffusion of di-interstitial was reduced to an effective 3D mechanism, was carried out.

The research was funded by the Russian Science Foundation grant № 23-7201090, https://rscf.ru/project/23-72-01090/

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FORMATION AND EVOLUTION OF RADIATION DEFECTS UNDER LOW-TEMPERATURE NEUTRON IRRADIATION

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In the study of processes occurring in materials, the rate of radiation damage and the damaging dose are usually used as characteristics of exposure to neutron irradiation. This is often not enough to describe the evolution of a microstructure, since it depends not only on the number of point defects generated, but also on their mutual configuration. Everywhere, calculations of the damaging dose are carried out according to a standardized scheme, which makes it possible to compare the effect of irradiation on materials in different reactors. However, verification of these calculations on experimental material is practically not carried out, since (i) the dynamic stage (formation of a cascade, the time of the stage is $10^{-16} \div 10^{-15}$ s) is followed by (ii) the kinetic stage (within $10^{-10} \div 10^{-9}$ s) at which the cascade evolves in the area of its formation and then there is (iii) the thermodynamic stage – interaction with point defects that have entered the matrix from different cascade regions (during the rest time of the irradiation). Only after that, the object becomes available for experimental research. At the same time, initial conditions have a significant impact on the evolution of the microstructure and, as a consequence, the properties of the irradiated materials. The problem of the correct description of the effect of neutron irradiation at the dynamic and kinetic stages remains relevant.

The system is least susceptible to changes at the thermodynamic stage in the case of cryogenic neutron irradiation, when both vacancies and interstitials do not have thermal mobility. Such work was carried out at the IWW-2M reactor in the period 1987–1998, but later the technology turned out to be temporarily unclaimed and was lost. Currently, the IWW-2M reactor has the possibility of low-temperature neutron irradiation, in which the interstitials are mobile, and vacancies are practically unable to migrate through the crystal.

The main purpose of the presented work was: (i) to conduct low-temperature neutron irradiation of Cr, as a representative of the BCC structure, (ii) to describe the evolution of radiation defects in it using the developed apparatus, and (iii) to verify the calculated characteristics of point defects and their complexes accumulated during irradiation, based on experimental results of post-reactor studies.

In the paper, the elastic interaction model is used to calculate the energies (i) transferred by neutrons to a primary knocked-on atoms and (ii) of colliding ions during interaction with each other. The following were obtained: (i) the energy spectrum of the primary knocked-on atoms, (ii) the number of cascade regions, their size distribution and the number of point defects contained in them. At the same time, not molecular dynamic calculations were used, but the apparatus of statistical thermodynamics. Within the framework of the approach used, the rates of accumulation of single point defects, as well as their double and triple complexes by the end of the kinetic stage were calculated.

The calculated characteristics were compared with the results of dilatometric dimensional changes associated with the release of vacancies from the irradiated sample, as well as with the results of microstructural studies using transmission electron microscopy.

The research was carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme "Structure" No. 122021000033-2)

INJECTION-ENHANCED ANNEALING KINETICS OF POINT AND GROUP RADIATION-INDUCED DEFECTS IN GaN LEDs

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Injection-enhanced annealing is widely used for bipolar devices and is attractive in particular in that the annealing of radiation-induced defects can occur at significantly lower temperatures if compare to conventional temperature annealing. For example, high-temperature annealing of GaAs samples irradiated with 1 MeV electrons can intensively proceed only at about 200 °C. Meanwhile, in case of injection-enhanced annealing of such samples, it would be observed under the temperature of liquid nitrogen (77 K) [1]. The same is true for many other semiconductor materials such as SiC, InP, etc. with GaN being the less studied among them [2,3]. Injection-enhanced annealing is believed to be used as a method to increase radiation resistance of bipolar devices. On the other hand, this effect makes it more difficult to estimate their radiation resistances. To the authors' knowledge, the available works do not pay much attention to the differences between the processes of annealing the defects induced by various types of ionizing radiation. Thus, this work is aimed at experimentally investigating different injection-enhanced annealing processes of radiation defects in modern gallium-nitride heterostructures.

GaN LEDs were studied with peak electroluminescence wavelengths of 365 nm and 450 nm. The LED active region contains quantum wells which allow significantly increasing device efficiencies. An essential advantage of LEDs as objects of research is that recording of optical characteristics enables obtaining data directly from the active region. Nuclear reactor, neutron generator (14 MeV neutrons), and ^{60}Co γ-quantum isotopic source were used as ionizing radiation sources. Since fast-neutron and gamma-quanta runs are highly larger than samples sizes, the formed defects in all three cases were uniformly distributed over the volume. To study the kinetics of injection-enhanced annealing, time dependence of electroluminescence power was measured while passing 1 – 20 A/cm^2 direct current through the diodes arranged on an aluminum heat remover. This allowed completely excluding the influence of temperature on injection-enhanced annealing.

In the study, injection-enhanced annealing of heterostructures irradiated with gamma-quanta and neutrons was shown to have significantly different kinetics: in the former case the samples were completely recovered, and in the latter one only 30-50 % of all defects were annealed (at a current density of 4 – 20 *A/cm*^{2}). The kinetics of injection-enhanced annealing was found to have the second order of reaction. Also, a component almost immune to annealing was additionally observed in annealing of neutron-induced damage. The revealed differences are likely to be conditioned by the presence of group defects (radiation clasters) in the samples irradiated with neutrons which are resistant to injection-enhanced annealing. The obtained experimental results are described by this hypothesis using the Gossik model.

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JOINT ACTION OF PULSED ION BEAMS AND PLASMA ON TANTALUM SURFACE

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A combined effect of pulsed ion and plasma fluxes on the surface layer of tantalum sheet samples was studied using two Plasma Focus installations, differing in stored energy E: PF-1000 (E up to ≈ 1 MJ) and PF “Vortex" (E ≈ 5 kJ), using deuterium or helium as a working gas. The ion power density was q ~ 10^{11} W/cm^2 and q ~ 10^9 W/cm^2 at pulse durations τ = 100 and 20 ns, respectively. The intensity of the plasma exposure was about an order of magnitude less than that of the ions, and the duration was 2-3 times longer.

It was found that in the microstructure of the surface layer of samples irradiated in PF Vortex, there are many craters – traces of the implanted gas, while in the structure of samples irradiated in PF-1000, their number is insignificant. The observed differences are related to the difference in the size of the vaporized layer in the compared experiments. When irradiated in a more severe mode in the PF-1000 installation, the layer with implanted ions completely evaporated. In a less severe irradiation regime in the PF Vortex, deuterium or helium implanted in Ta contributed to the boiling of the melt of the surface layer and the creation of additional stresses in it after solidification.

X-ray structural studies of the samples showed texture changes in the near-surface layers after irradiation in PF. The main feature of the changes is an increase in the intensity of reflexes from the family of planes {211} in comparison with both the original cold-formed and the reference annealed samples. The formation of the texture is associated with a directional heat sink during crystallization and cooling of the molten layer.

It was found that when irradiated in a more rigid mode in the PF-1000 installation, the microhardness of Ta practically does not change, and irradiation in the PF Vortex installation in a less rigid mode contributes to its increase. The reason for the observed effects may be the predominance in the first case of the role of the thermal effect of radiation fluxes, and in the second – the dominance of the process of implantation of working gas ions and the effect of stresses arising during ultrafast crystallization and cooling of the molten surface layer.

The influence of the type of working gas (deuterium or helium) on the microstructure, texture and microhardness of the surface layer in tantalum samples after irradiation in the PF Vortex is estimated. There was no difference in changes in surface morphology and texture when using deuterium or helium. At the same time, the microhardness of the surface layer increases significantly more when using helium as a working gas than when using deuterium. At the same time, with an increase in the number of pulse effects N in the studied range (up to N = 30), the effect of hardening of the remelted layer increases, and more significantly when using helium.

The work was carried out according to state assignment No. 075-01176-23-00

MULTISCALE APPROACH TO MODELLING OF RADIATION CREEP AND RADIATION SWELLING IN METALS

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Materials of nuclear, thermonuclear and hybrid systems must withstand temperature, mechanical and radiation loads during their operational lifespan without losing their functional properties, and be compatible with their environment (coolant, etc.). The operating conditions of materials of thermonuclear and hybrid systems partially overlap with the operating conditions of materials of nuclear reactors (temperatures, mechanical loads, damaging doses – dpa), so there is a desire to transfer the existing extensive developments in relation to materials of nuclear reactors to thermonuclear and hybrid applications.

Despite the mentioned overlap of part of the operating conditions, there is no such intersection with respect to another part of the operating conditions (e.g., differences in neutron spectra), which limits the possibility of direct transfer of experimental data on the behavior of materials under irradiation in one type of installation to installations of another type. A possible way to bridge the gap between the available and necessary data on the behavior of materials in the facilities being developed is to build physically based models of the material that describe its response to external influences (neutron, mechanical, thermal, etc.). Such models will provide a deep understanding of the physics of radiation-stimulated processes occurring in materials and will have predictive power, in contrast to models with weak or absent physical justification, which are able to describe any experimental data, but are not able to predict the behavior of the material when the operating conditions of the material change.

The use of a purely theoretical approach to the description of phenomena occurring in materials is limited by the structural complexity of the objects being modeled; therefore, in practice, computational modeling methods based on theoretical methods are used. Since no modeling method can fully cover spatial and temporal scales, a multiscale approach has been developed in which each computational method is applied at a specific spatial and/or temporal scale, using as input parameters data provided by other lower-scale computational models. The output data of the model of the considered scale, in turn, are the input parameters of the model of a higher scale.

Only the combined use of a multiscale modeling approach and comprehensive experimental research will allow for a complete understanding of the physics underlying changes in material properties during operation: models provide a rational explanation of experimental observations based on fundamental physical laws and possible mechanisms, while experimental data allow for validation and calibration of the models.

In this work, within the described approach, a multiscale model of radiation-induced deformation of metals is proposed; its validation and calibration are carried out based on comparing its results with a number of experimental data regarding such radiation phenomena as radiation creep and radiation swelling in BCC (Fe, V) and FCC (Cu) metals.

STABILITY OF THE ALLOYS WITH YTTRIUM OXIDES ADDITIVE UNDER ION IRRADIATION WITH FISSION FRAGMENTS ENERGIES

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High entropy alloys (HEA) are considered as perspective constructive materials for nuclear power facilities. Extensive research is ongoing with respect to their structure and mechanical properties under irradiation conditions simulating reactor environment [1,2].

The present work is dedicated to the Fe-Cr-Co-Ni based material obtained by spark plasma sintering (*SPS)* process at 980°C with additional alloying by yttrium oxides particles. The fission fragment impact simulation is accomplished by 150 MeV Xe ions with fluences up to 10^{14} cm^{-2} at IC-100 cyclotrone.

Transmission electron microscopy and X-ray diffraction studies showed that SPS leads to the formation of FCC phase of FeCrCoNi with grain size up to 1 micron. The nanosized oxide particles of different type containing yttrium in the structure are also registered. Ion irradiation leads to particle amorphization and stalking faults defects formation. Correlation between nanohardness and fluence value was observed. The role of radiation-induced structure changes for mechanical properties is discussed.

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STUDY OF MECHANICAL PROPERTIES AND FRACTURE FEATURES OF FERRITE-MARTENSITIC STEEL EP-450 IRRADIATED BY NEUTRONS IN THE BN-350 REACTOR

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Fast reactor core materials require steels and alloys resistant to high-energy neutron fluxes and capable of maintaining sufficient medium-temperature strength. EP 450 ferritic-martensitic steel, containing 11-13.5% chromium, is used as an acceptable material for cladding and covers of fuel assemblies (FA) of fast reactors with sodium coolant. Its competitive advantage is the high resistance to swelling and creep, especially at elevated core temperatures. At the same time, one of the problems of ferrite-martensitic steels is that with increasing dose of neutron irradiation the brittle-ductile transition temperature increases, which leads to a sharp decrease in ductility at relatively low temperatures typical for operation.

In this work, EP 450 (1Cr13Mo2NbVB) steel were investigated and samples cut from hexagonal wrappers of fuel assemblies of BN-350 reactor unirradiated and irradiated with neutrons to 50.4 dpa, heat treatment was carried out before irradiation — 1050°C for 30 minutes followed by tempering at 720°C for 1 hour. For uniaxial tensile tests, specimens with geometric dimensions of the working part 10×3.5×0.3 mm were used. The tests were carried out at room temperature, strain rate — 0.5 mm/min. The structure features were investigated using Hitachi TM-4000 PLUS electron scanning microscope and JEOL JEM-2100 transmission electron microscope. Vickers microhardness was determined using an eVick-1A microhardness tester (indenter load 50 g).

As a result it was revealed that irradiation of EP-450 steel with fast neutrons leads to a decrease in ductility and increase in strength of the material, while the uniform deformation of the alloy irradiated to 50.4 dpa decreases catastrophically to 1-2% due to the effect of low-temperature radiation embrittlement. The deformation, in this case, was limited within a few ferrite grains favorably oriented to the loading axis. According to fractographic studies of the fracture zone, the fracture in un-irradiated steel is ductile, while that of the steel irradiated to 50.4 dpa is brittle-ductile or brittle depending on the irradiation temperature. The paper discusses the influence of irradiation parameters on the strength, ductility and fracture of EP-450 steel.

THEORETICAL STUDY OF RADIATION-INDUCED SWELLING IN COPPER, VANADIUM AND AUSTENITIC STEEL IRRADIATED WITH NEUTRONS

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So far there are two well-developed swelling theories. One of which, was developed soon after the discovery of void swelling, is fully determined by the dislocation bias, i.e., preferential absorption of self-interstitial atoms (SIA) by dislocations. The dislocation bias is indeed an important mechanism; moreover, it solely determines swelling accumulation during electron irradiation with energy ~ 1 MeV. However, it does not explain swelling accumulation during neutron irradiation since defect production in the case is qualitatively different: in addition to single vacancies and SIAs migrating three-dimensionally, small interstitial loops migrating one-dimensionally are also produced, which is accounted in so-called Production Bias Model (PBM) [1, 2].

The qualitative difference in swelling accumulation in the cases of electron irradiation and neutron irradiations was demonstrated in [3], and was devoted to swelling accumulation in Cu irradiated with electrons, protons, and neutrons at low radiation dose (up to 0.01 dpa). The data presented in [3] are analyzed in this presentation based on calculations taking into account both the mechanisms: dislocation bias and production bias. The results obtained by the calculations demonstrated good agreement with the experiment [3].

Vanadium alloys are considered as promising materials for the manufacture of fuel element claddings in fast neutron nuclear reactors and blankets for thermonuclear installations. In this presentation, the results of numerical modeling were compared with known data from experimental study [4] carried out in pure vanadium irradiated at a temperature of 370°C to a radiation dose of 1.3 dpa.

Experimental swelling data measured in stainless steel (316) for the fast neutron nuclear reactors internal components [5] were also compared to the results of cluster dynamic approach for irradiation doses of up to 100 dpa. Obtained computation results showed reasonable agreement with the experimental data.

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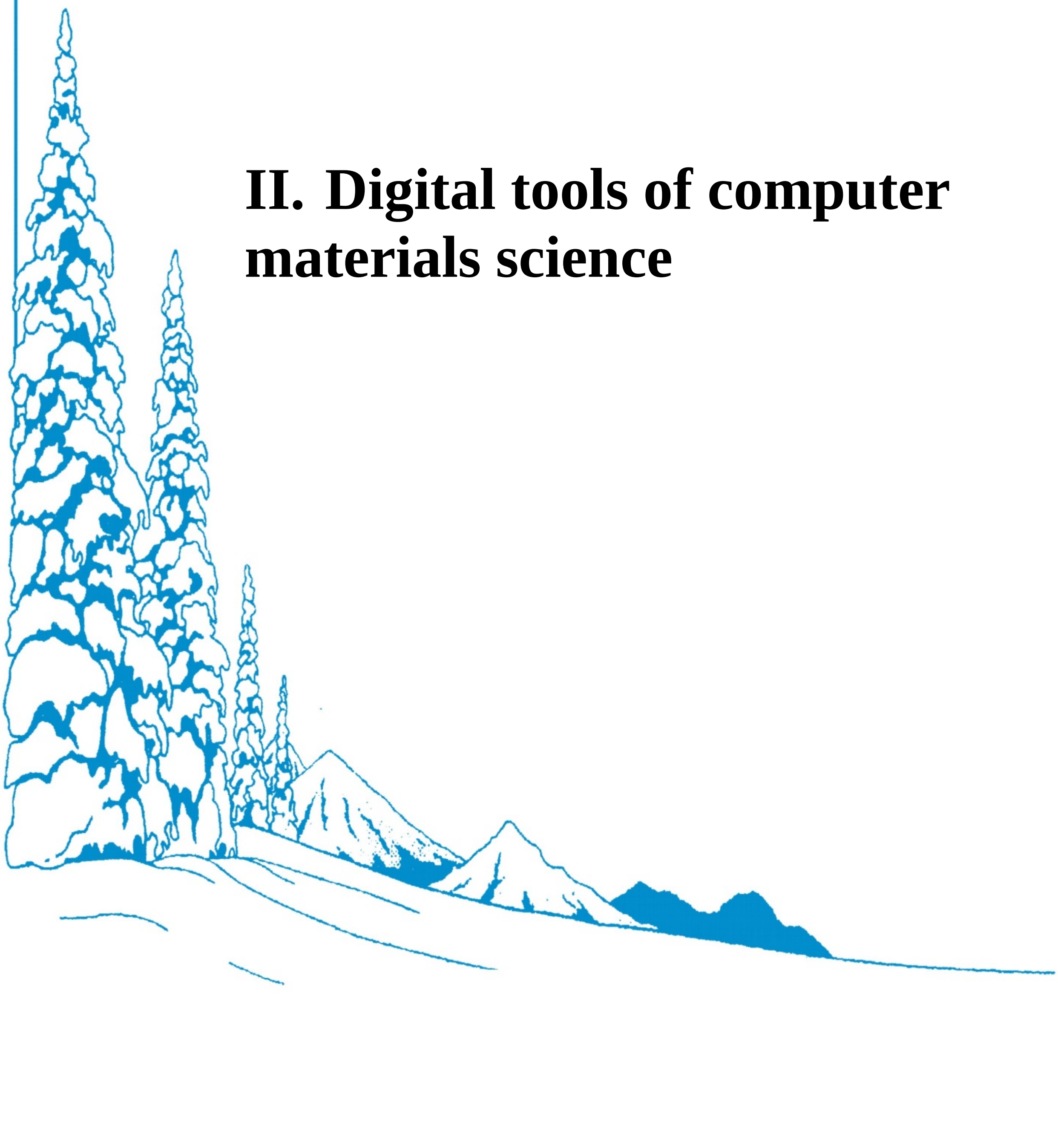

II. Digital tools of computer materials science

FINITE ELEMENT MODELING OF CASTING PROCESSES, HEAT TREATMENT AND STRUCTURE FORMATION OF CAST WORKPIECES

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In the modern world technologies develop at incredible speed, science and technique are closely intertwined, the use of effective modeling methods is becoming more important. One of these methods is the finite element modeling (FEM), which finds its application in a variety of industries. It is worth noting that FEM is one of the most accurate and universal methods of modeling, which allows you to study complex physical and chemical processes and phenomena. The FEM method is based on the division of the studied area into many final elements, for each of which a system of equations describing the studied process is solved. Due to its versatility, FEM method can able you to simulate a variety of objects and processes.

The work considers the importance of FEM and its role in the optimization of technological processes used both in laboratory conditions for the manufacture of samples and in large - capacity fertilious metallurgical production. The algorithm for the preparation of models in modern CAD systems, the stage of preparing the calculated nets and the construction of an array of elements, as well as the necessary boundary conditions and analysis of the data obtained are described.

Studies have been carried out to assess the influence of calculation parameters and thermodynamic characteristics of the simulated material on possible casting defects in the finished casting and the main approaches to optimizing casting equipment and technological parameters of the casting and heat treatment process have been demonstrated.

FIRST-PRINCIPLES STUDY OF THE PROPERTIES OF RADIATION DEFECTS IN SILICON

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Defects in semiconductors, particularly in silicon, can cause energy levels in the band gap as a result of irradiation. These defects can actively affect the transport of charge carriers, particularly through the generation and recombination of carriers via defect levels in the band gap. Among the numerous known defects in silicon, experimental data demonstrate that not all defects are equally effective in degrading the performance of electronic devices [1]. Therefore, we are interested in modeling the recombination of charge carriers through defect levels in silicon devices, specifically the probability of capture and emission of carriers, characterized by a capture cross section. The experimental measurement of cross section values is complicated by many factors, making the theoretical calculation of cross sections from first principles an important task [2].

This study presents the results of first-principle modeling of some of the main radiation defects in silicon: vacancy, double vacancy, and triple vacancy. The calculations were carried out within the framework of density functional theory using the hybrid functional of the exchange-correlation energy, HSE06. The local atomic structures of the defects were analyzed, and a description of their changes during carrier capture was presented. For the triple vacancy, the possibility of having two atomic structures depending on the charge state of the defect is shown. Additionally, the formation energies and the position of the defect energy levels in the band gap were calculated.

A static approximation was used to calculate the capture sections in the work. Phonon matrix elements were calculated in the one-dimensional approximation, taking into account the anharmonicity of oscillations [3]. As a result, the values of the capture cross sections of both majority and minority carriers at defect levels were calculated. A comparison of the calculated and available experimental values was carried out, showing good agreement.

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MODELING OF THE KINETICS OF SECONDARY PHASES FORMATION IN MULTICOMPONENT SYSTEMS BY METHODS OF COMPUTATIONAL MATERIALS SCIENCE

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The kinetics of the formation of secondary phases in multicomponent systems during radiation treatment was studied by methods of atomistic modeling using low-rank interatomic potentials (LRP) [1] and thermodynamic modeling using the Thermo-Calc program code [2]. Atomistic modeling with LRP was performed for Fe-Cu, Fe-Cr and Fe-Cr-Si-Ni-Mn systems. Formation of precipitations was carried out by the means of Thermo-Calc program code for systems Fe-Cu, Fe-Cr-Si-Ni-Mn and chemically close to Chs139 and EP823 steels. The influence of radiation-enhanced diffusion, interstitial clusters and ballistic mixing was taken into account in both types of computations. The empirical parameters of calculations using the Thermo-Calc program code (interfacial energy and additional Gibbs energy for phases) were selected on the basis of the results of secondary phases formation obtained using LRP.

The obtained values of the concentration and the average size of the precipitates of secondary phases are consistent with the published experimental data for the studied systems. It was shown that for different types of irradiations (for example, ion and neutron), the ratio between the number of ballistic and diffusion jumps was different. This had a strong effect on the dose dependence of the concentration and the average size of the precipitations for different types of irradiations.

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MONTE CARLO MODELING OF LOW-ENERGY ELECTRONS KNOCKED-OUT BY IONS OF MODERATED ENERGIES IN SILICON DEVICES

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We consider an action of Si^+ ions with moderate energies initiated by a neutron irradiation on a bulk silicon and SiO_2 as well as on interfaces “metal/silicon” and “metal/oxide/silicon”. Using the Monte Carlo calculations [1], we modeled the motion of the considered ions and subsequently determined the spectra of knocked-out primary and secondary electrons inside the slabs of different materials. We also found out an influence of oxide layer thickness and also a contribution of an intrinsic electric field as a function of an applied voltage on a number of electrons transferred through the oxide slab. Using our method, we could take into account the spatial and temporal scales of the described phenomena, which we cannot achieve by the known specialized approaches of classical molecular dynamics (eFF) or quantum modeling (TDDFT). The processes of elastic electron-electron collisions, ionizations of an atom by ion or by electrons, electron capture, optical phonon excitation in silicon dioxide were considered on the base of physical models introduced in the package of Geant4/MicroElec [2]. This package was modified by the authors for the four aims: to correct electron stopping power of silicon ions, to be able to use many volumes filled by different materials, to track the transitions of particles between the invented volumes and to set up local electric fields in these volumes.

Unless the direct modeling of Si^+ motion in silicon, SiO_2 and metal slabs, we have additionally carried out computation of mean energy per electron-hole pair for a monoenergetic electronic beam decelerated in bulk silicon or their oxide. We have shown that the mean energy per electron-hole pair behaves non-monotonously with the energy of an electron in the beam as was previously described for X-ray photons absorbed in silicon [3]. In the limit of maximum considered electron energy, the mean energy per electron-hole pair becomes close to the well-known constant of 3.62 eV/pair [4].

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MULTI-SCALE MODELING OF THE EFFECTS OF SWIFT HEAVY IONS IN SOLIDS

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A combined Monte Carlo (MC) and Molecular Dynamics (MD) approach enables us to study in detail effects of different stages of swift heavy ion (SHI) track formation. The MC model TREKIS [1] describes excitation of the electronic system and energy transfer to the lattice providing initial conditions for the MD simulations of subsequent lattice response. We discuss here the kinetics of individual track formation, tracks overlap and surface modifications in some amorphizable (YAG, Mg_2SiO_4) and non-amorphizable (Al_2O_3, MgO, CaF_2, CeO_2, ZrO_2) solids irradiated with SHIs. Transmission electron microscopy analysis of samples irradiated with high-energy heavy ions is used to validate the developed model and to investigate the link between the basic properties of the studied materials and the kinetics of structural changes of the targets. We demonstrate the following:

1) The size and morphology of individual latent tracks and tracks overlap at high fluences are strongly affected by recrystallization of the transiently disordered zone [2].

2) Protrusion of molten material and a final structure of surface defects induced by an SHI are governed by mobility of target atoms, surface tensions and recrystallization of a material during the ultra-short cooling period [4].

3) A target thickness affects formation of surface defects under SHI irradiation: the thinnest layers form a through hole, semispherical and spherical hillocks are created after an ion impact at medium thicknesses, whereas nanoparticle emission occurs from thick layers [5].

4) Impact of an SHI under a grazing incidence results in formation of a groove-like structure vs. a chain of nanohillocks depending on material and irradiation properties.

5) Irradiation of nanocrystlline non-amorphizable materials significantly affects the morphology of grain boundaries, which leads to the aggregation and enlargement of nanograins [5].

The study was supported by the Russian Science Foundation №23-72-01017, https://rscf.ru/project/23-72-01017/

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SIMPLIFIED ATOMISTIC BASED KINETIC MODEL FOR SWELLING PREDICTION

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One of the main materials for existing reactors and candidate materials for next generation reactors are austenitic steels [1]. In austenitic steels, one of the key problem is swelling, which can reach value 5% at doses 30-40 dpa and significantly limits their service life of both as core materials and internals. Swelling phenomena is also observed in steels of the ferritic and ferritic-martensitic classes, but at higher doses.

To understand the key properties of material, which determines swelling, it is important to develop various theoretical and experimental methods for swelling prediction. Neutron irradiation remains expensive and time consuming, but is necessary to justify the safety of the materials used. Accelerated testing based on ion irradiation is now actively used to probe candidate materials [2–4]. At the same time, the correspondence between ion and neutron irradiation remains not fully understood [2–4]. In this regard, it is relevant to develop models and programs for swelling prediction [5], comparative analysis of ion and neutron irradiation, approximation and extrapolation of experimental data and analysis of the swelling mechanisms in materials.

In this work, simplified kinetics with several self-consistent models is proposed for swelling prediction [6]. It is based on the rate theory and atomistic simulation, while focusing on the description of experimentally observed bubbles and voids evolution and swelling. In this way, several models are proposed. They include the self-consistent accounting for the vacancy diffusion coefficient and the formation energy, models of heterogeneous bubbles nucleation, interstitial cluster sink and spatial inhomogeneity of sinks. Parametrized model shows the reasonable agreement with experimental data on AISI CW 316 steel, irradiated at various temperatures and doses in fast reactor EBR-II. The influence of interstitial cluster sink and dislocation annealing on temperature dependence of swelling is discussed.

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SWELLING MODEL WITH EXPLICIT SPACE DISTRIBUTION OF SINKS

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The microstructure of the material plays a key role in swelling. The surface, grain boundaries, dislocations, dislocation loops, bubbles, and pores are sinks for mobile defects and impurity atoms, in particular for interstices, vacancies, and helium atoms. When calculating swelling within the framework of the mean field theory, the microstructure of the material is considered as a term in the kinetic equations with a certain rate constant, which is determined by the magnitude of the drain force and the diffusion coefficients of defects. Thus, the entire volume of the material is described on average by a certain value. When analyzing swelling using mean field theory, to match the pore size distribution function, it is sometimes necessary to introduce the distribution of drainage forces [1], which effectively reflects the heterogeneity of the distribution. The actual microstructure of materials is a significantly heterogeneous environment in which the density of wastewater can vary significantly from place to place. The mean field theory allows one to take into account the distribution of runoff only on average, which imposes restrictions on the calculated dependencies.

Also, average values, for example, the amount of swelling, may not be reproduced. Since the function of swelling from the runoff force is nonlinear, the value of swelling from the average is not equal to the average of the swelling values. As a result, it is fundamentally impossible to reproduce the dependency. An example is the region of high temperatures, when the dimensions of the critical nucleus are large. When considering average drainage forces, bubbles may not reach a critical size and pores will not appear. If there is a distribution of drainage forces, then in some places the critical size will be smaller, and some pores will form. As a result, swelling will decrease less sharply depending on temperature.

Also, as an example of the experimentally observed effect of heterogeneity on swelling, it is worth citing the results of ion irradiation. During ion irradiation, due to the influence of the surface as a drain, a zone without pores is formed near the surface. The boundaries of this zone are selected empirically; the characteristic region is from 100 to 300 nm.

To correctly determine the concentration of defects far from the drain, it is necessary to carry out calculations based on solving diffusion equations. In this case, the drains can change dynamically due to the appearance of bubbles and pores. For this purpose, a model was developed to calculate the influence of the nonuniform distribution of microstructural defects on swelling in structural materials.

At the initial stage, the spatial distribution of sinks is determined: surfaces, dislocations, and irradiation conditions are also set. Next, the spatial distribution of runoff is used to calculate the runoff at each point in space. A diffusion calculation is carried out for mobile defects. In this case: interstices, vacancies, helium atoms. Next, the concentrations of defects are used to calculate the kinetics of bubble nucleation, bubble growth, their transition into pores, and pore growth. After this, the effluent distribution is updated to take into account the change.

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THE INFLUENCE OF THERMODYNAMIC CHARACTERISTICS AND MESH SIZE ON THE ACCURACY OF MODELING CASTING DEFECTS

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One of the most important aspects of the development of competitive technologies in the modern world is the use of CAD/CAM/CAE systems in the preparation of production and production. CAE systems (computer-aided engineering) allow solving computational problems on structural strength, modeling of heat and mass transfer flows, aero- and hydrodynamics, etc. In this paper, one of the main problems of modeling accuracy is considered from the point of view of setting boundary conditions and the size of the calculated elements.

The paper analyzes the influence of the calculated elements size and the thermodynamic characteristics of the melt on the speed of calculations and the reliability of the results on the example of the finite element calculation of the casting operation of alloy 17CrNiMo6 (an analog of alloy structural steel 20KHN2M). The preparation stages of the calculation, the analysis of the dependence of the results on the varied design parameters are given, the sizes and localization of possible casting defects are demonstrated, as well as possible ways to optimize casting equipment to prevent them.

USE OF THE PHOTOGRAMMETRICAL RECONSTRUCTION OF THE FRACTURES DURING THE FRACTOGRAPHIC EXAMINATIONS — ADVANTAGES AND FIRST RESULTS

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The paper presents the results of the fractographic analysis of a standard depleted-uranium sample after the mechanical tensile testing (figure 1). The photogrammetrical reconstruction of the sample fracture surface at high magnification followed by the fracture quantitative characterization and analysis were used in the studies (figure 2).

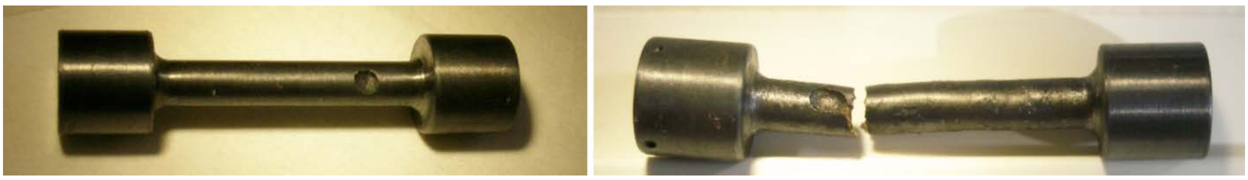
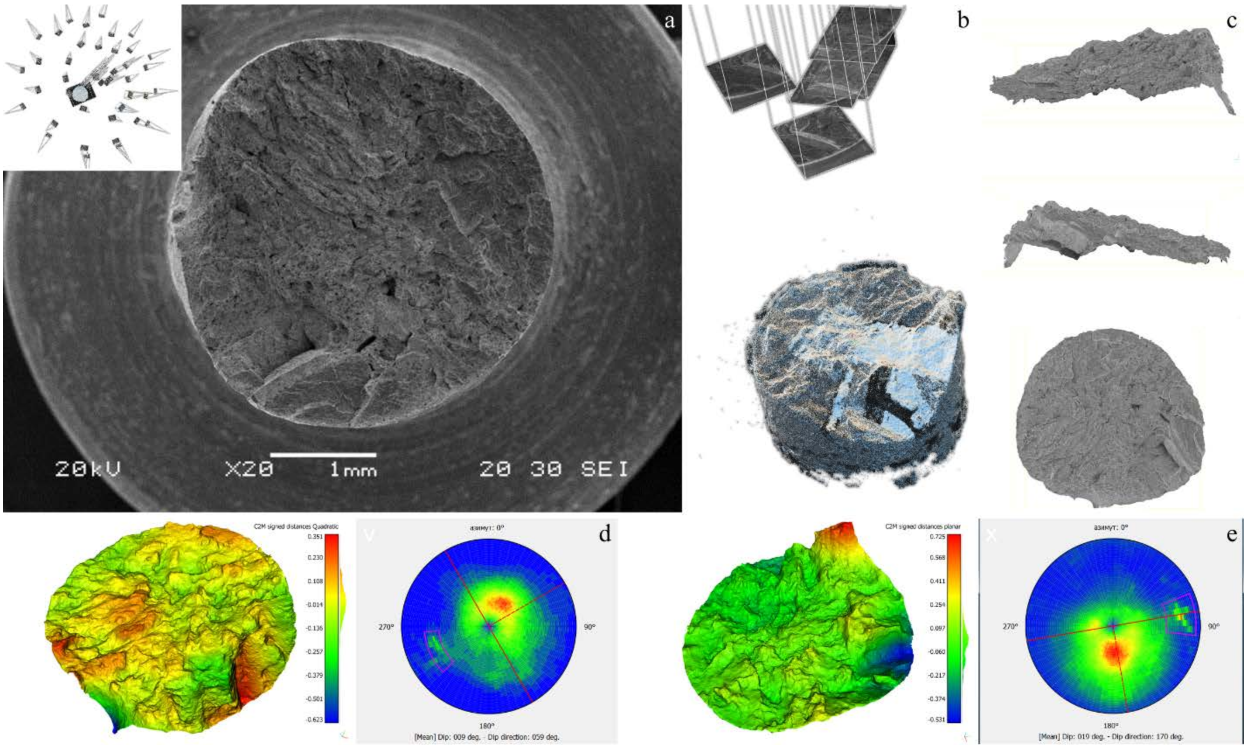


Figure 1 — Standard depleted-uranium sample before and after the mechanical tensile testing

Use of the proposed methodical approach is being developed and improved to complement the conventional fractography with a quantitative analysis. It is in demand for studies of fractures in the rapidly-oxidizing material samples.



a — one of the original photographs and the photographing scheme; b — unfinished digital model of one of the surfaces; c — some projections of the digital model; d — maps of heights and normal lines of the fracture within the first segment of the sample; e — maps of heights and normal lines of the fracture within the second segment of the sample

Figure 2 — Photogrammetrical modeling of the fracture surface

ZIRCONIUM PHASE DIAGRAM FROM AB INITIO MOLECULAR DYNAMICS

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The paper presents analysis of precision of a phonon-based free energy calculation technique (Temperature Dependent Effective Potential method)[1] in comparison with the thermodynamic integration method within classical molecular dynamics. It was shown that the use of the second and third order force constants is insufficient for accurate calculations of free energies at elevated temperatures due to noticeable anharmonic contributions to lattice vibrations. On the other hand, reliable calculations of the crystal phase equilibrium lines requires free energy accuracy higher than 1-3 meV per atom. Based upon the obtained results the Temperature Dependent Effective Potential technique is applied to the detailed study of the solid-state Zr phase diagram from *ab-initio* molecular dynamics with the account for up to the fourth order force constants. The calculated zirconium phase diagram is in good agreement with experiment and the α, β, ω triple point was determined at $P \approx 8.3$ GPa, $T \approx 790$ K.

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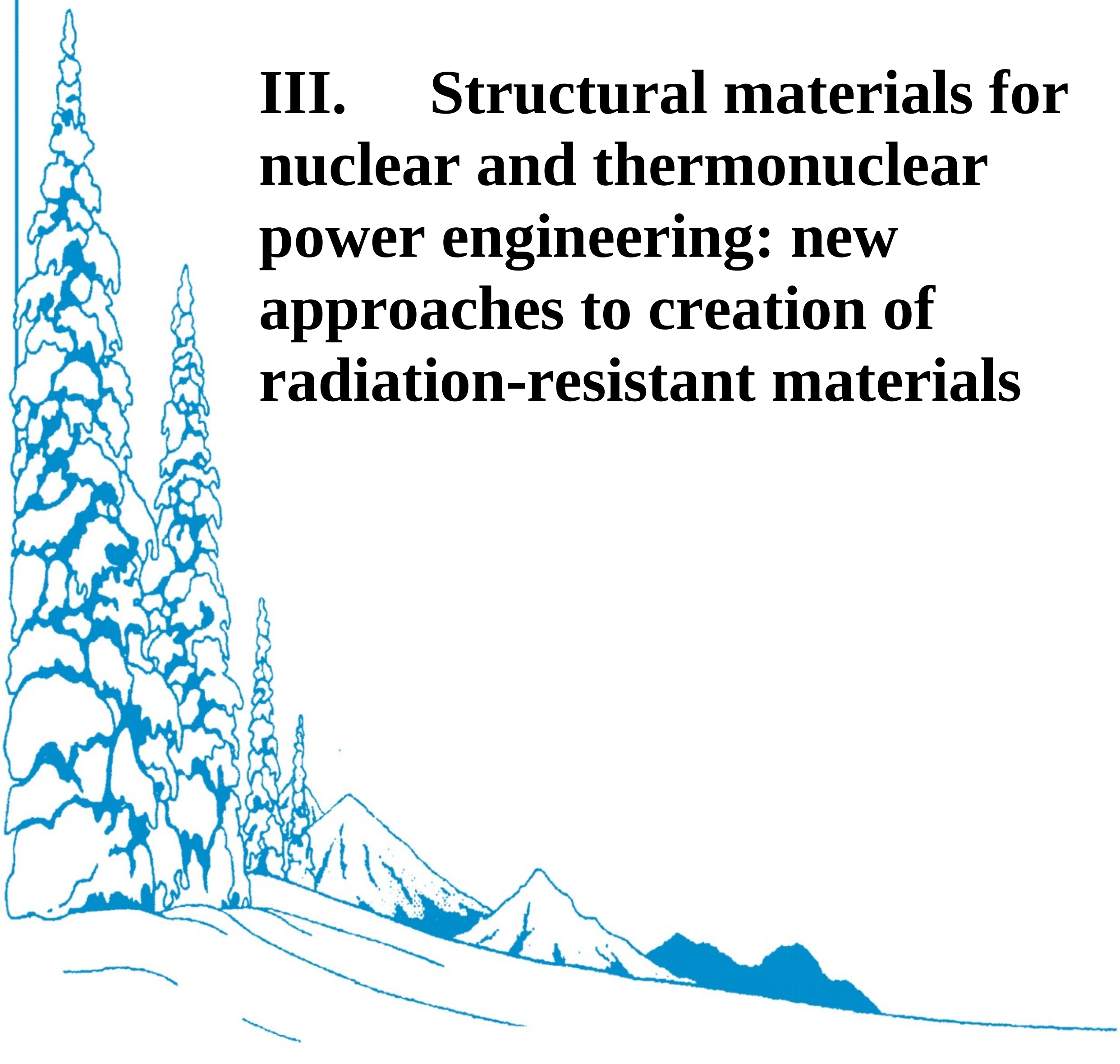
III. Structural materials for nuclear and thermonuclear power engineering: new approaches to creation of radiation-resistant materials



ALLOYING OF ALUMINUM BY BORON WITH HIGH DEGREE UNIFORMITY

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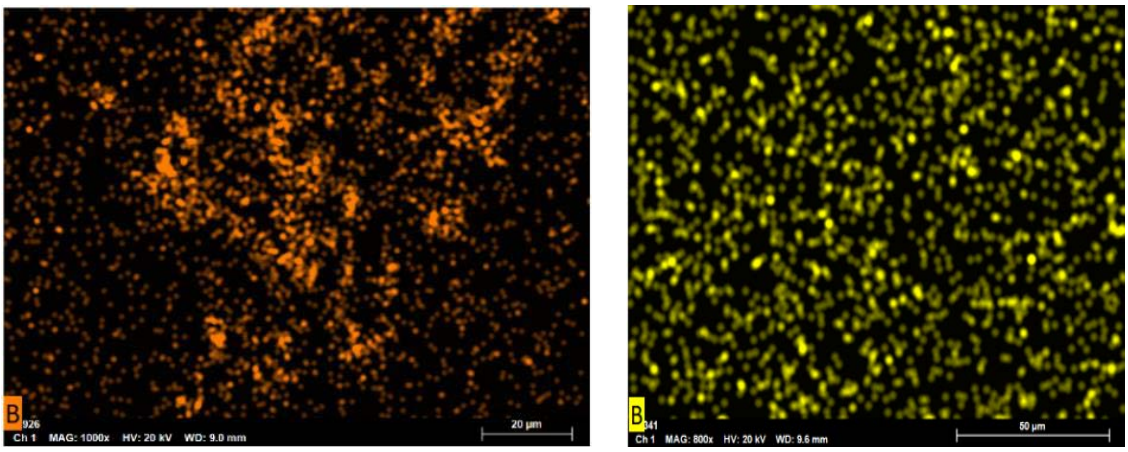
The work demonstrated the possibility of combining the process of converting boron powder into a nano-sized state with its simultaneous introduction into the aluminum melt. It has been shown that the method of processing micron boron powders with arc discharge plasma makes it possible to obtain particles with an average size of 4–11 *nm*. Thus, many processes using nanodispersed powders can be combined with the process of their production, which avoids the difficulties associated with storing such highly reactive materials. The results of plasma alloying of aluminum in the melt with nanosized boron particles are presented. Generating a flow of arc argon plasma over an aluminum melt with micron-sized fullerene and boron powders introduced into it made it possible to obtain an alloy containing boron uniformly distributed throughout the volume. To introduce boron, a plasmatron [1] with a plasma-forming and, at the same time, transport gas – argon – was used. Fullerenes, which were used as the most effective reducer of aluminum in the oxide film, were supplied through one jet, and boron was supplied through the other. Quantitative X-ray fluorescence analysis of a sample of areas with a diameter of 20 *μm* showed that boron is distributed into aluminum with a degree of uniformity of the component: 19±5.6 *wt.%* for the standard sample (Fig. 1a) and 7.8 (±2.5) *wt.%* for the sample we obtained using the above technology (Fig. 1b).



(a) (b)

Figure 1. Photographs (magnification 1000x in mapping mode):

a sample of a standard ligature (a); the aluminum–boron sample (b)

The research was carried out within the state assignment of Kirensky Institute of Physics, FSBSI "Federal Research Center "Krasnoyarsk Science Center SB RAS". The authors thank M. Zhizhaev, A.M. Tokmin, V.A. Lopatin, M.R. Kastyuk for conducting analytical studies, incl. using equipment Center for Common Use of the Krasnoyarsk Science Center SB RAS.

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COMPREHENSIVE ANALYSIS OF THE NANOSTRUCTURE OF OXIDE DISPERSION-STRENGTHENED STEELS

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The characterization of the nanostructure of oxide dispersion strengthened (ODS) steels requires a comprehensive analysis using complementary techniques. In this work, the methods of transmission electron microscopy (TEM), atom probe tomography (APT), small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS) have been applied to several ODS steels. The studied steels have different alloying systems differing in the content of Cr, V, W, Al, and Zr, produced in Japan, Republic Korea and Europe. Previously, it was shown that ODS steels contain high number density of nanosized oxides and clusters detected with TEM and APT. So, there is a question about separation of oxides and clusters with different microscopic techniques. Local techniques like TEM and APT do not provide high accuracy in the number density of inclusions due to their inhomogeneous distribution.

It is shown that most of the studied steels contain oxide inclusions and nanosized clusters enriched in O and Y, as well as V, Ti, Al, and Zr, depending on the initial steel composition. TEM and APT provide detailed information about the inclusion types and their size distribution, while SANS and SAXS allow for measuring the average density of inclusions in large volumes of material with the highest accuracy. The importance of the correct determination of inclusion types for hardening calculations is shown. The results of these calculations are compared with microhardness measurements. The calculated values of hardness for the studied steels are in the range of 2.7– 4.3 GPa, which is well confirmed by microhardness measurements.

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EFFECT OF NEUTRON IRRADIATION ON MICROSTRESSES IN AUSTENITIC STEEL

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Austenitic class steel of Cr16-Ni15 type is used as fuel element cladding in fast neutron reactors.

Swelling is the main problem that limits the use of this class of materials at high burnup.

The factors that inhibit swelling are [1]: an increase in the stability of the solid solution, the phase stability of the released MeC-particles and the stability of the dislocation structure; an increase in the boron content of the solid solution, and cold deformation by 20-25%, which forms a cellular structure with the presence of strain microtwins.

These factors are the main causes of microstresses in the material, causing microdeformation of the crystal lattice.

Radiographically, such stresses are manifested in the change of interplanar distances and in the broadening of interference maxima.

Integral control of factors inhibiting irradiation swelling is possible by determining the effect of irradiation conditions, such as temperature and irradiation dose, on microstrain.

The paper presents the results of X-ray diffraction studies of the influence of neutron irradiation in the BN-600 reactor on the microstresses in steel of the Cr16-Ni15 type.

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ENHANCED IRRADIATION TOLERANCE OF A MEDIUM ENTROPY ALLOY VIA PRECIPITATION AND DISSOLUTION OF NANOPRECIPITATES

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High/medium entropy alloys (HEAs/MEAs) are good candidates for nuclear applications due to the excellent mechanical properties, good corrosion resistance and radiation resistance. In this work, a novel cobalt-free MEA was developed by introducing $L1_2$ nanoprecipitates. The microstructure evolution and radiation tolerance were evaluated after bombarded using 3 MeV Fe^{11+} ions at 500 ^{o}C. The evolution of nanoprecipitates was closely related to the irradiation dose, and dominated by irradiation-enhanced diffusion and ballistic dissolution mechanism. For the solid-solution MEA (without $L1_2$ nanoprecipitates), irradiation hardening occurred due to the irradiation-induced formation of precipitates, voids and dislocation loops. However, in MEA with $L1_2$ nanoprecipitates after aging, irradiation induced dissolution and reprecipitation of nanoprecipitates were observed. Different from the solid-solution MEA, the hardness kept almost unchanged in the aging sample after irradiation. The swelling rate of the solid-solution sample after irradiation is 9.4×10^{-6} %/dpa, while no swelling occurs in the aging sample under the same irradiation condition. Besides, the average size and number density of dislocation loops in the aging sample decreased by ~ 40% and ~ 28%, compared with the solidsolution sample. The precipitation and dissolution of nanoprecipitates substantially improved the radiation tolerance of the cobalt-free MEA.

IRRADIATION EFFECTS IN STEELS AND ALLOYS

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Pre-existing precipitates, twin boundaries, and grain boundaries all can act as defect traps, enhancing the irradiation tolerance, such as reducing the swelling rate/hardening and preventing radiation-induced precipitation. In recent years, our group mainly focuses on the effects of pre-existing precipitates and twin boundaries on the irradiation tolerance in the newly-developed precipitate-strengthened ferritic steels and high entropy alloys. Various kinds of ions, including Ne^{20+}, Au^{2+}, Fe^{11+}, He^{2+}, protons and electron, were used to irradiate the steels and alloys. The microstructure evolution and mechanical properties were subsequently examined by transmission electron microscope (TEM), atom probe tomography (APT), nanoindentation and micro-tensile test. In steels, irradiation-enhanced precipitation and coarsening of pre-existing nanoscale precipitates were observed, depending on the irradiation dose. The precipitation and coarsening of nanoscale precipitates are responsible for the changes in hardness. In high entropy alloys, a rather low swelling rates were observed after irradiation due to the existence of pre-existing precipitates and twin boundaries. The irradiation-induced segregation level is obviously suppressed in the HEAs due to the sluggish atom diffusion. In the meantime, the high-density nanoprecipitates have dual functions: (I) They can increase the surface area of particles capable of adsorbing defects, and improve the ability of the alloy to suppress the coarsening of He bubbles. (II) The reduction of matrix SFE caused by precipitation inhibits the transition from a faulty loop to a perfect dislocation loop, prolongs the latency of the dislocation loop and delays its growth.

MASS SPECTROSCOPIC REGISTRATION OF MODIFIED TUNGSTEN ISOTOPES WITH INCREASED MASSES

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According to [1], the processes of cold fusion and nuclear decay can be realized with the participation of compact massive electron (ee) pairs that have opposite spins and are connected by contact interaction described by hadronic mechanics [2]. The existence of such pairs is supported by experiments [3], which established the existence of atoms with increased masses for all titanium isotopes.

In this work, a mass spectrometric analysis of the surface layer of a titanium anode after an arc discharge in air was carried out using a tungsten cathode. It is significant that only tungsten with an increased mass of atoms was found on the anode. The table below shows (in aem units with an accuracy of hundredths) the masses of modified m^* and ordinary m atoms of tungsten isotopes, with m^* corresponding to the maximum values of the broadened peaks of the mass spectrum. The resolution and calibration of the spectrometer ensure the reliability of the data.

Table. Values of ordinary and modified atomic masses for five stable isotopes of tungsten

m*(aum)	180.20	182.07	183.07	184.10	186.12
m (aum)	179.95	181.95	182.95	183.95	185.95
$\Delta m = m^* - m$ (aum)	0.25	0.12	0.12	0.15	0.17

Note that the mass increment Δm, in accordance with estimates [1], falls within the expected range of values m_{ee} mass of (ee) - pairs 0.04 aum $\leq m_{ee} \leq$ 0.4 aum. The absence of tungsten atoms with ordinary masses on the anode is interpreted as a consequence of a decrease in the binding energy with the cathode material for modified tungsten atoms. This change in binding energy seems natural, since the capture of massive electron pairs (occupying deep electronic states near nuclei and partially shielding their charge) is chemically equivalent to a transition to atoms with a lower charge number. Since the estimate of the lower limit of the mass (ee) - pair $(m_{ee})_{\min} \approx 0.04$ aum, it is possible that the modified atoms captured several (ee) - pairs (no more than four for the main isotopes of *W*). Then, in chemical terms, the modified atoms of the main isotopes of tungsten can be close to the atoms *Hf, Yb, Er, Dy*. Judging by the molar heat of evaporation, the binding energy for atoms of these elements is less than that of *W*.

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MICROSTRUCTURE EVOLUTION OF STEEL Cr16-Ni19 TYPE UNDER NEUTRON IRRADIATION AT INITIAL STAGE OF RADIATION SWELLING

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Studies of fuel element cladding are carried out mainly in accordance with safety justification programs during normal or trial operation of reactor fuel assemblies, therefore samples with maximum operating parameters are selected. Model development involves describing processes from the initial stage. There are not enough materials to verify this stage. The purpose of experimental studies of the evolution of the microstructure under neutron irradiation of steel type Cr16-Ni19 c.d., currently used as the main material for the fuel element claddings in BN reactors, was to obtain results in a wide range of conditions for verification of the developed models at various stages of fuel element operation.

The studies were carried out on samples of the cladding of one fuel element in order to minimize the possibility of the influence of the initial heterogeneity of the material after operation in the BN-600 reactor. The displacement rate varied over two orders of magnitude at as close a temperature as possible, and six samples were studied. The microstructure of an unirradiated steel sample of type Cr16-Ni19 c.d., manufactured using the same technology as the irradiated material, was also studied.

The main elements of the microstructure under study, intended for verification of the model, were used: dislocation structure – its qualitative and quantitative description (dislocation density, where possible); characteristics of porosity (qualitatively – relations with other elements, quantitatively – histogram); the second phases precipitations - qualitatively (type, composition, lattice, relations with other elements).

It has been shown that irradiation at a temperature of ~370°C with a displacement rate G=0,05×10^{-7} dpa/s leads to the transformation of the initial cellular dislocation structure into a separately located dislocations network, while the signs of the cellular structure are partially preserved in the form of weakly ordered clusters interacting dislocations. The radiation-induced dislocation loops with stacking faults ranging in size from 5 to 50 nm exhibits in the structure. The solid solution separation occurs in the material: nickel and silicon segregate on dislocations and grain boundaries. A radiation-induced γ′ phase is formed from elements segregating on dislocations. Small gas-vacancy bubbles are observed, formed predominantly on dislocations and dislocation loops; the bubble size does not exceed 3 nm.

Increasing the generation rate of atomic displacements from 0,77×10^{-7} dpa/s to 7,48×10^{-7} dpa/s does not qualitatively change the structural picture. Along with small pores, larger voids appear, distinguished into two systems of voids of “medium” and “large” sizes. In addition to the γ′-phase, precipitation of the G-phase and complex FCC carbides are observed both in the matrix and along the grain boundaries.

In the work, the approximation was accepted that the irradiation temperature in the studied range (370...410)°C is the same, and the dependences of the characteristics of various types of voids (average size, concentration) on the displacements rate were plotted. The dependence of the integral porosity of the material on the displacements rate is obtained. With increasing dose rate, an increase in porosity values is observed from hundredths of a percent to ~0.6% at a dose rate of 7,48×10^{-7} dpa/s.

MÖSSBAUER ANALYSIS OF THE STRUCTURE EVOLUTION OF THE EP823 AND EP823-ODS STEELS UNDER NEUTRON IRRADIATION IN CONDITIONS OF MECHANICAL STRESS IN THE BN600 REACTOR

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The influence of mechanical stresses on the structure evolution under neutron irradiation in the ferritic-martensitic steel EP823 and its EP823-ODS modification hardened by yttrium and titanium oxides was studied using Mössbauer spectroscopy with a resonance detection and electron microscopy. Irradiation of the samples in the form of fuel claddings was carried out in the BN600 fast neutron reactor at a temperature of 505 °C with a dose of ~ 85 dpa. During the irradiation process, austenite steels have swelled causing stress development inside the fuel element tube and size variation for both filler and tube where this filler has been placed.

Earlier it was shown that irradiation of the EP823 steel leads to solid solution decomposition, accompanied by a decrease in the effective concentration of chromium in the matrix and the formation of carbides and an intermetallic χ phase [1]. In the current work, it was established that additional mechanical stresses during irradiation of the EP823 and EP823-ODS steels significantly accelerated these processes. At the same time, the change in the degree of decomposition and the magnetic texture parameter $A^{2,5} : A^{1,6}$ revealed correlation. The intensification of the decomposition processes, as well as the increase in the magnetic texture parameter, is determined by the degree of mechanical stresses and their anisotropy, characterized by a difference in the values of relative plastic deformation of the sample along and across of the fuel cladding tube surface.

The research was carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme “Structure” No. 122021000033-2)

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PROSPECTS FOR IMPLEMENTATION OF HIGH-ENTROPY ALLOYS AS RADIATION-RESISTANT STRUCTURAL MATERIALS

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Currently, high-entropy alloys (HEAs) are suggested as structural materials for the next-generation nuclear reactors. One of the main challenges in their development is the lack of appropriate radiation-resistant steel and/or alloys for pressure vessels, intermediate heat exchangers and core devices. Two other issues are appropriate qualifications of these materials and high-temperature design methodologies. In such experimental facilities, most of the cores have consisted of both graphite and ceramic fuels, which significantly limit the use of metal structures for control systems and the pressure vessels. The selection of materials for advanced nuclear reactors must simultaneously satisfy several critical characteristics, including resistance to radiation (greater than 200 dpa), hot corrosion, both hydrogen and liquid-metal embrittlement, creep, spalling, swelling, and thermal fatigue, as well as high-temperature strength and dimensional stability. For such materials, a more complete evaluation of the mechanical properties, including creep behavior, radiation hardening and the stress-corrosion cracking behavior is required. It is difficult to achieve a combination of both excellent high temperature strength and low temperature ductility. In addition, results of both heat and thermomechanical treatment must be studied in detail for promising candidates. Thermal stability, especially the microstructural, is of vital importance during long-term operation at high temperatures. Also, the change in temperature during reactor operation must be taken into account. Thus, the mechanical characteristics of HEAs need to be assessed after long-term aging to determine their stability at elevated temperatures.

According to some researchers, HEAs exhibit ‘excellent’ resistance to radiation swelling and damage at various structural levels. Also, they may be exposed to high ion irradiation doses up to about 100 dpa. The key reason for this phenomenon has been stated their sluggish diffusion. As a result, moving of atoms implanted by irradiation is restrained. Moreover, higher stresses at the atomic level contributes to the ‘self-healing’ mechanism. Respectively, HEAs are characterized by improved radiation resistance due to structural features, especially chemical disorder, and unique internodal lattice distortion. They retain great phase structural stability under electron or ion irradiation. With an increase in the number of components, the probability of short-range recombination of radiation defects in a multicomponent alloy increases, which makes it possible to effectively resist to the formation of voids by a large number of vacancies. However, as can be inferred from comparing by the authors the requirements for the structural materials for the advanced nuclear reactors with the results achieved for HEAs [1], some challenges still exist, making it difficult to use them for these purposes in the near future.

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SET UP FOR PLASMA-CHEMICAL PRODUCTION OF COMPOSITE MATERIALS

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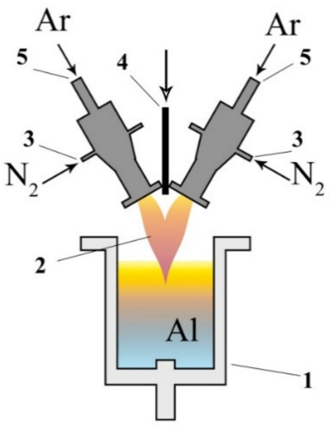
The work presents a set up based on a two-jet plasmatron. One jet is used to introduce a substance that reduces the metal in the oxide film, and the other is used to introduce a composite component.



(a) (b)

Figure.
Schematic diagram of stabilization of plasma flows of a two–jet plasma generator (a):

1 – graphite crucible, 2 – arc discharge, 3 – tangential input of insulating gas, 4 – capillary for supplying a substance, 5 – input of plasma–forming gas;

photograph of a plasmatron in operation (b)

The set up operation is demonstrated using the example of introducing boron into aluminum. Famously, boron-based alloys and composites are used in atomic energetic for thermal neutrons attenuation (the thermal neutrons absorption cross section for boron is 3600 *barn*). Using this set up, a composite material (aluminum alloy with boron evenly distributed in it) was obtained. Plasma introduction of boron into aluminum was carried out using two series-connected plasma generators that we had previously developed [1]. Argon was used as a plasma-forming gas, which is also a transport gas for the boron introduction. Helium was used as a buffer and transport gas for introducing a substance that reduces aluminum in the oxide film (fullerenes). It was shown that the introduced boron particles treated with plasma have an average size of 4–11 *nm*, while the average size of the initial particles is 100–1000 *nm*.

The research was carried out within the state assignment of Kirensky Institute of Physics, FSBSI "Federal Research Center "Krasnoyarsk Science Center SB RAS". The authors thank M. Zhizhaev, A.M. Tokmin, V.A. Lopatin, M.R. Kastyuk for conducting analytical studies, incl. using equipment Center for Common Use of the Krasnoyarsk Science Center SB RAS.

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STRUCTURE AND CREEP CHARACTERISTICS OF THE CHS-139 AND EK-181 MARTENSITIC STEELS

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In the current work, long-term high-temperature tests under the load of Russian advanced reactor martensitic steels CHS-139 and EK-181 were carried out. The samples for creep tests were made of fuel cladding tube with a diameter of 6.9, 9.3, and 10.5 mm and wall thickness of 0.4 and 0.5 mm, respectively. The creep characteristics for transverse and longitudinal samples were compared. The characteristics of long-term strength, ductility, and creep rates at 650, 670, and 700 °C under stresses of 60, 80, 100, and 140 MPa were determined.

In the CHS-139 and EK-181 steels, a polygonized lath martensite structure with a high dislocation density (up to 10^{11} cm^{-2}) prevailed in the initial state. Carbides of the $Me_{23}C_6$ type with a size of 50.200 nm were located along the boundaries of martensitic plates and inside them. Dispersed carbides of the VC type (~ 5 nm in size) were also present inside the martensitic plates.

After high-temperature exposure (during creep tests) in the structure of all steels the following occurred: (i) the destruction of a part of the plates boundaries and an increase in the width of the plates, (ii) a decrease in the density of dislocations, (iii) the formation of a block-like and subgrain structure, (iv) the emergence of new grains. In the composition of CHS-139 steel, as the most alloyed with carbon and other carbide-forming elements, carbides formed during tempering stabilized the boundaries of all types (plates, blocks, subgrains, grains). Therefore, CHS-139 steel showed the best results when tested for creep compared to EK-181 steel.

It was shown that longitudinal samples of CHS-139 steel, made of a tube with a diameter of

9.2 mm and a wall thickness of 0.55 mm, had a higher creep resistance compared to longitudinal samples, made of a tube with a diameter of 6.9 mm and a wall thickness of 0.4 mm. Transverse samples of CHS-139 steel, made of a tube with a diameter of 6.9 mm and a wall thickness of 0.4 mm, had a higher long-term strength during high-temperature tests at 700 °C. And when tested at 670 C, higher values of long-term strength were observed in transverse samples made of a tube with a diameter of 10.5 mm and a wall thickness of 0.5 mm.

The research was carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme "Structure" No. 122021000033-2)

STRUCTURE AND PROPERTIES DEGRADATION OF VVER-1000 REACTOR PRESSURE VESSEL MATERIALS AND ITS IMPACT ON SERVICE TIME

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Changes in structural-phase state of VVER-1000 reactor pressure vessel (RPV) materials (steels) during the operation process within the regular lifetime as well as within extended lifetime (60 years and more) are reviewed. Extending the RPV lifetime is possible only after thorough studying of RPV steels structure evolution under conditions of radiation at working temperatures. It is essential to understand the changes in volume density and average sizes of radiation defects and radiation-induced structural elements. It is also essential to know the radiation embrittlement mechanisms.

In the current research, analysis of existing literature data and results of experiments performed in NRC "Kurchatov institute" was conducted. Information about evolution of RPV steels structure during the reactor lifetime was gathered. Extended dose dependencies of changes in structural parameters of RPV materials are given. Rate of changes of grain boundary segregation, strength characteristics and critical temperature of brittleness for RPV materials due to irradiation was determined.

Based on analysis of structural-phase state tendencies changing of VVER-1000 RPV materials at service times of 60 and more years the following conclusions can be made:

- At service times of 60 and more years the rate of grain boundary phosphorous segregation is significantly decelerated, while approaching the equilibrium segregation level. This leads to reducing the input from non-strengthening mechanism into the radiation embrittlement;
- Growth rate of radiation-induced precipitates average size and volume density is decelerated, while volume density of dislocation loops continues to grow. This may lead to the continued yield strength growth, although its growth rate will be decreased;
- Thus, it is expected that the input of the strengthening mechanism in radiation embrittlement at service times of 60 and more years might prevail;
- Growth rate of critical temperature of brittleness shift (ΔT_c) is also expected to decelerate at long-term operations;
- By calculation-experimental method it was shown that the lifetime of VVER-1000 RPVs can be extended beyond 60 years by means of re-assessment and, in some cases,

by recovering annealing;

- Decision to extend the lifetime of every particular RPV should be done individually.

STUDY OF THE EFFECT OF Fe ION IRRADIATION ON THE NANOSTRUCTURE OF OXIDE DISPERSE-STRENGTHENED STEELS BY ATOM-PROBE TOMOGRAPHY AND TRANSMISSION ELECTRON MICROSCOPY METHODS

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In advanced nuclear and thermonuclear reactors, core materials should have high radiation resistance and heat resistance at temperatures up to 650 °C and doses up to 200 dpa (displacements per atom). Oxide dispersion-strengthened (ODS) steels containing homogeneously distributed thermally stable nanoscale oxides in their matrix are promising materials capable of meeting these requirements [1-2].

In this work, three ODS steels 10Cr ODS, KP-3 ODS and Eurofer ODS in the initial state and after irradiation with Fe^{2+} ions with energy 5.6 MeV at temperature of 500°C and damaging doses up to 100 dpa. The study was carried out using modern methods of transmission electron microscopy and atom-probe tomography [3].

Oxide inclusions and clusters were found in the initial state of the steels. The average size of oxides ranged from 3 to 6 nm and their number density ranged from 2×10^{22} m^{-3} to 13×10^{22} m^{-3}. The number density of clusters ranged from 16×10^{22} m^{-3} to 32×10^{23} m^{-3} and their average size ranged from 2 to 4 nm [4].

The study of samples irradiated to 100 dpa at 500°C showed a significant decrease in the number density of oxide particles in 10Cr ODS (~ 5 times) and KP-3 ODS steels (~ 4 times) [5]. At the same time, in Eurofer ODS the number density of oxide particles remained within error range. The number density of clusters sharply decreased only in Eurofer ODS, and in 10Cr ODS and KP-3 ODS, on the contrary, increased.

A series of studies has shown that Eurofer ODS steel also has stable oxide particles in the region of intermediate operating temperatures due to the interaction of subsystems of clusters and oxides.

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STUDY OF THE RADIATION HARDENING MECHANISMS OF HEAT-RESISTANT OXIDE DISPERSION STRENGTHENED STEELS IN ACCELERATED TESTS USING ION IRRADIATION AND ULTRAMICROSCOPIC ANALYSIS

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Oxide dispersion strengthened steels (ODS steels) have significantly higher heat resistance than traditional ferritic-martensitic steels due to a significant number of uniformly distributed oxides. Such materials are being developed for a number of nuclear applications: the first wall of future thermonuclear reactors, materials for the cladding of fuel elements in fast neutron reactors, and for use in other IV generation reactor installations [1-2]. These materials can withstand temperatures up to 700°C and are expected to withstand radiation swelling of up to 200 dpa [3]. The mechanical properties of ODS steels significantly depend on the characteristics of the nanostructure: the size and spatial distribution of dispersed inclusions. In turn, the choice of alloying additives and thermomechanical processing modes have a direct impact on it’s characteristics. Quantitative analysis of oxide inclusions in ODS steels requires the use of several complementary microscopic analysis techniques, such as transmission electron microscopy (TEM) and atom probe tomography (APT).

The increased operational properties of ODS steels are significantly depends on oxide nanoinclusions (particles and clusters) uniformly distributed in the matrix. That's why the study of the stability of the nanostructure of ODS steels, including under irradiation is paid much attention by researches [3, 4].

The goal of this work is a systematic comprehensive study of radiation-induced changes in Russian ODS steels EP-450 ODS and EP-823 ODS in region of low-temperature radiation embrittlement from 350°C to 500°C in the dose range from 30 to 100 dpa. EP450 ODS steel has a larger number of oxide particles and smaller clusters in the initial state, than EP823 ODS steel. The formation of a large number of radiation-induced Si-Ni-Mn clusters is observed in EP823 ODS steel after irradiation up to 30 dpa. There is no such effect in EP450 ODS steel. Nanohardness measurements show that the main differences in the behavior of steels occur at high irradiation temperatures at doses up to 60 dpa, but at a doses of 100 dpa both steels show a tendency to soften.

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THE PHASE FORMATION PATTENS IN THE VVER-TYPE REACTOR PRESSURE VESSEL STEELS

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One of the degradation mechanisms of nuclear reactor pressure vessels (RPV) is radiation hardening due to formation of radiation-induced precipitates. In this regard, this paper investigates the peculiarities of phase formation in various RPV steels depending on operational factors (neutron fluence, flux, irradiation temperature and steel composition). For this purpose, atom probe tomography studies results obtained over the last decade in NRC "Kurchatov institute" for RPV steels of operating Russian reactors, as well as Russian-made steels being developed have been accumulated and analysed.

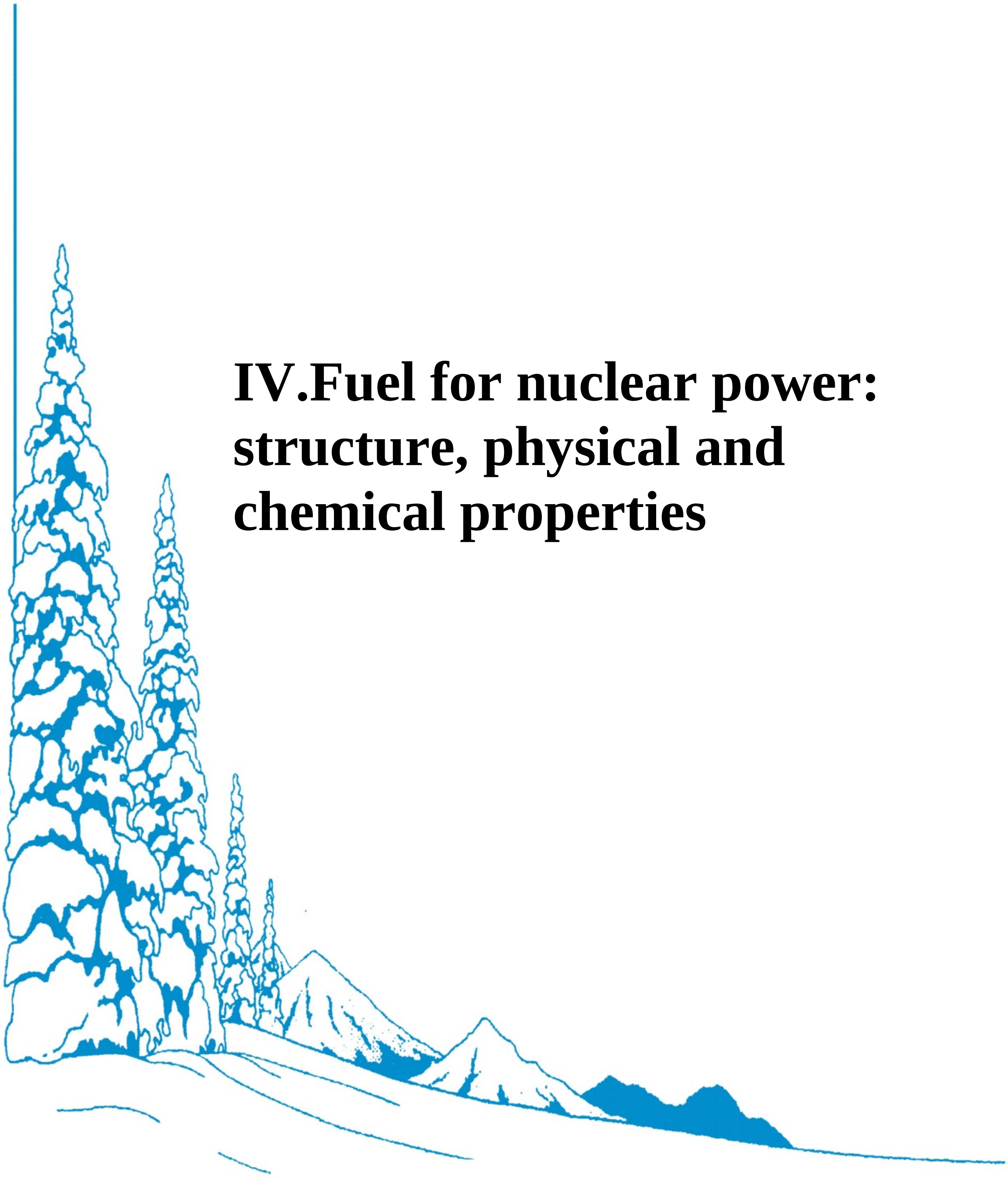
RPV steels with low Cu content (VVER-1000 RPV steels) were studied to show that 300 °C irradiation leads to the formation of Ni-Si-Mn precipitates by radiation-induced mechanism, mainly on point defect clusters formed in cascades. These cascade clusters act as sinks for radiation-induced segregation (RIS) of Ni, Mn, and Si atoms and, at sufficient RIS level, form a precipitate nucleus. Further growth of precipitates is determined by the diffusional mobility of atoms. All this is determined by both the steel composition and the operating parameters (fluence, flux, irradiation temperature).

Thus, increased Ni and Mn content in steel (VVER-1000 welds compared to base metal) leads to the higher number densities of precipitates caused by a higher level of RIS in them, required for precipitate nucleation on cascade clusters of point defects. At the same time the study shows that for materials with lower concentrations of Ni and Mn (1.0–1.3 wt.% Ni and 0.4–0.5 wt.% Mn) precipitate nucleation at the initial stage of irradiation occurs heterogeneously mainly on sinks (dislocations) with their fraction decreasing as the fluence increases, since it leads to an increase in the RIS level. In the steel with increased Ni content up to 5 wt.% but with ultra-low Mn content ≤ 0.03 wt.%, it is possible to suppress the formation of Ni-Si-Mn precipitates under irradiation.

An increase in the fast neutron fluence (and irradiation time) leads to both an increase in nucleation sites number and the level of RIS, which leads to an increase in the density and size of precipitates. The composition of precipitates correlates with the alloy composition.

Increasing the fast neutron flux (i.e., decreasing the irradiation time at the same fluence) leads to an increase in nucleation sites number (increasing the number of point defect clusters, at a close RIS level). This determines a higher density of precipitates of smaller sizes due to less time for diffusion processes to occur.

The study of materials irradiated at different temperatures showed that at low irradiation temperatures (50–130°C) precipitates are not formed, which is due to the low level of RIS and low diffusional mobility of atoms, while the number of sites for precipitate nucleation increases. At high irradiation temperatures (400°C), cascade clusters of point defects are hardly formed. Therefore, precipitates can emerge on heterogeneous sinks - dislocations and grain boundaries by thermodynamic driving force along with radiation-enhanced diffusion. The composition of precipitates in this case corresponds to equilibrium phases.



IV.Fuel for nuclear power: structure, physical and chemical properties

A SEARCH OF ELECTODES' USED IN ELECTROCHEMICAL REDUCTIONAL REEXTRACTION OF Pu AND Np POROUS LAYER PRODUCTION TECHNOLOGY

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One of FSUE Mayak PA areas of work is nuclear reprocessing. Spent fuel reprocessing is based on PUREX, which consists of dissolvement of fuel in nitric acid, extraction of Pu and Np in organic solvent made up of 30 % tributyl phosphate and synthetical saturated hydrocarbons, continued by reductional reextraction of plutonium into the aqueous phase. Typical reducing agents include hydrazine, hydroxylammonuim nitrate, ferrous sulphamate, nitrous acid, U(IV), ascorbic acid, hydrogene etc. U(IV) outstands other reducing agents used in industry as it can be produced directly during nuclear reprocessing.

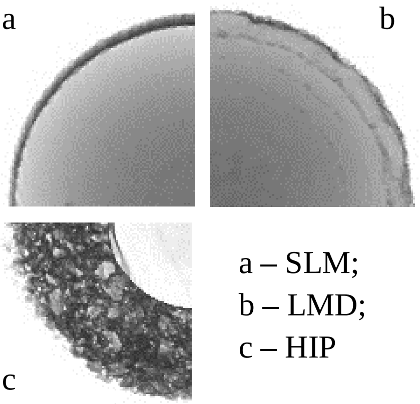
U(IV) on FSUE Mayak PA is produced by electrochemical method based on passing of a direct electric current through the electrolyte. The electrodes are mounted into the blocks. The cathode is a titanium louver. The anode assembly consists of the «anodic rack», where cylindric titanium electrodes are placed. The electrode is a titanium rod with a layer of porous titanium formed on it (titanium blank). The antimony and tin oxides coating is applied on the porous layer to provide resistance to corrosion.

The technology of forming of porous titanium layer which would provide the opportunity of titanium blanks' serial production for newly designed anode assemblies was to select. The three different technologies were considered with this purpose:

- selective laser melting (SLM);
- laser metal deposition (LMD);
- hot isostatic pressing (HIP).

The anodic tin-antimony coating was formed by the technology developed on FSUE Mayak PA.

The quality of formed porous layer and the thickness of anode coating were researched by the microscopic methods of analysis. The titanium blanks with the tin-antimony coating applied on it were fragmented and its cross-sections were analyzed.



Picture 1 – Cross-sections of analyzed titanium blanks

The results of microscopic research had shown that working layer of titanium blanks made by SLM and LMD technologies (Pic. 1 a, 1 b) did not exceed 50 micrometers, while the titanium blank made by HIP technology had fully porous working layer (Pic. 1 c) with thickness of about 3 millimeters.

The anodic coating with thickness more than 100 micrometers was applied on each titanium blank, though coating of blanks made by SLM and LMD technologies formed only on the surface of porous layer. Anodic coating applied on the porous layer made by HIP technology in its turn formed in the whole volume of the porous layer.

Thus, among the considered technologies HIP is the most suitable for forming porous layer. The batch of these electrodes is currently being tested in the model electrochemical reduction of uranium solutions apparatus.

APPLICATION OF THE METHOD OF ORIENTATION MICROSCOPY TO STUDY THE STRUCTURAL-PHASE STATE OF IRRADIATED ZIRCONIUM ALLOYS

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Up to the present time zirconium-based alloys are actual materials in various fields of industry, in particular nuclear industry. Unique physical-mechanical, corrosion properties allow to use zirconium alloys in aggressive conditions of the core zone of thermal nuclear reactors [1...2].

One of the main problems of zirconium-based alloys used in nuclear power engineering is the high propensity of the material to hydrogenation. Due to the low solubility of hydrogen in the α-Zr crystal lattice (0.034 ppm at 293 K), its penetration into the product leads to the release of hydrides, which can lead to serious degradation of mechanical properties and, consequently, to the possibility of damage and destruction of products during operation in a nuclear reactor [3].

This work is devoted to the possibility of applying the EBSD method to the analysis of changes in the structural-phase state of products made of Zr-2.5% Nb alloy after operation in thermal neutron reactors [4].

Samples from Zr-2.5%Nb alloy after operation in a nuclear reactor on thermal neutrons (coolant - water) were used as the material of the study. The studies were performed on a scanning electron microscope MIRA3 FEG-SEM equipped with an Oxford Instruments Nordlys Nano electron backscattered electron backscattered detector (EBSD) and a programme for processing the obtained results.

As a result of the conducted studies with the help of scanning electron microscopy and orientation microscopy (EBSD) the possibility of determining the structure parameters (grain size, alloy recrystallisation fraction) and texture, as well as revealing the phase composition of the material (α-Zr, β-Zr, β-Nb, ZrH and $ZrH_{1,66}$) depending on the part of the product (deformed tube or welded joint zone) was shown.

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ESTIMATION OF INSTANT PERMISSIBLE VALUES OF LINER'S ADMIXTURE IN MAGLIF DEVICE FUEL

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One of the problems of fusion devices is the rational selection of material for the "reactor" walls. These reactor surfaces are the "front line". Under extreme thermonuclear burning conditions, the fuel mixture may contain an admixture of wall material that affects the burning behavior. At the same time, the electronic component of the impurity creates additional radiation losses, and therefore the use of low-*Z* material makes it possible to reduce them. However, the ion component can actively participate in energy production by interacting with fuel particles. It affects burning efficiency depending on the temperature of the fuel burning area.

This work considers a particular type of reactor – MagLIF device, which is described in detail in [1, 2]. Here, a metal liner with fuel inside is affected by a high current discharge, as a result of which the system turns plasma and, due to magnetic compression caused by the current, turns into a plasma cord, while then a strictly time-synchronized laser pulse is directed from the end of the liner. Due to this, additional compression occurs in the plasma cord system and a wave of thermonuclear burning region is launched. In this compressed region the density and temperature reach the orders of values of 10^{23} *particles per* cm^3 and *tens of keV*. In addition to fuel particles, there will be particles of material from the metal liner. A fully ionized admixture will be actively involved in the burning process of the compressed region.

In this work, based on the burning picture presented in [3], an estimation of the instant permissible (threshold) values of the liner's admixture for effective burning under extreme conditions of MagLIF devices is made. This instant indicator shows what maximum part of the liner mixture in the fuel can be at a certain time moment to still maintain temperature increase of the burning area with "contaminated" fuel. Based on the example of calculations of the traditional types of fuel burning in the MagLIF device, it was estimated that the most energy-efficient fuel type DT allows the presence of beryllium liner admixtures in the fuel up to values of several tens of percent. Other fuels DD and D^3He are also considered.

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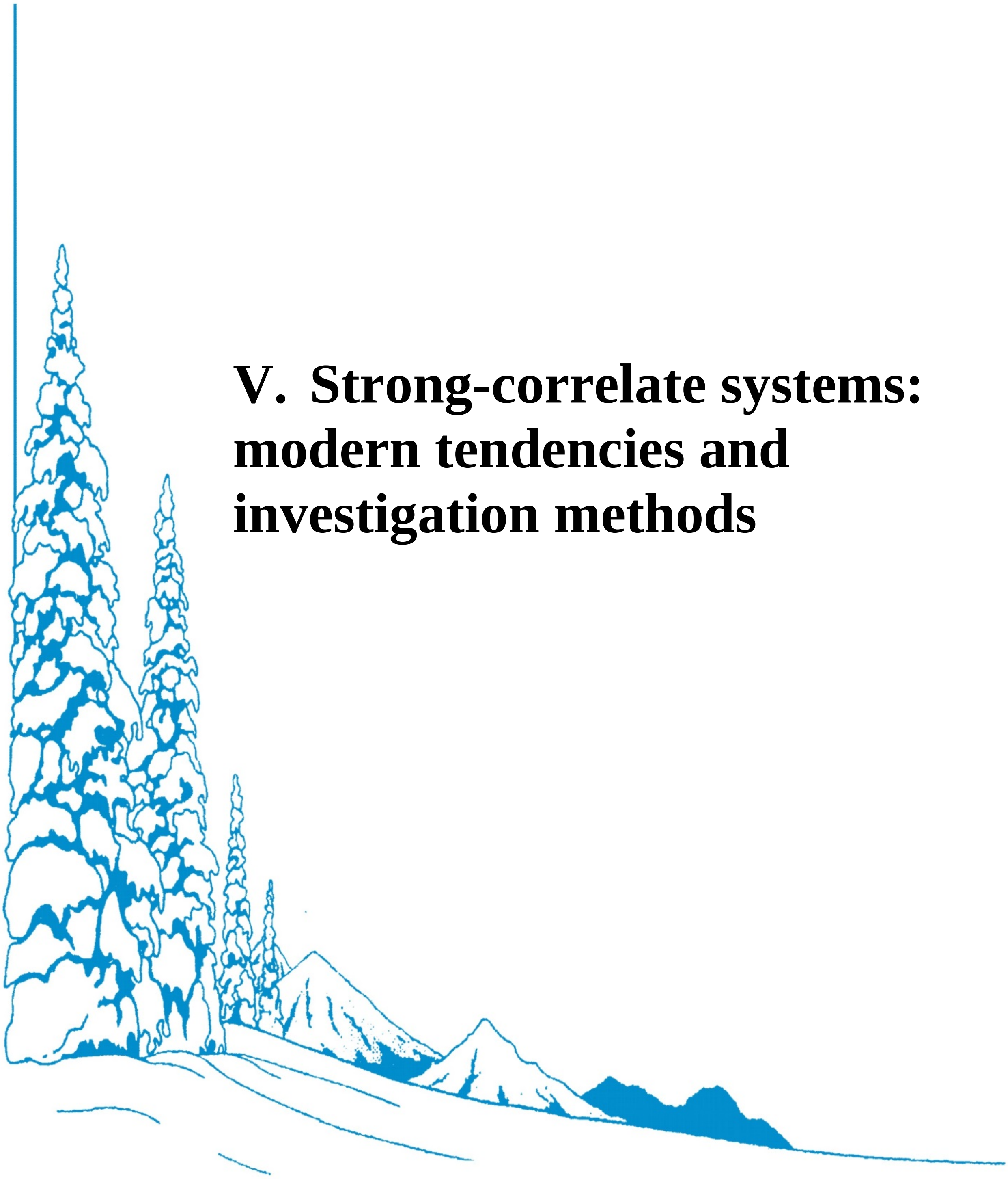

V. Strong-correlate systems: modern tendencies and investigation methods

TOPOLOGICAL ANALYSIS OF Li^+ CATIONS MIGRATION PATHS IN LITHIUM-VANADIUM BRONZE $Li_{1+x}V_3O_8$ (x = 0.1, 0.2, 0.3)

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Lithium-vanadium bronze $Li_{1+x}V_3O_8$ is one of the most attractive cathode materials for lithium-ion batteries. Lithium vanadium bronze $Li_{1+x}V_3O_8$ has a high potential (~3 V) and high theoretical specific capacity (~374 mAh/g) [1] that is associated with the possible intercalation of three additional Li^+ ions per formula unit ($LiV^{5+}{}_3O_8 + 3Li^+ \rightarrow Li_4V^{4+}{}_3O_8$) [2]. However, Li-ion migration properties in $Li_{1+x}V_3O_8$ have not been fully studied yet despite its key role in electrochemical performance. The main limitation of $Li_{1+x}V_3O_8$ structural studies by X-ray methods is their low sensitivity to light elements such as lithium and oxygen. On the other hand, vanadium is practically invisible in neutron diffraction experiments due to small coherent scattering cross section. In order to study the crystal structure of $Li_{1+x}V_3O_8$ (x = 0.1, 0.2 and 0.3) we used combination of neutron and x-ray diffraction techniques. Simultaneous Rietveld refinement of x-ray and neutron diffraction patterns made it possible to clarify the structure of $Li_{1+x}V_3O_8$ (x = 0.1, 0.2 и 0.3) and determine the distribution of lithium atoms over crystallographic positions. The Voronoi–Dirichlet approach implemented into the program package TOPOS [3] was employed to find Li migration map. The Li+ diffusion process in $Li_{1+x}V_3O_8$ (x = 0.1, 0.2 and 0.3) was found to be one-dimensional along the [010] crystallographic axis due to hop between nearby vacant sites.

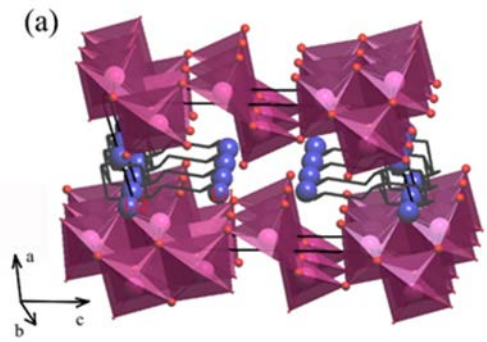

Fig.1. Unit cell and conductivity map in crystal structure $Li_{1+x}V_3O_8$ (x = 0.1, 0.2, 0.3).

The results were obtained at IMP Neutron Material Science Complex within the state assignm ent of Ministry of Science and Higher Education of the Russian Federation (theme "FLUX" No. 122021000031-8).

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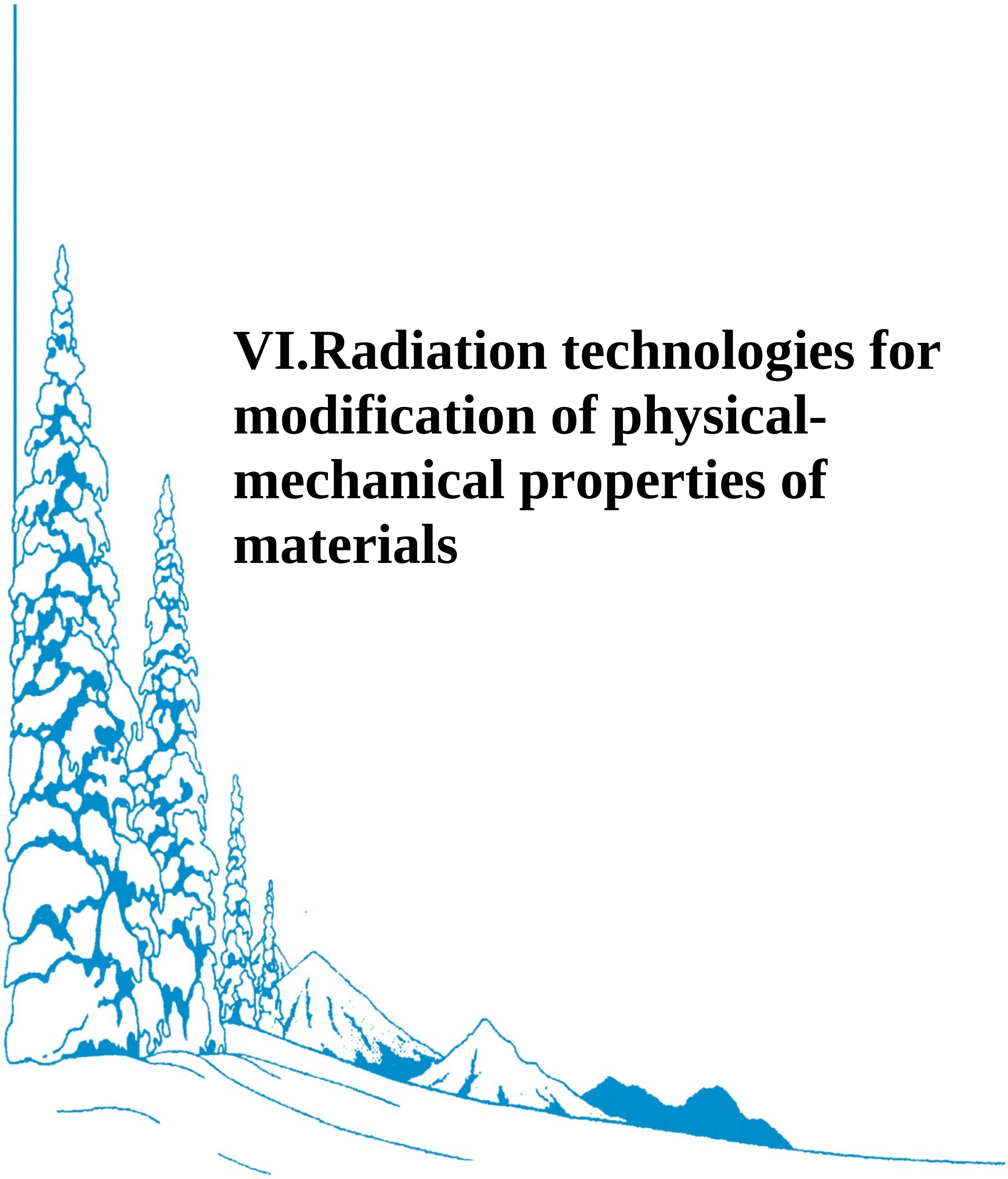

VI.Radiation technologies for modification of physical-mechanical properties of materials

FEATURES OF FORMATION OF SURFACE LAYERS OF TITANIUM ALLOY VT6 UNDER CONDITIONS OF PLASMA TREATMENT OF N^+ IONS

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Titanium alloys are widely used in various fields of technology due to their high strength, ductility and low biotoxicity. An urgent problem is the development of technologies for modifying the surface of titanium alloys to increase their hardness, wear resistance, corrosion resistance and biocompatibility [1]. One of the widely used methods of modification of titanium alloys is ion-plasma treatment of their surface. In particular, methods of diffusion saturation with nitrogen in the plasma of glow and arc discharges are used [2, 3], as well as irradiation with ion fluxes [4]. In most cases, nitriding is carried out at high (800 – 900 ºC) temperatures for many hours. However, at high temperatures (exceeding the temperature of polymorphic α→β transformation), nitriding of low-alloy titanium alloys leads to the growth of crystallites, a change in the microstructure and, as a consequence, a decrease in the operational properties of the material [5].

Therefore, it is necessary to search for solutions that allow nitriding of titanium alloys under mild conditions (glow discharge, short processing time, relatively low temperatures) in order to ensure the preservation of the structural-phase state and properties of the material in the volume of products. The constructive simplicity of the nitriding installation is also important, so that the developed technology can be applied in production in the future. In order to understand the mechanisms of the nitriding process and its purposeful regulation, comparative comprehensive studies of the surface morphology, composition, structural-phase state and mechanical properties (microhardness) of the surface layers of a titanium alloy during nitriding in a glow discharge plasma, depending on the exposure temperature, have been carried out in this work. The samples were heated to temperatures of 300, 500 and 700 °C.

The work was performed under state assignment No. 121030100002-0 from the Russian Ministry of Science and Higher Education. The equipment of the Center for Physical and Physical-Chemical Analysis Methods and Studying the Properties and Characteristics of Surfaces, Nanostructures, Materials, and Products shared research facilities of the UdmFRC UB RAS was used in the study.

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FORMATION OF A CARBON FILM ON THE SURFACE OF A METAL ALLOY OF THE Cu-Ni SYSTEM UNDER ION IRRADIATION CONDITIONS

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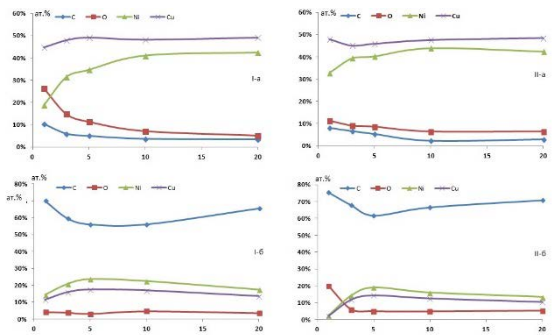
In this paper, the features of segregation processes in the surface layers of Cu-Ni alloy samples initially in a highly deformed state (after rolling), as well as samples subjected to pre-annealing in a vacuum furnace at a temperature of 600 °C. are investigated. A comparative analysis of Cu-Ni alloy samples irradiated with C^+ ions, as well as sequentially treated with O^+ and C^+ ions, was carried out. The main purpose of this work was to determine the conditions for the formation of a carbon layer as a result of high-energy irradiation of samples with carbon ions. The irradiation of the samples was carried out under the same conditions. Carbon ions were implanted with an energy of 30 keV and a dose of 10^{18} ions/cm^2. To determine the effect of surface contamination, some of the samples were pretreated with oxygen ions up to a dose of 1.3×10^{17} ion/cm^2. From the data of X-ray diffraction analysis, it can be seen that as a result of annealing of the initial rolled samples, the diffraction peaks narrow, which indicates an increase in the size of the crystallites in the sample and a decrease in microdeformations. In addition, annealing leads to a significant redistribution of the peak intensities of the Cu-Ni phase, which indicates the presence of texture in both the initially rolled and annealed sample. On the diffractograms of all samples, in addition to the lines from the Cu-Ni solid solution, one can also see peaks from other phases, possibly oxides or carbides of nickel or copper. The surface layers of the samples before irradiation contain about 50 at% - Cu and 40% at% Ni. As a result of irradiation with carbon atoms, a carbon-rich layer (up to 80 at%) is formed in the surface layers that are chemically unrelated to the matrix atoms, which indicates the diffusion of carbon atoms in the radiation field as an element with a smaller radius. Successive irradiation with oxygen and carbon ions of the rejected samples formed a two–layer structure on the surface of the samples - an oxygen-enriched layer containing a large amount of copper and nickel oxides, and a subsequent layer enriched with carbon atoms.



Distribution of alloy components: I – rolled samples, II – rejected samples; a) before irradiation, b) after successive irradiation with oxygen and carbon ions

According to the results of the work, it was revealed that irradiation with carbon ions forms a layer on the surface that is inseparable from the matrix atoms, enriched with carbon atoms that are both in a chemically unrelated form and in the form of carbides (extremely low concentration), the thickness of the layer exceeds the depth of the carbon ion path, which is possibly due to a large dose of radiation.

INITIONALIZATION OF THE SHAPE MEMORY EFFECT BY IRRADIATION WITH FAST NEUTRONS

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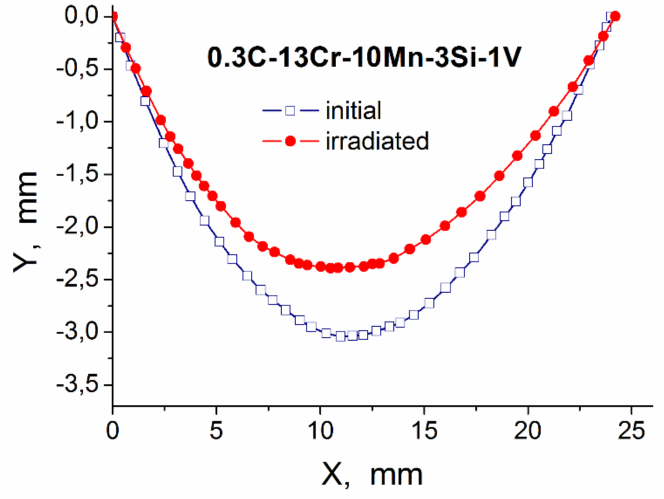
When studying impact of irradiation of titanium nickelide with fast neutrons, it was shown [1] that such treatment suppresses the shape-memory effect (SME) characteristic of this intermetallics and alongside gives rise to amorphization of the material.

The SME inherent in austenitic manganese steels is known to be related to the formation of deformational ε-martensite or deformatonal twinning and formation of martensite crystals with new orientational relationships. The extent to which this SME manifests itself essentially depends on the microstructure of the material, namely, presence of vanadium nanocarbides [2, 3] precipitating in the course of artificial aging of steels, which is accompanied by depletion of matrix with carbon. On the other hand, it was established that neutron irradiation can exert a significant effect on such subsytems of nanocarbides, which makes it possible to expect a kind of effect of the neutron irradiation on SME as well.



The middle line of the side projection of the sample before and after irradiation by fast neutron fluence of $6{\cdot}10^{19}$ cm^{-2}.

The band sample of austenitic steel 0.3C-13Cr-10Mn-3Si-1V was cold deformed to a shape of circular arc with a deflection of 3 mm and then irradiated by fast neutrons with a fluence of 6×10^{19} cm^{-2} in the vertical wet channel of the IVV-2M reactor at a temperature of 80 ºC. This material belongs to the class of the stainless manganese austenitic steels with the shape memory effect. The neutron irradiation was initially supposed to lower the SME upon the further heating in comparison with the reference sample.

But instead, the SME appeared immediately under irradiation showing a decrease in the deflection of about 21%. Check experiments confirmed that the lower limit of the SME in this material is 120 ºC with its absence at 80 ºC. This allows us to assert that the observed effect is the result of the neutron irradiation.

The results were obtained at IMP Neutron Material Science Complex within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme “FLUX” No. 122021000031-8).

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INVESTIGATION OF THE PROCESSES OF COMPOUNDS FORMATION Ti-Al UNDER LASER INFLUENCE

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The work considers the results of a study of the influence of focused pulsed laser radiation on the processes of forming Ti-Al compounds in multilayer films, depending on the selected laser radiation parameters.

The purpose of the work is to study the processes occurring in the material under study as a result of irradiation and to provide the necessary modes of laser exposure on the Ti-Al system for targeted modification of surface layers with intermetallides.

Studies were carried out on metal plates made of pure titanium "VT 1-0", on the surface of which a multilayer package of alternating three aluminum and three titanium layers was formed as a result of spraying (1st layer Al - 100 nm; subsequent Ti - 10 nm; Al – 10 nm; Ti – 10 nm; Al – 10 nm; Ti – 10 nm). Before spraying, the surface of the plates was subjected to mechanical and ion cleaning. The objects of the study were overall samples with a size of 10×10 mm with a thickness of 2 mm.

Laser exposure to the sputtered layers of the samples was carried out with a focused laser beam in an argon atmosphere. Surface treatment took place in the same pulse mode, but with different density of laser radiation power. The irradiation was carried out by scanning – by moving the laser beam in the selected area of the sample. The laser treatment zone was 10 × 10 mm in area.

"*Ldesigner F1*" fiber-optic ytterbium laser was used as radiation sources.

Analysis of the condition of the surface layers of the samples before and after laser exposure was carried out using atomic force microscopy ("*Solver-47 PRO*"), X-ray photoelectron spectroscopy ("*ES-2401*") and microhardness measurements ("*PMT-3*").

As a result of the studies, changes in the relief and topography of the surface of the samples, as well as changes in microhardness values from the initial state were detected. It was found that after laser exposure in the samples, elements are redistributed in the surface layers.

Possible mechanisms have been proposed to explain the observed changes in the alloy after laser exposure.

The work was carried out within State Task of the Ministry of Science and Higher Education of Russian Federation (No. 121030100002-0). In terms of conducting research by X-ray photoelectron spectroscopy, the work was carried out with the support of the Ministry of Science and Higher Education of the Russian Federation under Agreement No. 075-15-2021-1351. 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.

PHYSICO-MECHANICAL PROPERTIES OF Ti/Al AND Ni/Al MULTILAYER FILMS AFTER ION-BEAM MIXING

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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 [4-6].

In this work, the methods of X-ray photoelectron spectroscopy, atomic force microscopy and nanohardness measurement were used to study the morphology of the surface, the formation of the chemical composition and changes in the physical and mechanical characteristics of the surface layers of Ti/Al and Ni/Al multilayer films on the surface of titanium VT1-00 depending on the dose of argon ion irradiation ($5\cdot10^{15}$ - 10^{17} ion/cm^2).

The work was carried out within State Task of the Ministry of Science and Higher Education of Russian Federation (No. 121030100002-0). In terms of conducting research by X-ray photoelectron spectroscopy, the work was carried out with the support of the Ministry of Science and Higher Education of the Russian Federation under Agreement No. 075-15-2021-1351. 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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RADIATION-DYNAMIC EFFECTS UNDER CORPUSCULAR IRRADIATION. RADIATION SHAKING INSTEAD OF TEMPERATURE

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Nanoscale dynamic effects and processes occurring under cascade-forming types of irradiation of condensed matter with heavy ions, neutrons and fission fragments are considered. The role of these processes is beyond the scope of classical radiation physics of condensed matter. They were first reviewed in publications by the author and his colleagues, and later studied and confirmed, including by joint works with colleagues from Helmholtz-Zentrum Dresden-Rossendorf, Germany (see [1]). The sources of the recorded effects are the regions of passage of dense cascades of atomic displacements, thermalized in times of the order of one trillionth of a second (Thermal Spikes), with gigantic temperatures and pressures (T = 3000-6000 K, P = 5-40 GPa [1, 2]), which are sources of powerful post-cascade elastic and/or shock waves.

A theory has been developed of self-propagating (theoretically over unlimited distances) structural-phase transformations in metastable media [1-3], initiated by ion bombardment (due to “radiation shaking” by post-cascade waves). In practice, this provides [1, 2, 4, 5] an increase by at least 3-5 orders of magnitude in the linear scale of the impact of ionizing radiation on materials (including the depth of impact of ions); 2) a decrease in the temperature of radiation-initiated transformations by tens and hundreds of degrees compared to similar thermally activated processes; 3) an increase in their speed by several orders of magnitude compared to thermally and radiation-stimulated migration processes. It should be noted that the mechanism of radiation shaking is not related to radiation-enhanced diffusion.

Examples of radiation-dynamic (RD) processes in metals and alloys (intraphase and phase transformations) are considered. Specific applications concern the modification of resistive, magnetic, mechanical, resource and up to. properties of functional materials with the beams of accelerated ions [1, 2, 4, 5] Simulation studies of the radiation resistance of various materials have been carried out.

Rapid (within a few seconds) processes of formation in alloys of depleted and multiply enriched phases in chemical elements have been discovered [1, 3, 4, 5] during ion bombardment at temperatures significantly below the threshold of activation of thermal diffusion. That is of fundamental interest. The emerging states that are close to equilibrium [5] cannot be obtained by any other means. This makes it possible to detect theoretically predicted as well as unknown low-temperature phases (which are “things in themselves”) with unknown properties.

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THE EFFECT OF ALTERNATING IRRADIATION WITH O^+ AND N^+ IONS ON THE COMPOSITION, STRUCTURE AND ELECTROCHEMICAL PROPERTIES OF TITANIUM ALLOY VT6

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Ion implantation is a complex interconnected physico-chemical processes. To date, the role of physical and chemical processes has not been sufficiently studied. In our previous studies, it was shown that the accumulation of nitrogen to concentrations of 30-40 at.% in the surface layers of titanium alloy VT6 during implantation of N^+ ions is determined by titanium atoms [1]. Nitrogen accumulation is accompanied by the formation of titanium nitride TiN and its release in the form of phase inclusions over the entire surface. Comparative studies have suggested the predominant influence of chemical processes in the formation of surface layers, in particular, the chemical activity of titanium atoms to the implanted nitrogen [1, 2]. To confirm this assumption, in this paper it is proposed to irradiate the titanium alloy VT6 alternately first with O^+ ions, and then with N^+ ions. Preliminary irradiation with O^+ ions due to the higher chemical activity of oxygen to titanium atoms should lead to changes in the processes of accumulation of the implanted element and the formation of phase components of the surface layers during subsequent irradiation with N^+ ions. In particular, titanium atoms bound by oxygen into oxides as a result of preliminary irradiation with O^+ ions will determine to a lesser extent the accumulation of nitrogen and the formation of nitride phases, confirming the role of chemical processes in the formation of surface layers.

In this paper, a study of the chemical composition, surface morphology and electrochemical properties of titanium alloy VT6 in the initial state, after irradiation with O^+ ions and after alternate irradiation with O^+ and N^+ ions with radiation doses of 10^{18} and $3 \cdot 10^{18}$ ion /cm^2 of N^+ ions was carried out. It is shown that under the conditions of irradiation with O^+ ions, intensive oxidation of titanium atoms occurs, accompanied by the formation of titanium oxides and hydroxides with particle sizes from 100 to 200 nm. It was found that with subsequent irradiation with N^+ ions, nitrogen accumulation and the formation of titanium nitride TiN is carried out to lower concentrations than without pretreatment with O^+ ions. It is shown that during electrochemical tests in the range from the open circuit potential to 500 mV, a decrease in the oxidation rate of modified samples is observed by an order of magnitude. At high test potentials, the anodic oxidation currents of the modified samples exceed the initial values, which may be due to the oxidation of the phases of titanium nitride and oxynitride and the acceleration of the anodic release of oxygen and chlorine due to increased electrocatalytic activity of the modified surface.

The work was performed under state assignment No. 121030100002-0 from the Russian Ministry of Science and Higher Education. The equipment of the Center for Physical and Physical-Chemical Analysis Methods and Studying the Properties and Characteristics of Surfaces, Nanostructures, Materials, and Products shared research facilities of the UdmFRC UB RAS was used in the study.

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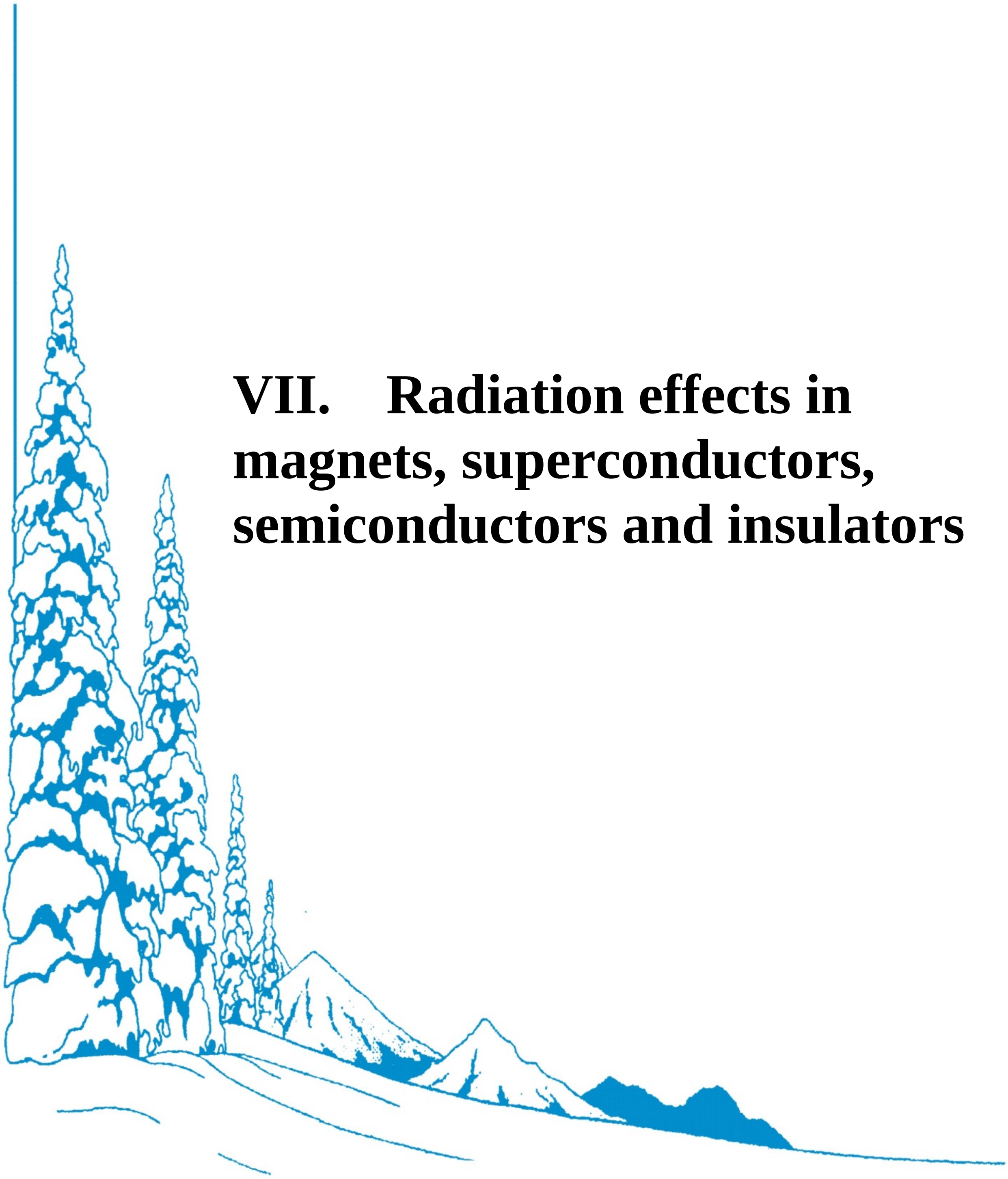
VII. Radiation effects in magnets, superconductors, semiconductors and insulators



CONFOCAL OPTICAL SPECTROSCOPY OF RADIATION DEFECTS IN $MgAl_2O_4$ CRYSTALS IRRADIATED WITH HIGH ENERGY HEAVY IONS

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Radiation-induced changes in microstructure and optical properties of $MgAl_2O_4$ remain a subject of continuous studies during last few decades. Its resistance against neutron irradiation being compared with alumina was evaluated somewhat as an excellent that is not common case for oxide ceramic. At the same time, demonstrating exceptional stability during accumulation of radiation defects produced in elastic collisions, $MgAl_2O_4$ spinel is rather sensitive to damage via relaxation of dense electronic excitations, having a relatively low threshold of latent track formation, about 7.5 keV/nm [1,2].

Overall intention of this work is to study the optically stimulated luminescence in $MgAl_2O_4$ single crystals in presence of latent tracks formed by swift heavy ions using laser confocal microscopy technique. Photoluminescence (PL) spectra from the near surface region of Bi (670 MeV), Xe (156 MeV), Kr (100 MeV) and Ar (44 MeV) ion irradiated specimens were recorded during excitation at 355 nm, 472 nm and 532 nm. It was found that PL spectra are always composed of broad overlapping bands positioned over the entire spectral range from the excitation wavelengths till 800 nm. It is suggested that such spectral composition might be due to excitation of antisite defects in disordered regions surrounding ion track core with following energy transfer to luminescent centers and radiative recombination. As possible luminescence centers, aggregate color centers and complexes of defect plus impurities are also considered. Experimental results have evidenced that structural state of ion track core (amorphous, or non amorphous) does not affect itself on the luminescence processes in high energy heavy ion irradiated $MgAl_2O_4$ crystals.

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INCREASING THE CRITICAL CURRENT OF HTSC COMPOSITES WHEN IMPLANTING MAGNETIC IONS

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Modern high-temperature superconducting tape composites have a fairly complex composite structure, which consists of a Hastelloy alloy-based substrate with a thickness of about 60 μm, several thin buffer oxide layers and a 2 μm layer of directly high-temperature superconductor (HTSC) $REBa_2Cu_3O_{7-x}$ (RE is a rare earth element, for example , Y or Gd)). The entire structure is covered with protective layers of silver and copper. Such superconducting materials exhibit enormous critical current densities (several MA units per square cm of cross-section) even at the boiling point of liquid nitrogen. At the same time, for many practical applications, the problem of increasing the critical current of HTSC tapes both in zero field and in magnetic fields and different temperatures remains relevant and requires a solution.

It is well known that an increase in the critical current is achieved through the creation of magnetic flux pinning centers—structural defects in the HTSC material. For this, various methods are used, from the formation of defects at the synthesis stage to radiation exposure, leading to the appearance of radiation defects of various types. At the same time, pinning can be enhanced by adding magnetic defects to the structural defects, which, due to additional magnetic interaction, will lead to an increase in the pinning force. Thus, we have previously shown that the implantation of magnetic Fe^+ ions can lead to an increase in the critical current of HTSC composites.

In this report, we provide detailed data on the effect of irradiation with magnetic Co2+ ions on the magnetization and critical current of HTSC composites. Irradiation of the samples was carried out with several fluences for 4 different modes of creating defects in which sequentially there was no implantation of ions, and then the concentration of magnetic ions in the HTSC layer increased until the mode of complete stopping of ions in the superconducting matrix (the Brag peak was in the middle of the HTSC layer). Different implantation modes were implemented by varying the thickness of the Ag layer, which led to different projective ion paths, which were previously calculated using the SRIM package. Before irradiation, all protective layers were removed, except for the Ag layer. It was shown that under certain irradiation conditions and implantation modes of magnetic Co^{2+} ions, an increase in magnetization and critical current is observed both in zero field and in fields up to 8 T (see Fig.). The report will analyze the results obtained and propose a physical model to explain the experimental data.

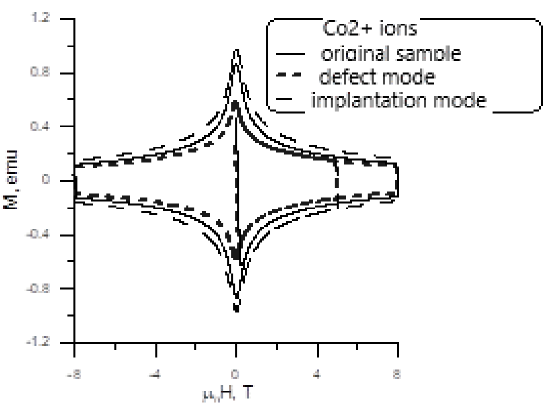

Fig. Increasing the magnetization of HTSC composites during implantation Co^{2+}

The study was supported by a grant from the Russian Science Foundation No. 23-19-00394, https://rscf.ru/project/23-19-00394/.

NUMERICAL ANALYSIS OF THE DYNAMICS OF RADIATION-INDUCED DEFECTS IN HTS COMPOSITES

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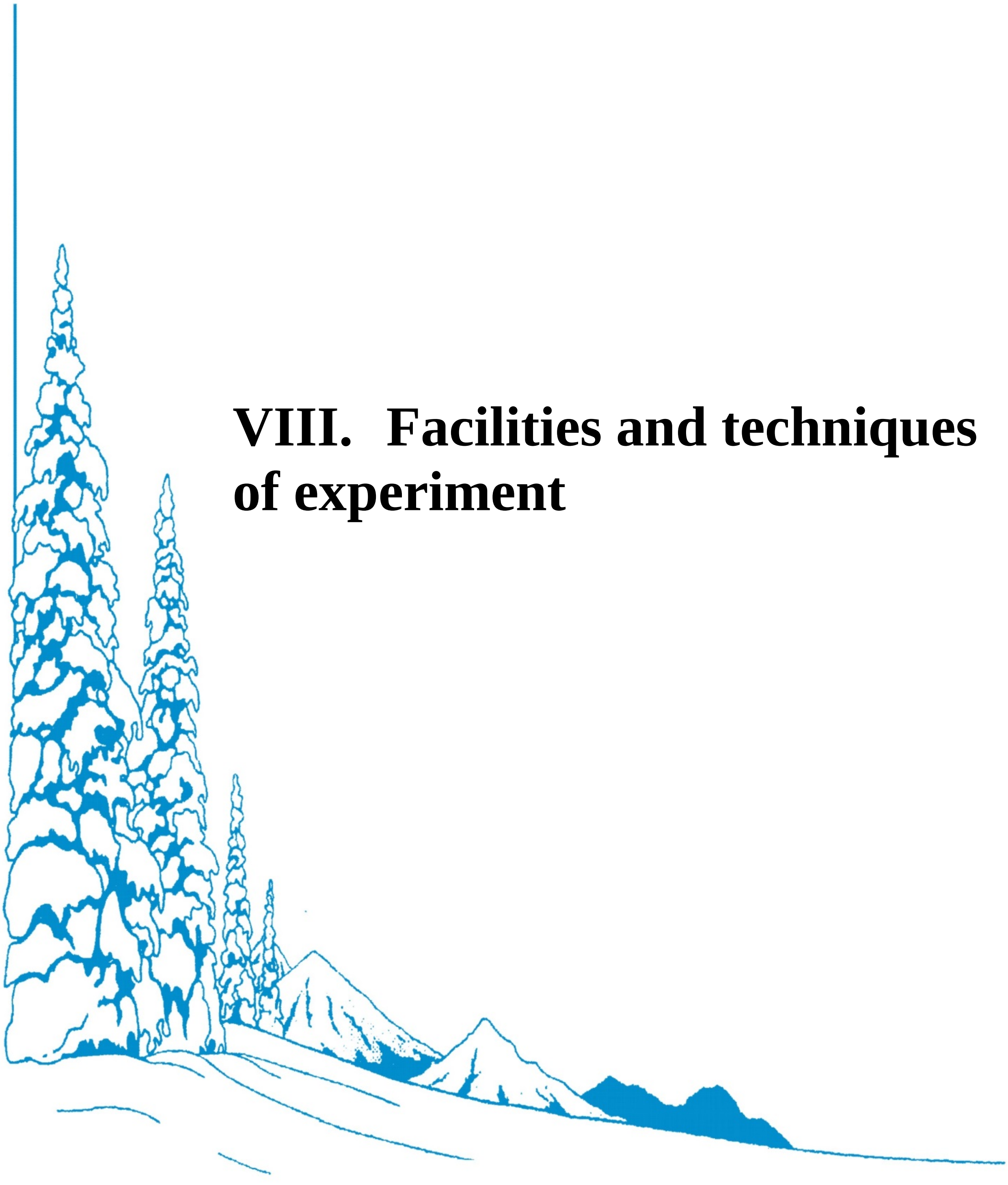
Under the influence of ionizing radiation, defects of various types are formed in the superconductor, which can serve as pinning centers for magnetic vortices. Ion irradiation at low fluences can lead to both an increase and a decrease in the critical current of high-temperature superconducting tapes based on the $YBa_2Cu_3O_{7-x}$ compound (hereinafter YBCO), while the increase in the critical current is associated with the formation of new pinning centers; decrease - may be associated with a decrease in the critical temperature with an increase in the concentration of defects and the overlap of their potential holes. At high fluences, volumetric pinning of Abrikosov vortices is determined only by radiation defects. In many cases, experimental research into the ionic effect on a material is hampered by the rather high cost of the process. It is also important to note that most methods of such research are destructive in relation to the target, since in order to study the resulting layers with impurities or structural defects it is necessary to destroy the target layer by layer. Computer modeling can significantly speed up the process of studying radiation defects (RD) in a substance, increase the radiation resistance of materials and offer effective methods for restoring their operational properties.

As part of this study, algorithms were developed for determining the parameters of radiation defects formed in $YBa_2Cu_3O_{7-x}$ by a powerful ion beam. The following system is considered as a starting point: a defect-free YBCO layer of thickness *h*, exposed to a flow of $^{132}Xe^{27+}$ ions with initial energy *E_Xe* and fluence *F0*, directed at an angle alpha to the target surface at temperature *T0*. Modeling of the described system is carried out using a multiscale approach, in which the results of calculations at the lower level are used for calculations at a higher level and further. Simulations of atomic displacement cascades in YBCO are performed using the molecular dynamics method. Modeling of the evolution of emerging defects and their interaction was carried out using the kinetic Monte Carlo method. A mathematical description of the model is presented, as well as the results of calculations of defect formation processes and an analysis of the kinetics of defects when a YBCO target is irradiated with $^{132}Xe^{27+}$ ions with an energy of 167 MeV at an angle of 90º to the target surface in the temperature range 1-100 K. The calculated displacement energy of oxygen in YBCO was ~10 eV, which is consistent with data from literature sources. Using the developed approach, it was found that the majority of defects are annihilated within the first picoseconds, at the stage of formation of a cascade of primary defects. Other radiation defects lead to changes in the crystal structure of the target and its properties. Clustering and defect kinetics were studied on a millisecond time scale. The temperature dependences of the concentration of radiation defects and the threshold energies of migration of radiation defects are presented, and the duration of the required thermal annealing of the samples is estimated.

The development of the calculation model was carried out within the framework of the State Assignment (project FSWU-2022-0013) with the support of the Ministry of Science and Higher Education of the Russian Federation

Calculations of the dynamics of radiation-induced defects in HTS composites were carried out with funding from JINR under the support program within the framework of the Ariadne collaboration.

VIII. Facilities and techniques of experiment



A NEW VERSION OF THE IMPLEMENTATION OF THE TASKS OF RADIATION MATERIALS SCIENCE - ON THE WORLD'S FIRST SATELLITE PROBE MICROSCOPE

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The presence of the so-called "proton belt" around the Earth at an altitude above 500 km above sea level has now begun to give us the opportunity to conduct new experiments in radiation materials science due to the discovery and successful testing of a new method, which was the development of traditional experiments in nuclear and thermonuclear installations [1]. The "proton belt" itself is known to contain protons with speeds up to 200 *km/s*, but the delivery of the studied samples to it together with analytical equipment has become news - not only because of the appearance of a fundamental possibility, but also because of the relatively affordable cost at the level of 100 *thousand US dollars* (2023). A modern scanning probe microscope "SMM-2000" with a resolution of up to 1 *nm*, was implemented in the form of a satellite of the Earth "Nanoprobe-1" with a size of only 300x100x100 *mm* (Fig.1), and on June 27, 2023, it was successfully launched into space at an altitude of 560 *km* at the beginning of the "proton belt". The copyright holder of the international patent [2] for this type of spacecraft is the Russian enterprise "PROTON Plant", Zelenograd, the manufacturer of these spacecraftes.

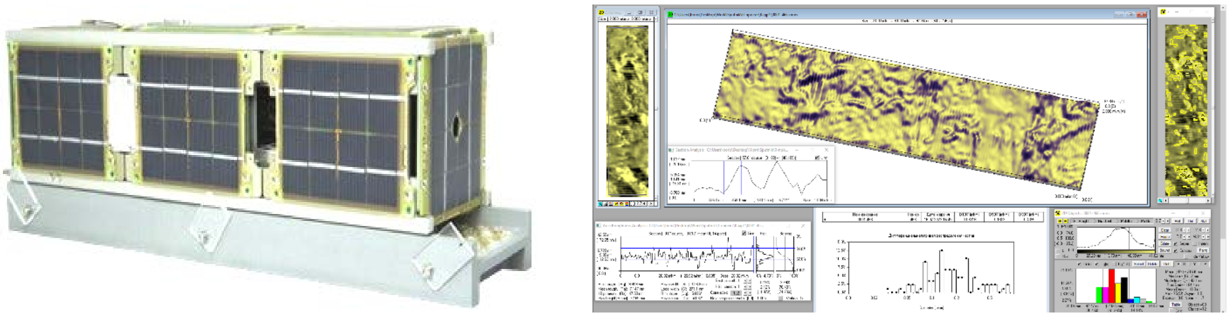

Fig.1. The world's first probe microscope satellite of the Earth (left) and the resulting frame in the size of 8 *microns* x 2 *microns* of the surface of the golden mirror after its exposure in outer space at an altitude of 560 *km* above sea level in the "proton belt" of the Earth.

This spacecraft is designed for more than two years of flights, while it can take more than a hundred high-resolution frames of the sample surface per day, transmitting these frames to Earth via radio waves available for reception by conventional antennas. There is still a lot of data to be taken and analyzed in the experiment currently being implemented, but even in the first frame a serious change in the surface of the sample is clearly visible: multiple potholes up to 30 *nm* deep appeared on the smooth surface of the golden mirror with a roughness Ra of no more than 1 *nm*. The launch of similar spacecraft with samples began to acquire a regular character [3], with the possible expansion of the number and types of analytical instruments on board.

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ADVANCED THERMOREFLECTANCE TECHNIQUES FOR NON-CONTACT MEASUREMENT OF MICRO-SCALE PHONON THERMAL TRANSPORT IN SWIFT HEAVY ION IRRADIATED YTTRIUM ALUMINIUM GARNET

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One promising design for next-generation nuclear fuel is based on inert matrix fuel (IMF) containing a low activation matrix (i.e. transparent to neutrons) as carrier for the fissile material. Yttrium aluminum garnet (YAG) $Y_3A1_5O_{12}$ – based ceramic composites are good IMF candidates [1]. To mimic the irradiation damage to inert ceramic matrices by fission products (FPs), the swift heavy ions (SHIs) derived from high energy ion accelerators, are typically employed to test the target matrix materials against radiation resistance. The SHIs with energies > 100 MeV impart damage to its near surface region down t*o several to tens of microns*, spanning electron ionization and nuclear displacement regimes of the bombarded ceramic. IMF ceramic, in addition to being radiation resistive to FPs, must also possess sufficiently high resistance to heat conductivity deterioration to corresponding radiation defects [2,3]. The thermal transport properties of irradiated IMF candidate materials need to be evaluated with corresponding micro-scale depth spatial resolution.

To perform such near-surface heat conduction assessment, we have assembled and tested in our laboratory continuum wave laser-based pump-probe thermoreflectance setup operating in two modes: frequency-domain thermoreflectance (FDTR) and spatially-domain thermoreflectance (SDTR) [4]. In the former approach, the pump and probe laser beams are focused into the same micron-size spot of the sample surface, while the modulation frequency of the heating (pump) laser beam is scanned over 0.3 - 100 kHz frequency range enabling measurement of the *cross-plane* thermal conductivity by thermally resolving both ion damaged and further lying undamaged regions on micrometer scale depth range. In the latter approach, the probe laser beam scans across the pump beam location in the radial plane of the sample surface at constant modulation rate, enabling the assessment of thermal anisotropy, i.e. the *in-plane* thermal conductivity [5].

We studied micron-scale depth resolved room-temperature thermal transport properties of YAG single crystal irradiated by 167 MeV Xenon ions with fluences $f = 2 \times 10^{11} - 6 \times 10^{12}\, cm^{-2}$. This ion fluence range was chosen to obtain both single ion track and partial tracks overlapping regimes in YAG crystal lattice.

Accelerator-drive SHIs penetrate into YAG crystal lattice and produce stable amorphous tracks along the ion paths [6]. The investigation of such track formation and their influence on YAG lattice shows how micro-scale phonon thermal transport in different dimensions in solids can be controlled by ion beam irradiation technique.

The multilayer heat conduction equation in cylindrical symmetry was used to extract the thermal conductivity of the damaged region of YAG. A semi-analytical model based on the

Klemens-Debye approximation [7] was used to model various phonon scattering mechanisms contributing to thermal conduction in pristine and irradiated YAG, with phonons being the major heat carriers in this insulating crystal.

The results of this investigation have shown that the thermal conductivity of irradiated YAG drops substantially at the highest ion fluence and the influence of tracks overlapping was observed, as expected. We assume that the formation of lateral amorphous tracks under SHI irradiation can potentially lead to anisotropic thermal transport behavior in YAG. Further exploration of this effect using SDTR approach might lead to new opportunities for adjustment thermal transport by ion-beam irradiation in dielectric materials and promote novel method of tailoring materials properties.

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APPLICATION OF ELECTRON SPECTROSCOPY METHODS FOR STUDYING THIN FILMS AND ION-MODIFIED MATERIALS

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Even in early works, for example, [1], it was shown that the satellite structure accompanying the XPS peak of C1s carries important information about the material. In particular, this was shown in the study of C60 fullerenes. Taking into account the relationship between the plasmon energy and the mass density of the substance in g/cm^3, it was determined that the fullerene density is 2,03 g/cm^3, which differed significantly from the values previously obtained by X-ray diffraction methods [2]. In the review work [3] in Chapter 6, it was also shown in detail that from the analysis of plasmon loss energies it is possible to determine both the mass and atomic density of carbon materials, in particular thin films of amorphous carbon.

The purpose of this work was to determine the mass density of magnetron sputtered carbon films, as well as carbon films subjected to subsequent pulsed implantation of argon and nitrogen ions. Based on the review work [3], the possibility of using brief analytical expressions to determine the mass density of known forms of carbon from previously certified samples was tested.

The mass density values of these materials were obtained, which showed satisfactory agreement with the reference data for the mass density values of carbon materials determined by the XPS method. Subsequently, these methodological results were used to characterize thin ion-modified magnetron films on the surface of glass or iron. It was shown that magnetron sputtered films, firstly, are highly disordered, and secondly, the films had a significantly lower mass density (on average 1,88 g/cm^3) compared to the known density of bulk graphite (2,26 g/cm^3), the target from which was used for magnetron sputtering. The same technique later made it possible to show changes in the mass density of a magnetron-sputtered thin carbon film under pulsed irradiation with ions of different masses and chemical reactivity.

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DEFINITION OF A DOMINANT MECHANISM FOR MICROCONTROLLER UPSETS INDUCED BY PULSED LOW-ENERGY PROTON RADIATION

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About 40-50% of all radiation tests now in progress in space applications focus on single-event effects (SEE). Logical-state upset in a memory cell induced by individual particles, the so-called single-event upset (SEU), is one of their manifestations.

Upsets induced by direct ionization from protons were first predicted in 1982 [1] and subsequently confirmed by the experimental work in 2007 [2] for low-energy protons generated by a static accelerator. More recently, many studies confirmed that the single-event upsets were induced by direct ionization from protons. At the same time, the reported cross sections of the upsets induced by low-energy protons exceeded the high-energy proton value by several orders of magnitude.

In the work presented, the feature of the experimental setup was a pulsed proton source based on a laser plasma source. Although the notion of the laser particle acceleration is not new, we know of no published data on the use of a source like this to study the microelectronics response induced by individual nuclear particles. In the authors' opinion, the source is generally promising. However, the problem of a high-density proton flux generated by the laser plasma source (on the order of 10^{13}–10^{16} $cm^{-2}\cdot s^{-1}$), which could result in the volumetric ionization effects, remained unsolved. It was necessary to verify the simulated cosmic proton (low-energy) radiation induced by the laser plasma facility.

In this regard, the purpose of the work was to determine, through analysis of experimental data, a dominant mechanism for upsets in the test sample induced by the pulse of low-energy protons.

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DETERMINATION OF THE MIGRATION ENERGY OF VACANCIES IN METALS USING LOW TEMPERATURE NEUTRON IRRADIATION

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The kinetics of the point defects formation in materials and their energy characteristics, in particular, the energy of migration and interaction with sinks, are necessary to describe radiation-induced processes occurring in reactor materials under neutron irradiation. To determine them, calculations are carried out using molecular dynamics methods and various types of interatomic potentials. The results obtained by different authors vary; the situation becomes much more complicated when they try to obtain them for real multicomponent reactor steels and alloys. The development and use of experimental methods for determining the characteristics of point defects generated by irradiation is an important problem in reactor materials science.

One of the methods used to register the temperature at which vacancies acquire mobility is the comparison of dilatometric heating diagrams of samples with vacancy concentration close to thermal equilibrium with a sample with their increased concentration. An effective method for accumulation of a large number of vacancies in a sample is low-temperature neutron irradiation, when the generated interstitials migrate and go to the sinks, in particular from the solid, and vacancies are practically deprived of thermal mobility and accumulate in the sample.

The report presents the results of experimental determination of vacancy migration energy in nickel and chromium samples after low-temperature irradiation in the reactor IVV-2M for 179 hours at a temperature of about 40÷45 °C. Along with obtaining a difference dilatogram - temperature dependence of the difference between the relative elongations of unirradiated and irradiated samples, the results of transmission electron microscopy and X-ray diffraction analysis of samples in the initial state and after low-temperature neutron irradiation are presented.

FRACTURE FEATURES OF IRRADIATED AUSTENITIC STEEL AT ELEVATED TEMPERATURES

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The fast neutron reactor is a key link in creating a closed fuel cycle for nuclear energy. The progress and successful operation of reactors of this type is due to the choice of structural materials and the step-by-step analysis and improvement of the functional characteristics of these materials [1,2]. The result of accumulated operating experience and improvement was austenitic steel with a Cr/Ni base (16:15), as well as its next generation with an increased Ni content of up to 19.5%. These steels have been successfully used and are being used as fuel cladding.

Increasing the burnup of nuclear fuel of present fast reactors is solved by increasing the duration of the fuel cycle [3]. This depends on maintaining the operability of the fuel claddings. Increasing the duration of the fuel campaign leads to an increase in the accumulated damage dose and increase changes in the structural state and local chemical and phase composition under irradiation at elevated temperatures. The radiation induced processes have a direct impact on the strength (mechanical) characteristics of austenitic steels and their fracture.

The use of scanning electron microscopy in the study of the fracture surface of irradiated samples can reveal the features of the ongoing deformation processes during tests [4].

A study was carried out of the characteristics of fractures of austenitic fuel cladding sleel after operation and mechanical tests at temperatures from 24 to 650 °C. The features of the fracture surface at different temperatures are determined.

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GLOVEBOXES AND GLOVEBOX LINES «SPECS GB»: MADE IN RUSSIA LABORATORY EQUIPMENT FOR LITHIUM BATTERY RESEARCH, DEVELOPMENT & PRODUCTION

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Spectroscopic system’s highly qualified, experienced and certified engineers deliver complex and diverse inertgas system solutions. Our combined process experience and proven solution capabilities enable our Russian customer base to meet the demands of today's emerging technologies.

Most commonly the presence of moisture and oxygen are the principal air components which shall be excluded from the process environment for lithium battery research, development & production. Therefore technologies are required which allow running processes under oxygen and moisture free conditions. Two predominant techniques have been established to address this specific problem – vacuum technology and inertgas technology. Whilst vacuum bases on the principle of creating nearly gas free environments by evacuating rigid structures to pressures less than 10-9 mbar, the inertgas technology selectively removes harmful components from the air resulting in a completely oxygen and moisture free working environment at ambient pressure. The main benefit between both approaches is that inertgas technology is compatible with all kinds of equipment, processes, and system enclosure sizes offering full auto and manual access at a fraction of the costs of normal vacuum systems. In case of the vacuum technology many tools are not vacuum proof, solvent containing materials cannot be processed.

Since its foundation in 2004 JSC «Spectroscopic systems» has been able to offer its comprehensive product portfolio of interdisciplinary systems which combine vacuum technology as well as inertgas technology. The core element of a well-designed inertgas-system is the «SPECS GB» gas purifier. This unit is a closed-loop system with integrated, fully regenerable scrubber units which selectively remove moisture, oxygen and solvents from an inertgas stream. Most commonly nitrogen, argon or helium is used as the process gas.

Specs GB systems are primarily used for the standard research and development of lithium ion battery technologies and our custom enclosures are used for critical dry production environments necessary for battery manufacturing. Boxes can help in maintaining a minimum-humidity atmosphere that will neither harm operators nor be disrupted by them. Our glovebox systems and custom enclosures also allow the ability to record and trace the production environment for enhanced quality control. Connected to the purifier is a gas-tight, hermetically sealed enclosure called a glovebox. These system come either in standardized sizes mainly used for research and development or in customized designs for industrial use.



INVESTIGATION OF IRRADIATION EFFECTS IN STRUCTURAL MATERIALS WITH ION ACCELERATORS

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The problems in selection of radiation-tolerant reactor materials based on reactor and accelerator irradiation are considered, associated with differences in the rates of damage dose accumulation and production of He and H. Current trends in the development of simulation studies at accelerators are presented. Using nuclear microanalysis methods, procedures for ion irradiation of structural reactor materials (SM) have been elaborated on the Tandem-3M accelerator at JSC State Scientific Center of the Russian Federation - IPPE. The stresses in the sample caused by temperature gradients and accumulation of implanted ions were calculated using finite element method for typical irradiation conditions. Calculations of neutron spectra in the BOR-60, MBIR, BN-800, BREST reactors, as well as the production rates of helium and hydrogen in SM during irradiation in these reactors, were carried out to take them into account during cyclic sequential accelerator irradiation of SM with metal ions, He and H.

Radiation phenomena in SM under reactor and accelerator irradiation are considered, with the main attention being paid to radiation-induced segregation and swelling.

The dependence of swelling on the composition of austenitic stainless steels - structural materials of VVER TOI internals - has been studied under ion irradiation. For subsequent reactor tests, the composition, which is the most resistant to swelling, was chosen. Using 18Cr10NiTi steel as an example, studies were carried out on the effect of helium and hydrogen on swelling in SM. It was shown that under triple cyclic sequential irradiation (Ni+He+H) swelling in this steel is significantly higher than under double one (Ni+He/H), i.e. a synergistic effect of helium and hydrogen in swelling of steel is observed for the conditions of their implantation corresponding to their accumulation in a fast reactor.

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PULSED IONIZING RADIATION DETECTION USING OPTICAL FIBER

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At present, there is a number of problems in the field of ionizing radiation (IR) recording related to the absence of fast detectors (< 1 ns resolution time), and recording of electrons and ultrahard X-ray radiation [1]. To solve these problems the trending fiber-optic sensors can be used. Such sensors have some advantages in terms of IR recording, in particular, resistance to interference, sensitivity to high-energy particles, capability to operate under high IR fluxes, and high resolution.

To apply fiber-optic sensors as IR detectors it is essential to have an idea of spectral-time characteristics of radiation-induced radiation (RIR) and the nature of this radiation. It should be also noted that at present the problems of combined luminescence and radiation-induced absorption (RIA) phenomena, peculiar to impulse IR effect, are rather neglected. The study of radiation effects in fiber optics, as used herein, is most relevant for optical gyroscopes, in which the length of fiber-optic waveguides is of order 1-5 km, for telecommunication fiber-optic lines, and fiber-optic IR detectors [1-2].

Then, the objective of the current work is to study RIR nature and spectral characteristics, and to develop a model to determine fiber-optic detector response with allowance for combined RIR and RIA phenomena.

The current work involved experimental tests of multi-mode silica and polymethylmethacrylate optic fibers with core diameter of 50 µm and 125 µm. These fibers were irradiated with 0.2 MeV, 1 MeV, and 6 MeV electrons in a pulsed mode. Spectral-time characteristics of radiation-induced radiation were measured at the output of fiber optics. In addition to electron energy, the beam incidence angle was varied. In the course of the work the application of the mathematical model based on the finite-difference method was considered to estimate a form of radiation-unduced emission pulse at the output of fiber optics.

As a result of experimental research it has been found that fiber's light response depends on electron beam incidence angle. It has been demonstrated that Vavilov-Cherenkov radiation considerably prevails in light response of the tested fibers. The increased electron energy results in higher intensity of short-wave subspectrum related to Vavilov-Cherenkov radiation. The developed model agrees with the experiment. It can be used for performance evaluation of systems comprising fiber lines, under the action of pulsed IR with arbitrary absorbed dose distribution along the line.

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THE EFFECT OF THERMAL NEUTRONS ON SINGLE-EVENT MEMORY CELL UPSETS

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Numerous research works, both foreign and domestic, demonstrate that single-event effects (SEEs) induced by individual neutrons are present in the state-of-the-art electronic component base.

The sensitivity of integrated circuit (IC) to SEEs is known to depend mainly on the VLSI manufacturing technique, as well as on neutron energy. As of today, there is a significant number of works on the IC sensitivity to fast neutron-induced SEEs. It should be noted that some papers [1, 2] demonstrate that SEEs can be induced not only by fast neutrons but also by thermal ones. The IC sensitivity to thermal neutrons can contribute significantly to the SEE cross section. Thus, paper [3] shows that cross section of single-event upset (SEU) from low-energy neutrons is comparable to that from fast neutrons.

The IC sensitivity to thermal neutrons is associated with nuclear reactions observed when neutrons interact with B^{10}. This problem is of the most immediate interest when speaking about the recording instruments of the nuclear power and research facilities. To prove the effect of thermal neutrons on the IC sensitivity, experiments are carried out with neutron sources whose spectrum contains a significant portion of low-energy (<0.1 MeV) neutrons.

The authors conducted an experiment on neutron generator with neutron energy of 14 MeV. In order to obtain thermal neutrons, polyethylene was used as a moderator. In several experiments, Cd with a thickness of 0.5-1 mm was used to evaluate the effect of thermal neutrons on the IC sensitivity to SEU. Cross section for neutron-Cd reaction in the low-energy (<1 eV) region was of the order of several kbarn. The static RAM (IS62WV1288BLL) was the object of this study.

The Monte-Carlo calculation of spectral distribution of neutrons that got through the polyethylene and Cd layers was performed using the PRIZMA code. Calculation data demonstrate that the experimental design meets the requirements of the original problem, namely, polyethylene effectively converts the 14-MeV neutrons to the thermal-energy region, while Cd absorbs thermal neutrons.

This study shows that in the presence of neutron radiation, memory cell suffers from single-event upsets. At that, the sensitivity of this very memory cell to SEU decreases approximately fivefold if a Cd foil is used.

The research findings prove that electronic component base can be sensitive to low-energy neutrons. And this conclusion should be taken into account when analyzing resistance of the devices to neutron radiation.

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THE PROJECT OF A CYCLOTRON COMPLEX FOR SIMULTANEOUS IRRADIATION OF MATERIALS WITH H, He, Me (Cr, Fe, Ni) IONS.

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The analysis of the literature data of recent years clearly demonstrates the "renaissance" of works related to modeling the effects of high-dose neutron irradiation using simultaneous irradiation with accelerated beams of hydrogen, helium and one of the metal ions. Simultaneous irradiation with hydrogen, helium, and iron (chromium, nickel) ions is a prerequisite for modern experiments on modeling structural disturbances caused by neutrons in materials of nuclear power plants. In world practice, such work is carried out on accelerators with particle energies that provide a thickness of the irradiated layer of at least 2 microns (to eliminate the surface effect) and allow receiving radiation damage doses up to 150 dpa and a concentration of helium and hydrogen up to 1000 ppm.

In Russia, the only accelerator that fully meets the modern requirements of the industry and allows the sequential irradiation of ion types listed above is 3MV Tandetron 4130 MC+(HC) (IPPE, Obninsk). A review of existing foreign facilities shows that there are no precedents in the world for creating a dedicated accelerator complex to solve the problem of simultaneous irradiation of target with three beams (optimization of the ratio of defect formation rates to the accumulation rates of helium and hydrogen). Such complexes were built gradually, as a result, existing facilities (JANNuS – France; TIARA - Japan; HZDR - Germany), having electrostatic accelerators in their base and created for nuclear analysis tasks (RBS, PIXE, NRA), are not optimized for radiation materials science tasks.

Currently, the federal project "Development of new materials and technologies for Advanced Energy Systems" is being implemented within the framework of the integrated program of Rosatom State Nuclear Energy Corporation (Development of Equipment, Technologies, and Scientific research of atomic Energy in the Russian Federation for the period up to 2024). One of the proposals to be implemented within its framework was a request for the creation in our country of a specialized center for simulation studies of structural materials based on an accelerator complex of electrostatic accelerators. The completion of the accelerator park of Institute of Physics and Power Engineering with Singletron 2MV and Tandetron 5MV machines would make it possible to create a center in Russia that is unique in its characteristics. But due to the change in the geopolitical situation in 2022, this proposal was not implemented.

Due to the specifics of this type of accelerators and the current situation of isolation of the Russian Federation from the supply of high-tech scientific equipment, considering the long-term professional experience of Joint Institute for Nuclear Research in the field of creating applied accelerator complexes and taking into account the world level of expertise of FLNR JINR (Dubna) in radiation materials science, an alternative idea for the center's basic accelerators seems possible.

An alternative to the complex of electrostatic accelerators can be the development at the JINR of a simultaneous triple irradiation facility based on three compact cyclotrons with proton energies of 0.5 MeV, helium 2 MeV and iron/chromium/nickel 21 MeV, which fully meets modern requirements for beam parameters in simulation experiments. An application complex with these parameters will allow obtaining high dose levels of radiation damage with a ratio of defect formation rates and accumulation rates of helium and hydrogen regulated during irradiation.

Specialists of the scientific and technological department of accelerators of the Flerov Laboratory of Nuclear Reactions have developed and propose for consideration the general concept of the center for simulation studies of structural materials based on three compact cyclotrons.

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