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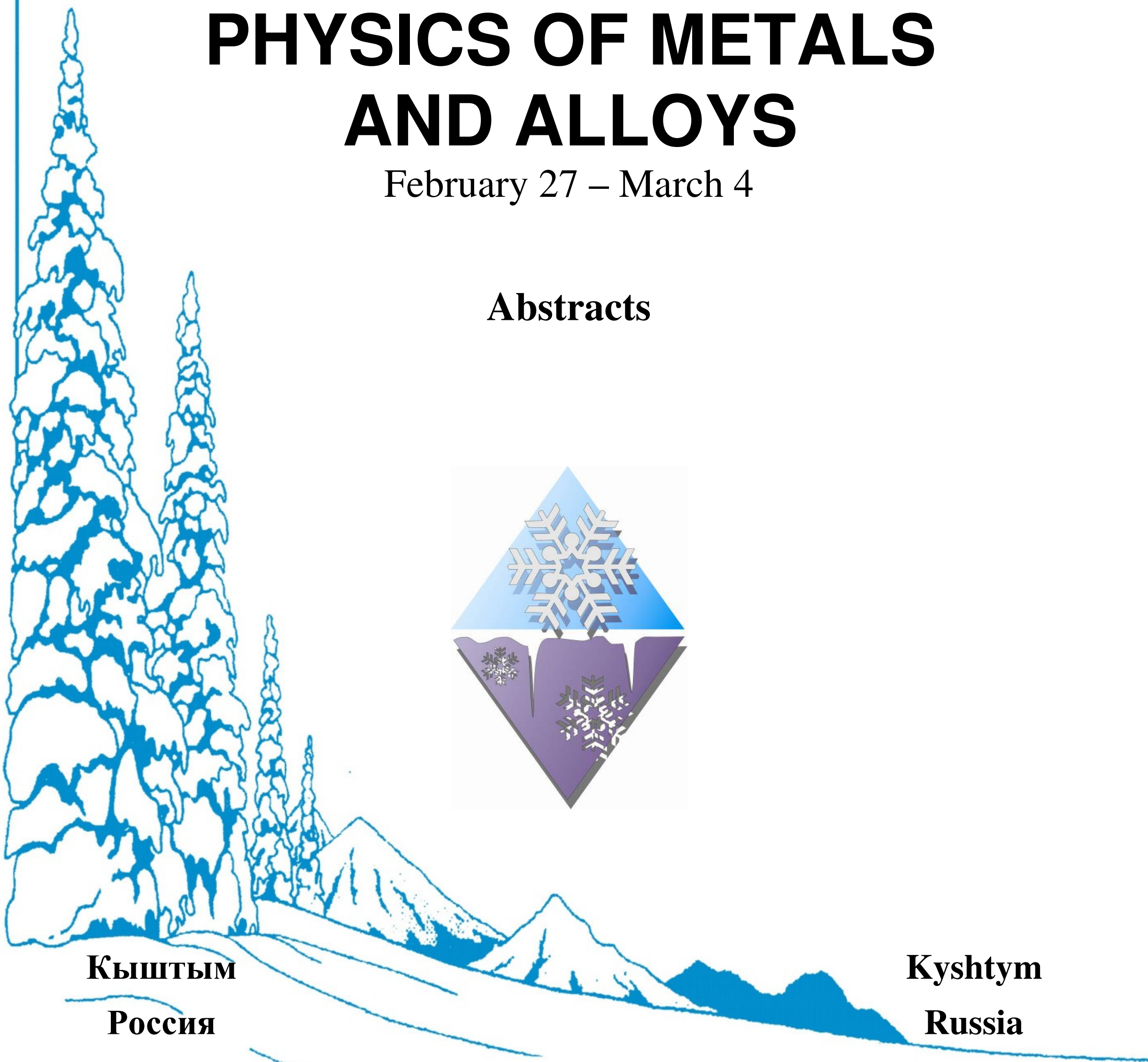
on

RADIATION DAMAGE PHYSICS OF METALS AND ALLOYS

February 27 – March 4

Abstracts



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Compiled by
Denis Perminov

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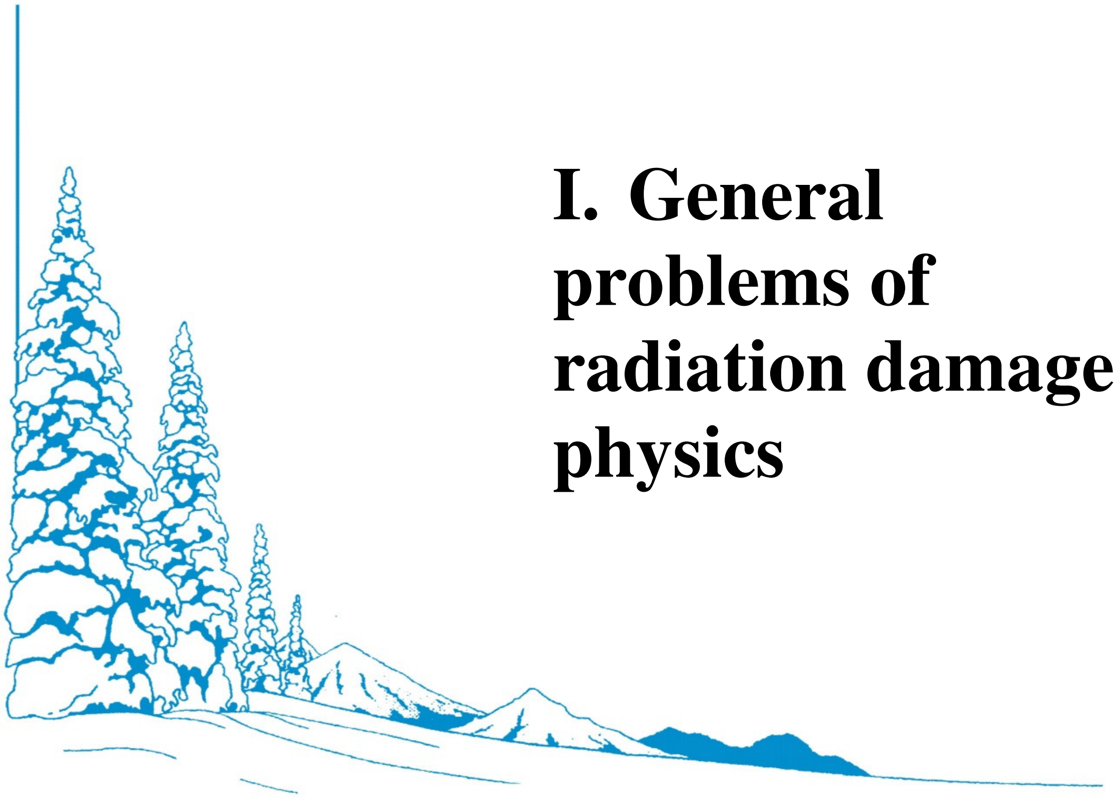

I. General problems of radiation damage physics

This Section is dedicated to most topical, as of now, problems of radiation damage physics of metals and alloys. It includes reports on specific features of the behavior of point defects in various alloys and compounds including Fe-Cr(Ni) systems, which are the basis of many radiation-resistant high-pressure-vessel materials. The program of the Section includes papers dedicated to investigations into specific features of the processes involved in the interaction of radiation- and deformation-induced point defects and their complexes with each other, and with impurity atoms, dislocations, interfaces, and grain boundaries using modern research methods at all stages of the formation of a complicated defect structure in nano- and submicrocrystalline metal systems. Also, the effect of these interactions on deformation- and radiation-induced processes is studied. Much attention is given to multiscale modeling of radiation processes in irradiated materials, analysis of structural and phase transformations, and the behavior of transmutated gas mixtures.

ATOMISTIC SIMULATIONS OF SUBSTITUTIONAL ELEMENTS SEGREGATION AT THE GRAIN BOUNDARIES AND DECOMPOSITION KINETICS

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Segregation of alloying elements at grain boundaries (GBs) has a significant impact on physical and mechanical properties of alloys, phase transitions, and on the formation of a microstructure. Although this problem is examined theoretically and experimentally for many years, the mechanisms of interaction of alloying elements with GBs and segregations formation remain subjects of debate. In particular, you cannot select one or more parameters, depending on the characteristics of GBs (misorientation angle, free atomic volume, the energy of the GB), or on the type of impurity atom (ion radius, the energy of dissolution), which determine essentially the segregation effect on GBs.

We examined the mechanism of segregations formation at GBs of different types, using the approaches of different scale levels: the calculation of segregation energy within density functional theory (SIESTA, PAW–VASP), molecular dynamics (MD) method, and Monte Carlo (MC) method. As the object of the study, Al alloys, alloyed with Mg or Zn, and also Fe–Cu alloys were used. The results obtained give an idea not only of the magnitude of the segregation energy, which determines the driving force of the process, but also on the width of the boundary area L_{GB}, which is enriched by impurity elements.

Based on *ab initio* simulations, we report on the nature of principally different mechanisms for interaction of Mg and Zn atoms with GBs in Al alloys leading to different segregation formation. The Mg atoms segregate in GB region with heterogeneous agglomerations due to a *deformation* mechanism of solute-GB interaction. In contrast to that, for the case of Zn atoms an *electronic* mechanism, associated with the formation of directional bonding, is dominating in the solute-GB interaction. As a result, for Zn atoms it is energetically beneficial to occupy interstitial positions at the very GB and to be arranged into thin layers along the GBs, thus weakening them.

Kinetics of the decomposition in the polycrystalline Fe–Cu alloy and formation of precipitates at GBs are investigated using atomistic modeling on different time scales: MC method, realizing the diffusion redistribution of Cu atoms, and MD method, providing atomic lattice relaxation. It was shown that for a small grain size (D ~ 10 nm) the decomposition in a bulk is suppressed, and coherently linked to the matrix Cu-reach precipitates are formed mainly on the GBs. The size and composition of the precipitates essentially depend on the GB type: small precipitates (1.2–1.4 nm) have an average composition of Fe–40 at.% Cu and are formed near the low–angle GBs. Larger precipitates of up to 4 nm with an average composition of Fe–60 at.% Cu are formed near the GBs of general type and triple junctions. The results help to explain the observed features of the GB enrichment in alloys subjected to severe plastic deformation. The results obtained represent a new approach to control GB segregation behavior and superior properties of UFG materials.

The results have been obtained using the computational resources of MCC National Research Center "Kurchatov Institute" (http://computing.kiae.ru).

DIFFUSION TRANSFORMATIONS IN STEELS AT LOWER TEMPERATURES IN THE PROCESS OF RADIATION AND DEFORMATION GENERATION OF POINT DEFECTS

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In the earlier Mossbauer and electron-microscopic investigations the possibility of anomalous dissolution of quite different disperse phases (intermetallic compounds, carbides, nitrides, oxides) at low temperatures in the process of radiation or deformation effect was shown. In particular, the deformation-induced dissolution of intermetallic compounds Ni_3Al with diameter about 4 nm in the matrix of austenite alloy Fe-35.4 Ni-9Al (at %) at cryogenic temperatures (below 77 K) under the high pressure torsion at 8 GPa which is followed by the deformation-induced precipitation of intermetallic compounds at the increase of deformation temperature to 473-573 K was investigated [1]. The measurements of nickel C_{Ni} concentration in Fe-Ni-Al matrix at dissolution or precipitation of high-nickel γ' phase of Ni_3Al was carried out mostly by the Mossbauer method which in this case gives more precise results than the electron microcopy or X-ray diffraction. The Mossbauer spectra were obtained in geometry on resonance radiation transmission with the energy 14.4 keV from the source Co^{57}(Rh). For the concentration analysis the obtained earlier dependence of the average field $\langle H \rangle$ on nucleus ^{57}Fe (at 293 K) on the nickel content: $C(\mathrm{Ni}) = 29{,}6 + 0.3\exp(\langle H \rangle/80)$ in Fe-Ni alloys with 29.6 – 43.5 at% Ni was used. In the process of studying the mechanism of radiation and deformation dissolution of intermetallic compounds of Ni_3Al or Ni_3Ti types in austenite Fe-36Ni-Ti(Al) steels the unexpected intensification of this process at cryogenic temperatures (77 K) was observed. The deformation dissolution was explained by the migration of Ni, Al or Ti atoms from the intermetallic particles to the matrix subsequent to the dislocations crossing the particles provided that these atoms passed to the interstitial positions with the decrease of migration activation energy almost by an order. The calculated values of the impurity atoms drift showed that the deformation-induced transition of atoms from Ni_3Ti particle (for example Ni) into the interstitial position in the form of crowdion (migration energy E~0.1 eV) lets them move by a diffusional way (for the appreciable distance ~1 nm and more) in the dislocation stress field even at temperature 77 K. Dumbbell pair diffusion (E~0.2 eV) subsequent to the dislocation is possible approximately at 173 K and higher and the diffusion according to vacancy mechanism (E ~ 1 eV) can occur only at higher temperatures, approximately 723 K and higher. To identify the forming at cryogen deformation (77 K) point defects (interstitial atoms and vacancies) the resistometric investigation in the model austenite Fe-36Ni alloy was carried out. The behavior of deformation-induced point defects at annealing was compared to their behavior after the low-temperature (70 K) electron irradiation. It was taken into account that the change of resistance during the annealing of the deformed or irradiated alloy at 77-140 K is connected with the migration of interstitial atoms whereas at temperatures higher than 200 K – with the migration of vacancies. Experimental data showed that at low-temperature deformation and subsequent annealing below 550 K the diffusion processes in Fe-36Ni alloy take place analogous to those that occur after the low-temperature electron irradiation. The formation and migration of interstitial atoms (77-140 K) and vacancies (200- 550 K) are observed. They cause the phase transformations explained by the short range atomic clustering and ordering of the high-nickel areas. Thus, when explaining the low-temperature deformation-induced diffusion of substitutional atoms in the iron-based investigated steels it is necessary to take into account the generation of interstitial atoms.

The disadvantage of world methods of production of the oxide disperse-hardened (ODH) steels is the extremely long (30 - 40 h) first stage of treatment – mechanical alloying of steel powder. The duration of the mechanical alloying process leads to the early wear and damage of mills, contamination of mixture with the wear products and weakness of quality of ODH-steels. In the new approach the low-stable at deformation iron oxides or even surface iron oxides in the form of thin film around the particles of steel powder but not the stable yttrium oxides with a high energy of interatomic bond are used to obtain ODH steels as the carriers of oxygen. The obtained results for the mechanism of deformation-induced dissolution of particles made it possible to optimize and simplify the production of the oxide disperse-hardened (ODH) heat-resistant reactor steels of new generation.

The work was fulfilled with the financial support of Russian scientific foundation (project № 14- 13-00908)

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DISLOCATION SINK EFFICIENCIES FOR RADIATION DEFECTS AND DISLOCATION BIAS IN δ-Pu

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When studying radiation properties of metals and developing their phenomenological models, there is a necessity of knowledge of dislocation sink efficiency values for self-radiation defects (RDs – self-interstitial atoms (SIAs), vacancies) and dislocation bias factor values (relative difference of sink efficiencies for SIAs and vacancies).

For δ-Pu, in the temperature range 200 K – 748 K and the dislocation density range 8×10^{11} m^{-2} – 2×10^{14} m^{-2}, sink efficiencies for self RDs and bias factors were determined for straight perfect screw, mixed and edge dislocations in ⟨110⟩{110}, ⟨110⟩{221}, ⟨110⟩{111}, ⟨110⟩{112}, ⟨110⟩{115}, ⟨110⟩{001} slip systems.

Sink efficiencies were calculated in the framework of multiscale approach with use of an object kinetic Monte Carlo (OKMC) method, anisotropic linear theory of elasticity (ALTE) and molecular statics (MS) method. Diffusion of RDs in model crystals containing dislocations was simulated by the OKMC method. Elastic interactions between RDs (elastic dipoles) in stable and saddle-point positions and elastic fields of dislocations were calculated within the ALTE. Elastic fields of dislocations were calculated by means of the ALTE. RDs dipole tensors were calculated in [1] by MS method using the interatomic interaction potential developed within modified embedded atom method in [2] (the potential parameter set with $t^{(3)} = 0$ [3] was used, which provides stability of fcc phase of Pu at 0 K).

The dislocation sink efficiency depends weakly on the dislocation slip system at a given angle between the dislocation and Burgers vector (in the limits of 14 % and 8 % for SIAs and vacancies, respectively, at 293 K). The dislocation sink efficiency decreases with temperature increase, its temperature dependence is well described by $\xi(T) = \xi_0[1 - AT^{-1}\exp(-T/B)]$, where A and B are fitting parameters and ξ_0 is the non-interacting linear sink efficiency. The dependence of dislocation sink efficiency on the dislocation density ρ_d at $\rho_d < 2\times10^{14}$ m^{-2} is well described by $\xi(\rho_d) = s\xi_0(\rho_d) + t(\rho_d)^{1/2}$, where s and t are fitting parameters.

All considered dislocations (edge, mixed and screw ones) are more effective sinks for SIAs than for vacancies. The dislocation bias values decrease with the temperature increase and the dislocation density decrease. For example, bias factors for screw and edge dislocations

— decrease from 11 % to 3 % and from (32 – 39) % to (10 – 14) %, respectively, with temperature increase from 250 K to 748 K at $\rho_d = 2\times10^{14}$ m^{-2};
— increase from 5 % to 10 % and from (16 – 20) % to (29 – 35) %, respectively, with dislocation density increase from 8×10^{11} m^{-2} to 2×10^{14} m^{-2}.

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EFFECT OF BOUNDARY CONDITIONS ON THE KINETICS OF HELIUM RELEASE FROM STRUCTURAL MATERIALS

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Gaseous products of nuclear reactions (specifically, helium) play a significant part in altering the material properties upon irradiation. It is known that atoms of inert gases promote the generation and growth of pores in irradiated materials and affect phenomena such as swelling, high temperature irradiation embrittlement, etc. Therefore, a study of the behavior of helium (its production, accumulation, retention, and release) within structural materials is fairly topical. In order to validate the methods of express imitation of accumulation and retention of helium within structural materials under reactor irradiation, we perform a comparative analysis of the spectra of the rate of gas release from samples of austenitic steel that were saturated with helium in different ways, i.e., through irradiation in a cyclotron, a magnetic mass - separation setup, the IRT-2000 reactor, the BOR-60 reactor, and using the so called tritium trick technique.

The effect of the presence of dislocations and grain boundaries on the release of helium from materials is evaluated. The results of the research conducted show that the kinetics of helium release from samples saturated with helium through the bombardment with alpha particles of different energies, which ensures the simultaneous introduction of helium and radiation defects (in wide ranges of helium concentration and radiation damage) into the material lattice, is similar to the kinetics of helium release from samples irradiated in reactors.

EFFECT OF RADIATION AND IMPURITIES ON THE GRAIN BOUNDARY DIFFUSION COEFFICIENTS AND GROWTH OF HELIUM BUBBLES AT GRAIN BOUNDARIES IN AUSTENITIC STEELS

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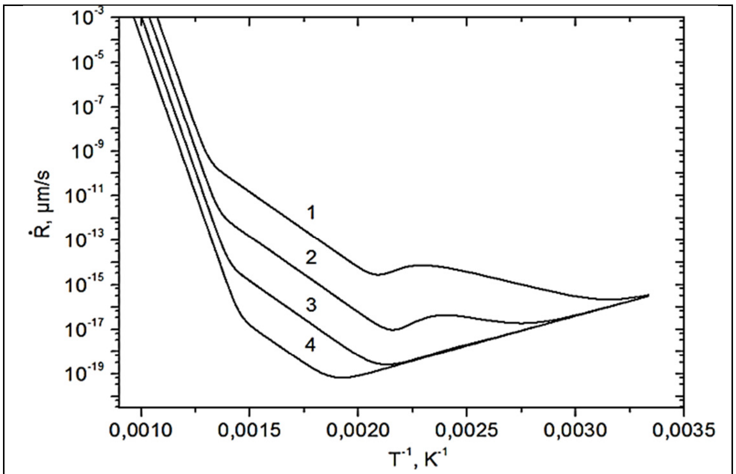
The influence of different types of impurities and alloying elements of different concentrations, the width of the grain boundary and the rate of accumulation of radiation dose on the kinetic characteristics of the own point of radiation defects (OPRD) in the grain boundary and radiation - enhanced grain boundary diffusion (REGBD) has been studied. The influence of these variables on the parameters of the processes of nucleation and growth of helium bubbles in the grain boundary has been analyzed.

Temperature dependences of steady-state concentration OPRD for materials with different binding energy complexes "OPRD – impurity atom" in the amount and in the grain boundary, the effective mutual recombination velocities STRD, influence the formation of impurity complexes on the acceleration of the REGBD has been studied.

The possibility of varying the characteristics of the complexes "OPRD – impurity atom", the concentration of alloying elements and impurities, irradiation parameters for suppressing the processes of high-temperature radiation embrittlement (HTRE) of austenitic steels has been analyzed.



The dependence of the rate of growth of the void size on the defect production rate. 1 - $K_0 = 10^{-4}$ dpa/s, 2 - $K_0 = 10^{-5}$ dpa/s, 3 - $K_0 = 10^{-6}$ dpa/s, 4 - $K_0 = 10^{-7}$ dpa/s

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EFFECTS OF Ti AND PLASTIC DEFORMATION ON DEFECT EVOLUTION IN ELECTRON-IRRADIATED AUSTENITIC STEEL STUDIED BY POSITRON ANNIHILATION

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Positron annihilation spectroscopy was used to study the formation and annealing of vacancy clusters in 16Cr15Ni3Mo austenitic steel and in the same compounds containing 1.02 wt % Ti. Defects were induced by electron (5 MeV) irradiation at 270-573 K. It was analyzed how a developed initial dislocation structure influenced the accumulation and annealing of vacancy defects in these steels. It was shown that vacancies interacted with titanium atoms. As a result, the Ti-containing steels exposed to radiation at temperatures from 270 to 423 K had an enhanced concentration of fine vacancy clusters decorated with titanium, which were thermally stable up to 450 K. A high initial dislocation density in the deformed steels led to a several-fold decrease in the concentration of vacancy clusters as compared to their concentration in the solution annealed state. The formation of fine TiC particles in Ti-modified deformed steel was monitored at the annealing temperatures from 850 to 1070 K. In the stainless steels, the positron trapping by dislocations was found to be blocked. This effect is caused by segregation of impurity atoms and nucleation of a precipitates at dislocations.

EVOLUTION OF INTERMETALLIC NANOPARTICLES AND VACANCY DEFECTS UNDER IRRADIATION IN Fe-Ni-Al AGEING ALLOY

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In work [1], we study the effects of intermetallic nanoparticles like Ni_3Al on the evolution of vacancy defects in the fcc Fe-Ni-Al alloy under electron irradiation using positron annihilation spectroscopy. Electrical resistivity measurements have been used as a testing method for characterizing the evolution in the underlying precipitate microstructure due to heat treatment and irradiation. It was shown that the nanosized (~4.5 nm) intermetallic precipitates homogeneously distributed in the alloy matrix caused a several-fold decrease in the accumulation of vacancies as compared to their accumulation in the pre-quenched alloy. This effect was enhanced with the irradiation temperature. The irradiation-induced growth of intermetallic nanoparticles was also observed in the pre-quenched Fe-Ni-Al alloy under irradiation at 573 K. Thus, resistivity measurement and positron confinement in ultrafine intermetallic particles, which we revealed earlier, provided the control over the evolution of coherent precipitates, along with vacancy defects, during irradiation and annealing.

The research was carried out within the state assignment of FASO of Russia (theme "Spin" No. 01201463330), supported in part by RFBR (projects No. 13-02-00359-a).

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INFLUENCE OF THE DAMAGE IRRADIATION ON THE LOW TEMPERATURE EMBRITTLEMENT OF METALS

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Dislocation mechanisms for the formation of the unstable state of low-temperature embrittlement (LTE state or cold brittleness) with the possibility for a brittle fracture (an avalanche spreading of the intragranular crack) of metals (mono- and polycrystals) with different crystal lattices (BCC, FCC, HCP) were considered. The conditions (without irradiation) of the LTE state formation and an avalanche spreading of intragranular crack (brittle failure) are connected with the stress-deformed state, the yield strength (the stress of the start moving of dislocations), the fracture breaking stress and mobility of dislocations in plastic zone of a crack (stress concentrator) of the fractured metal. The speed of dislocations in the plastic crack area determines the rate of crack spread. These conditions can be performed only for BCC and some of HCP metals, thus determining temperature area of the LTE states (cold brittleness) below the temperature of a ductile-brittle transition (V.M. Chernov, B.K. Kardashev, K.A. Moroz, Technical Physics, 2016, Vol. 61, No. 7, pp. 1015-1022).

The influence of a damaging irradiation on the LTE state (LTRE state) metals was considered. The radiation causes perturbations in metals which cause long-range dynamic stresses (elastic waves, "radiation jolting") that augment the mobility of dislocations and increase the stress relaxation rate in the plastic zone of crack (the area of the dynamic mobility of dislocations in the plastic zone does not occur). During irradiation unstable LTRE metal state with the possibility of brittle fracture (avalanche spread of the crack) is not formed (not formed the ductile-brittle transition temperature). In the process of low-temperature irradiation of materials (products) for all crystalline classes their crack resistance (ductility) increases, and a possibility of a brittle fracture (an avalanche spreading of the intragranular crack) are not realized (are suppressed).

LTRE state for irradiated metals that allowed for LTE states without irradiation (ferritic-martensitic steels, BCC and some of HCP metals and their alloys) are dangerous because of the arising of residual radiation hardening which increase the temperature of the ductile-brittle transition. Additional post-radiation annealing of irradiated metals lowers their temperature of a ductile-brittle transition because of reduction of concentrations and states of the radiation defects (reduction of the yield strength).

The non-damaging (absorbed) irradiation of metals (the energies lesser than the threshold displacement energy, gamma) will affect the conditions for the appearance LTRE states during the irradiation through the increasing temperature of the irradiation and via the occurring products of the nuclear reactions.

This work is supported by the Russian Foundation for Basic Research (Grant No 17-08-00656).

INTERACTION OF POINT DEFECTS AND ATOMS OF CARBON AT THE SEPARATION OF RADIATION DEFECTS IN Ni AT ELECTRON AND NEUTRON IRRADIATION

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It is performed the complex investigations of radiation damage of hardened and deformed Ni and Ni- 880 at. ppm C alloy under electron and neutron irradiation at the room temperature.

In pure nickel, with the deformation microstructure, both under electron and under neutron irradiation is observed separation of radiation-induced defects. A substantial part of self-interstitials annihilated when migrating to the dislocation sinks and there lead a greater accumulation of vacancies in the deformed nickel. Under electron irradiation separation of radiation defects have the maximum at degree of deformation of about 40%

When electron irradiation in the alloy Ni-C separation effect is observed, and when neutron irradiation there is no. This is due to the interaction of carbon atoms with radiation defects and effect of carbon on the formation of stable clusters consisting of carbon atoms and self-interstitials in the areas of displacement cascades. The main sinks for radiation-induced defects at the neutron irradiation are the areas with a high concentration of defects in cascades of atomic displacements.

The research was carried out within the state assignment of FASO of Russia (theme “Spin” No. 01201463330 and “Flux” No. 01201463334), supported in part by RFBR (projects No. 17-03-00223-a and No. 17-02-00204).

LATTICE DEFECTS IN PURE NICKEL AFTER IRRADIATION WITH FAST NEUTRONS AND SUBSEQUENT THERMAL ANNEALING (NEUTRON DIFFRACTION STUDIES)

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Samples of pure nickel have been studied by high-resolution neutron diffraction after irradiation to the maximal fluence 10^{20} n/cm^2 and subsequent isochronous annealing at the temperature 600°C. It is shown that up to small fluencies ~ 10^{19} n/cm^2, the predominant defects are interstitial atoms of nickel and vacancies homogeneously distributed over the sample volume. The lattice parameter grows because of a large contribution of interstitial atoms compared to the negative contribution of vacancies. At fluencies larger than 10^{19} n/cm^2, the radiation-induced diffusion results in the formation of clusters of Ni atoms, whose number and sizes increase with fluence. At the same time, their large number causes the predominance of the negative contribution of vacancies over that of interstitials, and the lattice parameter, passing through the maximum, decreases at the maximal fluence used in our experiments (see Fig. 1).

Temperature annealing recovers the structural parameters.

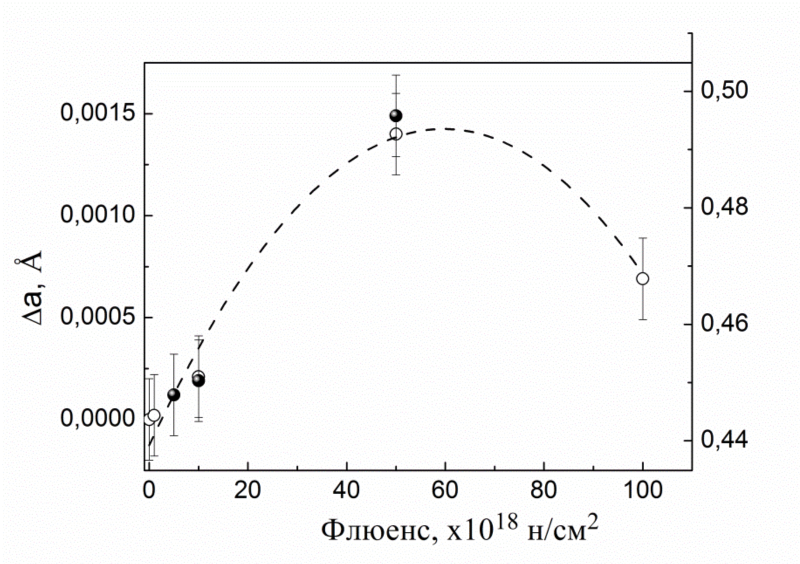

Fig.1. Dependence of the lattice parameter of nickel on fluence of fast neutrons. Open circles are neutron data, solid ones - X ray data.

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MD STUDY OF SELF-IRRADIATION EFFECTS ON DISLOCATION DYNAMICS IN δ-Pu

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Self-irradiation of fissile materials such as plutonium and its alloys continuously produces primary radiation defects in their crystal structure and decay products, for example, radiogenic helium, which tend to accumulate, diffusively migrate through the lattice, form clusters, and so on. The microstructure (morphology) of the point defects (the characteristic equilibrium size of defect clusters, their shape, clustered and isolated defect fractions) greatly influences the mechanical material properties. The paper proposes and implements an original idea of investigating equilibrium thermodynamics of radiation defect clusters within Molecular Dynamics (MD) with the Thermodynamic Integration Method (TIM) which calculates thermodynamic potentials for arbitrary interatomic interaction. It is for the first time that the method was here used to study radiation defect morphology and behavior in the crystal lattice. We studied how radiogenic helium behaved in Pu and fcc-Pu-Ga alloys and determined the equilibrium parameters of helium bubbles which agree well with experimental data. We also studied the behavior of clustered primary radiation defects in Pu-Ga alloys and obtained their equilibrium parameters. Using our newly developed stress relaxation method, we investigated dislocation dynamics under shear stresses down to strain rates close to zero. We thus evaluated Peierls stress and, accordingly, quasi-static elastic-plastic material properties. Simulations were done both in the absence of other defects in the structure, and in the presence of radiation defects of different morphology. Nanometer vacancy complexes and helium bubbles are shown to cause dislocation pinning which eventually makes the elastic limit higher. Our quantitative estimates for the effect of aging on the static elastic limit agree well with experiment. The techniques we have developed allow calculation technology to be extended to other active and structural materials for predicting their behavior under intense radiation.

MECHANISMS OF ALPHA PHASE FORMATION IN Fe-18Cr-10Ni-Ti STEEL AFTER IRRADIATION UP TO 150 DPA IN THE BOR-60 REACTOR

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Any reactor structural materials operate under difficult conditions with high damaging doses and stresses of various types which contribute to the deterioration of material properties.

To ensure reliable operation of non-replaceable reactor components and reactor in general, data obtained from special-purpose experiments on irradiation of samples are used as well as data from studying real elements that have been operated in the reactor for a long time.

The paper presents the results of microstructural investigations of Fe-18Cr-10Ni-Ti steel specimens, which were cut from elements of the BOR-60 reflector assembly irradiated up to the maximum dose of 150 dpa at temperatures from 330°C to 380°C.

Some specimens were cut from the mechanical testing samples irradiated at 420°C and 320-350°C. We obtained new experimental data on the evolution of the alpha phase in the Fe-18Cr-10Ni steel - a material of BOR-60 and VVER reactor internals. TEM of the specimens showed three types of the radiation-induced and radiation-stimulated phase in the material as a result of redistribution of the alloying elements under irradiation.

The data obtained can be used to justify the criterion of gamma-alpha transition in materials of VVER reactors internals at long operation to high damaging doses. These data will also be used to supplement the database on radiation resistance of the Fe-18Cr-10Ni-Ti steel required to justify life extension of BOR-60 reactor and VVER power reactor internals.

MODELING OF RADIATION DAMAGE IN MOLYBDENUM BY CLUSTER DYNAMICS

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Defect evolution of molybdenum and molybdenum alloys is considered under neutron and ion irradiation. By means of program Geant and SRIM, which are based on binary collision approxiamtion and Monte-Carlo method, the energy distributions of the primary knocked atoms (PKA) are calculated at particle energy. The formation of point defects and clusters due to PKA motion in crystal is simulated by means of molecular dynamics simulation (MD) [1]. Using of MD allows us to take into account crystal lattice effects and recombination and clustering of the defects at first stage of the cascade recovery. The following evolution of defects occurs for a long time and large space scales, therefore the modeling at such stage is considered by atomistic kinetic Monte-Carlo (KMC) [2] or cluster dynamics (CD) [3]. Atomistic KMC simulates the defect behaviour at atomic scale, taking into account the non-uniform distribution of defects in crystal and quite realistic interaction between them. In CD the interaction between defects is described in terms of mean field theory, i.e. the concentration of defects is uniform and reaction rates are calculated based on the theory of sink strength. The objects of CD are defect clusters of different sizes. This allows us to consider the nucleation process of clusters in much more details. CD is coarse method in comparison to KMC, but the computational cost of the last one sufficiently reduces of available time and space scales.

The results (size distribution of clusters) obtained by MD is used in CD as the input values of defect generation. Different situations are considered in order to reproduce different experimental conditions. First of all defect behavior in the bulk pure molybdenum is simulated, diffusion coefficients of point defects and clusters are used from [4]. In the second case the thin layer is considered, so the sink strength of surface is taken into account. More realistic models includes the influence of impurities on diffusion coefficients. Based density function theory calculation the influence of carbon is investigated, the mobility of interstitial clusters is drastically reduced. The influence carbon concentration on dislocation loop concentration and sizes are discussed. In order to investigate the role of temperature, several temperatures are considered. The increasing of temperature smooths over the impurity effects.

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POINT DEFECT MIGRATION IN THE TEMPERATURE GRADIENT FIELD

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During operation of fuel elements a wall thickness temperature gradient appears. It causes nonuniform conditions for the migration of point defects generated under neutron irradiation, thus causing radiation-induced structural changes through the cladding thickness. The paper aims to describe point defect migration in the cladding regarding active temperature gradient.

Point defect migration model [1] describes vacancy and interstitial atom movement in the temperature gradient field regarding variations of the point defect transition probability in different directions. Equations for steady vacancy and interstitial flows through the wall thickness towards the cladding tube axis and in the opposite direction have been obtained. It is shown that a steady wall thickness distribution of vacancies and interstitials occurs in the cladding exposed to neutron irradiation. The distribution of point defect concentrations in austenitic steel claddings under irradiation of fuel elements in fast reactor has been calculated. It is shown that the wall thickness temperature gradient causes vacancy concentration reduction at the internal surface and its increase at the external surface as compared with the central cladding area. It causes porosity characteristics variation developed at the external and internal surfaces.

Experimental results of radiation porosity investigation in austenitic steel claddings irradiated at different temperatures as a part of BN-600 reactor fuel elements are given. It is shown that at the internal surface there is a void-depleted area, and at the external surface an area with large voids appears. The calculation profile of vacancy concentration distribution at the internal surface correlates with the measured width of the void-depleted area.

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QUANTUM MOLECULAR DYNAMICS: PARALLEL REPLICA METHOD FOR ACCELERATED CALCULATION OF DIFFUSIVITIES

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Usually prediction of the radiation-induced degradation of steels and alloys is based on kinetic theory models [1,2]. The main advantage of this approach is the possibility of describing the evolution of the material on realistic timescales. However, such models require a large amount of data on the characteristics of the material, particularly diffusive properties of the system. But corresponding experiments often are very expensive or even impossible for technical reasons. In this case, diffusivities can be estimated from atomistic simulations.

Probably the most accurate of such methods is quantum molecular dynamics (QMD). On the other hand, QMD calculations are also the most expensive from computational point of view. Thus direct simulation of diffusion processes in solids can be carried out only at high temperatures, usually close to the melting point of the material. Evaluation of diffusivities at lower temperatures requires application of acceleration techniques, e.g. the parallel replica dynamics (PRD) [3].

In this paper, we explore the PRD algorithm and study the impact of its internal parameters on the simulation outcome. We determine the sources of the most significant errors and propose corresponding corrections. PRD algorithm was implemented in code and coupled to QMD package. The proposed approach was verified by calculation of self-diffusivities in aluminum. The results of accelerated modeling are in good agreement both with standard QMD simulations, and with experimental data. It is demonstrated that application of parallel replica dynamics allows to expand timescales accessible for QMD simulations, from a hundred of picoseconds to a few nanoseconds. Note, that the upper bound is dictated by available computation resources, rather than by restrictions of the method.

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RESULTS OF THE COMPUTER ANALYSIS OF THE LAYER-BY-LAYER FIELD ION MICROSCOPY IMAGES OF PLATINUM IRRADIATED WITH Ar^+ IONS (E = 30 keV)

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The field ion microscopy images of the surface atomic layers of metals and alloys, which were taken using tip emitters, include the image of thousands of atoms, which are located in both the sites of a regular lattice and regions with radiation defects.

This paper presents the results of the application of a specially developed algorithm and a computer program for the analysis of ionic field microscopy images to study the effect of Ar^+ ions (E = 30 keV) on the structure of the surface atomic layers of pure platinum.

The coordinates of atoms, the brightness of their images, and their sizes were determined. The curves of the distribution of the brightness and atomic radii were built. It is shown that the width of the distributions significantly increases as the distance to the exposed surface decreases. The number of atoms in the field ion microscopy images increases with distance from the irradiated surface.

Field ion microscopy images with only those atoms whose brightness (or radius) is in certain range were taken. These atoms can be highlighted in the ionic field microscopy images. The zones where irradiation-induced changes in the field microscopy images are mostly pronounced were determined. They are zones of the passage of the dense cascades of atomic displacements. Damaged zones include images of atoms with both abnormally low and abnormally high radii.

The work presents the layer-by-layer images of the surface layers of the irradiated platinum (from 1st to 5th and more distant). The possibility of reconstruction of the 3D-picture of the irradiated metal at a temperature of liquid nitrogen (T ~ 77 K) is shown.

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ROLE OF NANOSCALE DYNAMIC EFFECTS UNDER CASCADE-FORMING IRRADIATION

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Classical radiation physics is based on the description of migration of radiation defects with account of their interaction with atoms and lattice defects. It describes quite well the relatively slow processes that lead to radiation swelling, radiation creep, radiation embrittlement, radiation segregation, and others.

However, there is no adequate explanation for some well-known effects. They are primarily "low-dose" and "long-range" effects under ion (corpuscular) irradiation.

The studies made at the laboratory of ion beam exposures of the institute of Electrophysics UB RAS during last decades have revealed a crucial role of nanoscale dynamic effects in the physics of ionizing radiation impact on condensed materials. This can serve the base for the explanation of the above-mentioned effects and for development of unique technologies for the modification of bulk properties of materials (electrical, magnetic, mechanical and others) by surface radiation. The essence of radiation-dynamic effects is that the area of passage of the dense cascades of atomic displacements thermalized over the time of the order of 10^{-12} s and heated to 3000-6000 K (thermal spikes) are zones of explosive energy release that was not taken into account in the classical radiation physics.

Radiation shaking of condensed matters with post-cascade waves explains the effect of low doses, which consists in a significant changes in the structure and properties of materials at small number of displacements per atom and the long-range effects under corpuscular irradiation. These two effects represent two sides of the same coin.

As an evidence of the existence and the special role of the nanoscale zones of explosive energy release the temperature of these zones was experimentally determined for the first time, on the basis of analysis of spectral composition of the glow of the targets during their irradiation by argon ions [1, 2]. As other evidence of cascade dynamic effects it was obtained the atomic-scale field ion microscopy images of the zones of the passage of the dense cascades of atomic displacements. It has been defined geometrical dimensions of these zones and the number of surviving defects. In addition it was investigated the impact of Ar^+ and Xe^+ ions on the metal nanowires, the diameter of which (60 and 100 nm) is comparable to the diameter of the cascade areas (10-20 nm). The direct electron-microscopic images of nanowires and thermal spikes splashed out from the nanowires surface layers were obtained [3] (the times of splashing and solidification of these regions are comparable to each other).

Foundations for commercial technologies of the instant, within several seconds, cold radiation annealing of aluminum alloys were developed based on the nanoscale dynamic effects. Methods for improving the electrical and magnetic properties of materials were proposed. Radiation-dynamic effects play an important role in neutron irradiation and self-irradiation of fissile materials. They should be considered for nuclear safety while creating new materials for the application in nuclear power internals and materials used in outer space.

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SIMULATED STRESSED-STRAINED STATE OF A PRESSURIZED CONTOURED SPECIMEN

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The paper presents the results of simulating the stressed-strained state of a pressurized contoured specimen to investigate the irradiation creep processes [1, 2]. Distributions of the hoop stresses on the internal and external tubes are shown.

The main purpose of the calculations is to determine the strain and components of the normal stresses for the external and internal tubes of the pressurized specimen to investigate the irradiation creep processes.

Simulation of the stressed-strained state of the pressurized specimen is done by the finite element method with the use of the ANSYS Mechanical software.

The calculations showed that due to the gas pressure in the inter-tubular space, the hoop compressive stresses appear on the internal tube of the specimen whereas hoop tensile ones appear on the external tube. Axial stresses are approximately twice less than the hoop ones and confirmed by the analytical calculations using the formulae presented in PNAE G -7-002-86. Radial stresses are insignificant and do not greatly contribute to the stressed-strained state. So, they can be neglected in further research to analyze the stress-strain effect.

The described computational model of the pressurized contoured specimen can be used for creep calculations provided there is no any effect of radiation-induced swelling.

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SINK STRENGTHS OF MICROSTRUCTURE ELEMENTS FOR RADIATION DEFECTS IN BCC Fe AND V METALS

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When studying radiation properties of metals and developing their phenomenological models, there is a necessity of knowledge of sink strength values for self-radiation defects (RDs – self-interstitial atoms (SIAs), vacancies) and bias factor values (relative difference of sink strengths for SIAs and vacancies) of microstructure elements of different types.

For BCC Fe and V metals, in the temperature range 293 K – 1000 K, sink strengths for self RDs and bias factors were determined for microstructure elements of different types:

- low angle tilt boundaries (LATBs) – dislocation walls consisting of straight edge dislocations in slip systems <111>{110} and <111>{112} – with misorientation angles in the range from 1.5° to 10°, and the subgrain size (distance between two dislocation walls) in the range from 150*a* to 900*a*, *a* is the lattice parameter;
- square interstitial dislocation loops (DLs) with Burgers vector <100> and habitus plane {100}, dislocation segments along <100> directions, side length of the DLs in the range from 1,5*a* to 34,5*a*, DLs number density in the range from $(200a)^{-3}$ to $(5000a)^{-3}$;
- spherical vacancy voids (VVs) with diameters in the range from 2*a* to 20*a*, number density $(200a)^{-3}$.

Sink strengths were calculated in the framework of multiscale approach with use of an object kinetic Monte Carlo (OKMC) method, anisotropic linear theory of elasticity (ALTE) and molecular statics (MS) method. Diffusion of RDs in model crystals containing microstructure elements was simulated by OKMC method. Elastic interactions between RDs (elastic dipoles) and elastic fields of microstructure elements (LATBs, DLs, VVs) were calculated within the ALTE. Elastic fields of LATBs were calculated by means of the ALTE, and thereof of DLs and VVs – by means of MS method. To calculate elastic fields of DLs in Fe, interatomic interaction potential of Romanov et al., 2006 was used. To calculate elastic fields of VVs in Fe and V, potentials of Malerba et al., 2010 and Mendelev et al., 2007 were used, respectively. RDs dipole tensors in Fe and V were calculated by MS method using potentials of Romanov et al., 2006 and Romanov et al., 2012, respectively.

The values of LATB bias factor are several times higher for Fe than for V, change within 30% with the temperature change from 293 K to 1000 K, are approximately inversely proportional to the subgrain size, decrease on the order of magnitude with the misorientation angle increase from 1.5° to 10°. LATB bias factor values are much smaller than the corresponding values for uniformly distributed bulk dislocations.

In Fe, an DL bias factor increases with DL side length increase, saturating at the side length values greater than 20*a*, and weakly depends on the DL number density. At temperatures higher than 600 K, bias factor values for the smallest considered DLs are only a few percent, while thereof for the DLs with the side length values greater than 20*a* are tens of percent.

The values of VV bias factor weakly depend on the VV number density, their absolute values are significantly smaller for large VVs (diameter is greater than ~13*a*) than for small ones. Bias factor takes maximal values for VVs with diameters of 2*a* and 3*a* in Fe and V, respectively (48% and 44%, respectively, at 293 K; 28% and 7%, respectively, at 1000 K).

Some radiation properties of metals and their phenomenological models taking into account the results obtained were considered.

THE STORED ENERGY FINGERPRINTS OF RADIATION DAMAGE

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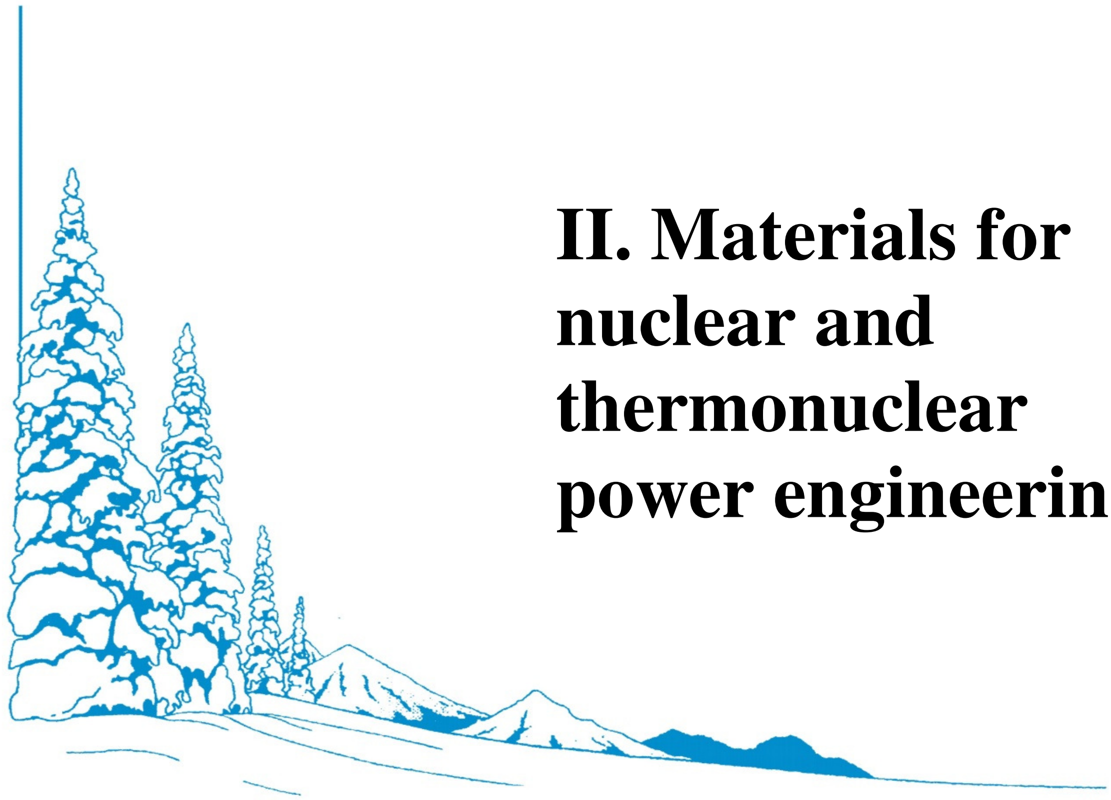
The current unit of radiation damage, the displacements per atom (DPA), is a calculated exposure parameter that does not directly yield the defect populations responsible for irradiation-induced material properties. Were an a posteriori measure of radiation damage to exist, it would help to answer numerous, lingering questions about the nature and effects of irradiation. We propose the use of stored energy fingerprints as this new unit of radiation damage. They can be measured after irradiation, and they yield information about the resulting defect populations. We present a combination of time-accelerated molecular dynamics (MD) simulations and differential scanning calorimetry (DSC) measurements, which together paint a more measurable picture of the multiscale nature of radiation damage. Potential applications range from settling the neutron/ion equivalency question, to quantitatively understanding dose rate effects, to using nanocalorimetry to verify historical uranium enrichment.



II. Materials for nuclear and thermonuclear power engineering

The most topical problem of today is development of new metal materials for fusion and fission-type reactors. Ion particular, the reactors currently under construction (BN-800) and future fast-neutron reactor projects (BN-1800) still expect the constructional materials showing high radiation resistance to withstand the damaging dose of 100-130 dpa, which would ensure the required level of nuclear fuel burnup. The Section includes a great number of material-science presentations on radiation-induced changes in physical and mechanical properties of different high-pressure-vessel materials (those currently in use and showing promise). A consideration will be given to material-science problems of high-temperature creep, swelling of fcc and bcc steels, and the effect of radiation on austenitic high-pressure-vessel steels, including the only "standard" austenitic ChS-68 steel for the BN-600 reactor fuel elements. The results obtained for real high-pressure-vessel materials are analyzed proceeding from the general principles of radiation physics of solids. This Section also includes papers by Russian and foreign investigators reporting the results of studies into the effect of oxide and intermetallic aging on the structure and the mechanical properties of high-alloy constructional steels. Primary emphasis will be on the recently developed steels strengthened with heat-resistant oxides (yttrium, titanium, and thorium).

ALLOYING OF STEEL AND GRAPHITE BY HYDROGEN IN NUCLEAR REACTOR

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It is known that in traditional energetic hydrogen is the firstprimary source of equipment damage [1]. This problem has high actuality for both nuclear and thermonuclear power engineering [2]. Study of radiation-hydrogen embrittlement of the steel raises the question concerning the unknown source of hydrogen in reactors [3-6]. Later unexpectedly high hydrogen concentrations were detected in irradiated graphite [7].

It is necessary to look for this source of hydrogen especially because many hydrogen flakes were detected in reactor vessels of Belgian NPPs [8,9].

As a possible initial hypothesis about the enigmatical source of hydrogen one can propose protons generation during beta-decay of free neutrons inasmuch as protons detected by researches at nuclear reactors as witness of beta-decay of free neutrons [10].

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CARBON CONTAMINATION, ITS CONSEQUENCES, AND ITS MITIGATION DURING CHARGED PARTICLE SIMULATION OF NEUTRON-INDUCED VOID SWELLING

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Self-ion irradiation of reactor structural materials at accelerated dpa rates has been used successfully to simulate the development of void swelling during neutron irradiation. The credibility of this simulation requires that factors that are atypical of neutron environments be taken into consideration and mitigated as much as possible. The major neutron-atypical variables arise from strong surface influence, strong gradients in dpa rate, injected interstitial suppression of void nucleation, compressive stress state and compositional redistribution.

However, it has recently become known that the bombarding ion beam entrains carbon, nitrogen and oxygen via Coulomb dragging and deposits these elements on the bombarded specimen. Carbon especially is deposited, ion-mixed and then diffuses into the ion damaged region. The results of a series of experiments conducted on pure Fe, model alloys and commercial alloys are presented that show the development of internal depth profiles of carbon, nitrogen and oxygen.

Carbon is known to have a strong effect on void swelling in neutron-irradiated steels and it is demonstrated in this presentation that beam-induced carbon contamination also depresses swelling during ion irradiation of HT9 ferritic-martensitic steel.

Monte Carlo modeling of the entrainment phenomenon is presented. An innovative method is then discussed that was developed to strongly reduce such contamination using multiple beam-deflection steps coupled with liquid nitrogen cooling.

COMBINED PLASMA-DEFORMATION METHOD OF NITRIDATION OF AUSTENITIC CHROMIUM-NICKEL STEEL

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Austenitic chromium-nickel steels are widely used in atomic industry. Significant flaws of austenitic chromium-nickel steels are low strength properties and tendency to frictional adhesion. These flaws are not improved by heat treatment. A promising method of hardening of austenitic stainless steel is low-temperature ion-plasma nitriding using electron beam plasma [1, 2].

Reducing the temperature stainless steels nitriding below 450 °C allows forming high strength corrosion resistant phase of supersaturated solid solution of nitrogen without the formation of chromium nitride. Chromium nitride embrittle and reduce the corrosion resistance of the surface layer. Lately successfully apply pre-processing of nanostructured treatment SMAT (surface mechanical attrition treatment) with the aim of acceleration nitrogen diffusion and increase the depth of the nitrided layer at a low temperature plasma nitriding [3]. Finishing friction treatment by sliding indenter is an effective method of nanostructuring and strain hardening of austenitic steels [4].

In the present work, comprehensive experimental research was carried out using methods of microhardness, scanning electron microscopy, profilometry, X-ray analysis and nuclear reaction method. Based on these researches good perspectives for the use of nanostructured friction treatment by the synthetic diamond indenter were showed to improve nitriding efficiency in the electron beam plasma. Increasing the depth of the hardened layer and improving the quality of nitrided surface (roughness reduction) at low temperature (350 °C) nitriding provided by combined plasma-deformation method of nitridation austenitic chromium-nickel steel including friction treatment followed after nitriding in electron beam plasma.

The work was done in the framework RFBR (project № 15-08-07947) and in integrated program of Ural Branch of the Russian Academy of Sciences (project № 15-9-12-45).

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COMPARATIVE EXAMINATION OF MECHANICAL PROPERTIES OF ChS-68 AND EK-164 AUSTENITIC CLADDING STEELS AFTER HIGH DOSE RATE IRRADIATION

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In the second half of the 21st century fast reactors with a fuel cycle on the principles of self-sufficiency and nuclear nonproliferation (BN-600, BN-800, BREST and others) will become the basis of nuclear energy.

Due to high irradiation temperatures and doses in fast reactors the development of structural materials for claddings with a set of specified mechanical and technological properties, compatible with coolant and fuel material, and stable under neutron irradiation is a topical issue for such reactors.

Nowadays 20% cold-worked austenitic steel ChS-68-ID (06Cr-16Ni-15Mo-2Mn-2Ti-V-B) is a standard material for BN-600 reactor claddings. With the use of this material BN-600 reactor lifetime has been changed over to the maximum fuel burnup of 12.5% FIMA and maximum damage dose up to 87 dpa. Cold-worked austenitic steel EK-164-ID (07Cr-16Ni-19Mo-2Mn-2Nb-Ti-B), developed at VNIINM, is less susceptible to swelling and is considered as a prospective material with an expected minimum damage dose of 110 dpa.

The paper aimed to investigate neutron irradiation effect on mechanical properties of BN-600 claddings made of ChS-68 and EK-164 austenitic steels.

The results of the mechanical properties determination for claddings made of these materials after operation at temperature in the range between 370 and 630°C and damage doses up to 80-95 dpa have been summarized.

Short-term mechanical properties have been determined according to the results of two testing methods: uniaxial tension of annular cladding specimens and loading of tubular specimens with internal pressure of the plastic aggregate. Annular specimen testing shows a conservative estimate for the cladding operating capacity, though giving rather statistically representative comparative values for strength and plasticity characteristics of specimens irradiated in different conditions. Tubular specimen testing shows more adequate determination of mechanical properties in actual loading conditions, though giving less statistically representative data due to large-scale specimens.

Specimens of different claddings for mechanical tests have been selected so that their irradiation temperatures were close, and damage doses slightly differed. As a result dose dependence of mechanical properties of ChS-68 and EK-164 steels for different irradiation temperatures has been shown.

Comparative investigation of mechanical properties of ChS-68 and EK-164 steels based on the results of tubular specimen testing shows high strength and plasticity values for claddings made of both steels at temperature in the range between 20 and 600°C and damage doses up to ~90 dpa: tensile strength is over 600 MPa, total elongation is over 1-2%. At operating temperatures the plasticity of the cold-worked EK-164-ID steel cladding is higher than that of the cold-worked ChS-68-ID steel cladding.

Low-temperature and high-temperature radiation-induced embrittlement of cladding materials, typical for both steels, has been found during tests. High-temperature radiation-induced embrittlement is more typical for cold-worked EK-164-ID steel claddings.

CORROSION DAMAGES OF EK-164 STEEL CLADDINGS OPERATED IN FAST REACTOR

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Corrosion damages of internal and external cladding surfaces occur during fuel assembly operation in fast reactors and are one of the factors limiting cladding operating life. Metallography is a conventional method of cladding corrosion investigation. At JSC "INM" a method of corrosion damage investigation with scanning electron microscopy has been developed. The investigation aimed to obtain experimental data on damages of different EK-164 steel cladding areas at the side of fuel composition and sodium coolant.

The investigation has been carried out with TESCAN Mira 3LMU scanning electron microscope (SEM) equipped with X-Act 6 energy dispersive X-ray analysis system (Oxford Instruments) providing surface topography analysis, as well as elemental composition analysis of matrix areas, grain boundaries and precipitates. The paper gives the results of the investigation of EK-164 steel cladding areas after fuel assembly operation in BN-600 reactor medium enriched area to maximum damage dose of 95 dpa at irradiation temperatures of 430…600 °C. It is shown that the cladding material interaction with the fuel composition takes place at the cladding internal side, and at the external side with the sodium coolant. In some areas corrosion damages were found to be nonuniform in penetration depth along the cladding internal surface perimeter. At grain boundaries the cracking with their spalling takes place. It is shown that the palladium grain boundary diffusion is found inside the steel, thus generating particles in boundaries and changing their composition. Moreover, at the fuel composition side there are corrosion damages of cladding material grains. EK-164 steel interaction with the sodium coolant at the external side in the investigated temperature range causes generation of an oxide layer and a layer depleted in doping elements: chromium and nickel. Corrosion damage distribution along the core height has been compared with gamma spectrometry results.

Corrosion damage depths both at the internal and external sides of EK-164 steel claddings have been compared after operation in fuel assemblies in high and low enriched areas of BN-600 reactor [1], [2].

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CREEP ANALYSIS OF THE AUSTENITIC STEEL SPECIMENS IRRADIATED IN THE BOR-60 REACTOR AT 330-350°C

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The paper reports on research into irradiation–induced creep of the pressurized contoured specimens irradiated in the BOR-60 reactor at temperatures of 330-350°C up to the various damage doses [1, 2].

The paper goal is to experimentally determine the effect of the stress pattern on the creep strain in Fe-18Cr-10Ni-Ti austenitic steels under neutron irradiation in the BOR-60 reactor.

The effect of compressive and tensile stresses on the creep of Fe-0.08C-18Cr-10Ni-Ti steel is compared. The results can be used to verify the models of the effect of various stresses on the irradiation–induced creep.

The analysis of the standard and co-axial pressurized Fe-0.08C-18Cr-10Ni-Ti austenitic steel specimens irradiated in the BOR-60 reactor shows that the length and diameter of the pressurized specimens increase linearly as the damage dose rises. The creep modules computed for Fe-18Cr-

10Ni-Ti steel show good agreement with the creep modules for Fe-18Cr-9Ni-based austenitic steels.

The research results are used in the strength calculations done for the VVER-1000 baffle and new VVER-1200 designs.

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CREEP CHARACTERISTICS OF RUSSIAN FERRITE-MARTENSITE STEELS INCLUDING DUO MODIFICATIONS

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Long-term high-temperature load tests (on the transverse microsamples cut out of the fuel element cladding) of Russian reactor steels with BCC lattice after quenching and high-temperature tempering at 720 °C resulting in the precipitation of carbides of $Cr_{23}C_6$ and VC type in ferrite-martensite structure have been carried out in this work. The characteristics of long-term hardness, plasticity and creep rate at 650, 670 and 700 °C and stresses of 60, 80, 100 and 140 MPa were detected. It was stated that according to the decrease of creep rate the reactor steels are arranged in the following order: (EP-823 and EP-900), EK-181, (EP-450 and ChS-139), EP-450-ODS. It was shown that in the process of long-term holding under a load in the reactor steels with BCC lattice there occurs the degradation of lath martensite structure with the decrease of density of dislocations and formation of dislocation–free subgrains as well as the coarsening of chromium-containing carbide phase $M_{23}C_6$. The reason of heat resistance of ChS-139 steel at creep testing is the larger than in the other steels content of carbon (0,21 mass%) that provides the increased amount of $Cr_{23}C_6$ type carbides making the migration of grains and subgrains difficult. The second reason of the high heat resistance of ChS-139 and EP-450 steels is the maximal summary content of high-melting elements Mo, W, Nb, V, Ta (2,40 - 2,52 mass%) which restrict the development of diffusional softening processes.

Among the tested steels the highest characteristics of long-term hardness and creep resistance belong to the oxide disperse-hardened steel EP-450-ODS containing the most heat-resistant yttrium-titanium oxides in ferrite matrix with the average size 5 nm which grow in size in the process of long-term tests. At 700 °C and stress 100 MPa the samples of EP-450-ODS steel withstand without damage for more than 28000 h that is by two orders more than the time for all nonoxide steels with BCC lattice.

The work was fulfilled on the subject “Structure” with partial financial support of the project UB RAS (№ 15-9-2-16).

DEFORMATION-INDUCED STRUCTURAL PHASE TRANSFORMATIONS IN NITRIDE DISPERSION-STRENGTHENED HIGH-NITROGEN 22CrMn1.24N CHROMIUM STEEL

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Structural and phase transformations in high-nitrogen 22CrMn1.24N steel during isothermal annealing and subsequent intensive cold deformation in rotating Bridgman anvils at room and cryogenic temperatures were investigated by Mossbauer spectroscopy. The steel was manufactured by casting with nitrogen counterpressure.

Aging at 723 C and 823 K, 30 min and intense cold deformation lead to cyclic precipitation (during annealing) and dissolution (during shear under pressure) of chromium nitrides in the austenite matrix.

Full polymorphic $\gamma \to \alpha$ transformation with precipitating of chromium nitrides CrN in the BCC matrix with 19.6 at.% Cr was the result of annealing at 923 K, 2.5 h. Few percent chromium growth in BCC matrix took place in the shear under pressure experiment at 573, 292 and 77 K. More complete decomposition of chromium nitrides in the case of deformation at cryogenic temperatures is associated with the weakening dynamic of ageing competing with the nonequilibrium processes of dissolution.

The work was performed at financial support from Russian Scientific Foundation (project № 14-13-00908).

DEPENDENCE OF THE DEGRADATION OF THE VIRTUAL RPV STEEL ON THE NEUTRON IRRADIATION DOSE RATE

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Problems of the neutron irradiation dose rate on the PWR RPV steels degradation influence are analyzed.

Estimation of the dependence of the RPV embrittlement versus neutron irradiation dose rate is carried out in a rough approximation for imaginary virtual steel by means of the averaging of the “chemical” radiation embrittlement coefficient A_F=800 (P+0,07Cu) [1].

Actual radiation embrittlement coefficient was determined experimentally on the basis of normative dependence $\Delta T_F = A_F (F \times 10^{-18})^{1/3}$ [2].

Experimental results consists of 5 sets with intensities range of 130-1100 (test reactors), 30-40,7 (WWER 440-213), 12,5-29,7 (WWER 440-213 with dummies), 1,3-6,9 and 0,2-1,3 (templates and trepans) in 10^{12} $cm^{-2}s^{-1}$ units that intensities were differing by factor of 5000.

As a result dependence of the A_F dependence versus neutron irradiation dose rate was received as A_F=17,8+9,5/φ, where φ – intensity in 10^{12} $cm^{-2}s^{-1}$ units.

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DETECTION OF THE OSCILLATIONS IN KINETICS OF THE REACTOR PRESSURE VESSEL STEEL DAMAGE

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Fast neutron intensity (flux) influence on reactor materials radiation damage is a critically important question in the problem of the correct use of the accelerated irradiation tests data for substantiation of the materials workability in real irradiation conditions that is low neutron intensity.

Investigations of the flux influence on radiation damage and experimental data scattering reveal the existence of non-monotonous sections in kinetics of the reactor pressure vessels (RPV) steel damage. Discovery of the oscillations as indicator of the self-organization processes presence give reasons for new ways searching on RPV steel radiation stability increasing and attempt of the self-restoring metal elaboration.

This fact actualizes the problem of more precise definition of the RPV materials radiation embrittlement mechanisms and gives reasons for search of the ways to manage the radiation stability (nanostructuring and so on to stimulate the radiation defects annihilation), development of the means for creating of more stableness self recovering smart materials.

Anticipated results:
- theory of the RPV steels radiation degradation mechanisms evolution;
- more adequate models of the radiation embrittlement development;
- improvement of surveillance specimens programmes;
- methods and means development for representative accelerated irradiation of the RPV materials;
- search of the ways for creating of the stable to irradiation self-organizing RPV materials.

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EFFECT OF HIGH-ENERGY HEAVY ION IRRADIATION ON THE MICROSTRUCTURE OF OXIDE DISPERSION STRENGTHENED STEEL

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Advanced steels that are now under development, have complex heterogeneous structure with many different nanoscale inclusions. Energy dissipation in such structures is non-trivial and can lead to local changes in the structural-phase state of the material. The stability of such steels under the high-energy radiation impact requires systematic studies using ion irradiation in a wide range of masses and energies, allowing varying the level of ionization energy loss and the resulting effect on the material.

Oxide dispersed strengthened (ODS) steels are considered to be potential structural materials for fusion and fission power plants and for other applications at high temperatures, including cosmic applications. ODS alloys are supposed to have higher creep strength and radiation resistance at elevated temperatures than conventional base alloys. These exceptional mechanical properties of the material are provided by the presence of large number of nanooxides in microstructure of the steel. Irradiation with swift heavy ions results in high energy dissipation in the lattice along the particle track (electronic stopping power). Rapid deposition of released energy brings to drastically changes in the oxide particles microstructure.

Research of ODS Eurofer steel irradiated with Xe (1.2 MeV/amu up to total fluence $1*10^{14}$ ions×cm^{-2}) and Au ions (5.6 MeV/nucleon up to total fluence $5*10^{12}$ ions×cm^{-2}) was carried out in this work by methods of high resolution transmission electron microscopy. Processes of tracks formation within oxide particles at investigated conditions were analyzed. The effects of high and low (100 keV/nucleon) energy impact on nanoscale state of ODS steel were compared.

EFFECT OF THE THERMAL ANNEALING ON HEAT CONDUCTIVITY OF GR-280 GRAPHITE EXPOSED TO HIGH FLUENCE

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Work is devoted to research of effect of high-temperature annealing on heat conductivity of GR-280 graphite irradiated at 450-650°C to fluence of $(0.5\text{-}1.5)\cdot 10^{26}$ m^{-2}. Heat conductivity has been measured by a method of laser flash. Annealing of radiation defects carried out at temperatures of 600-1200°C. As a result of the done work the dependence of heat conductivity from temperature and duration of annealing has been acquired. It is shown that the heat conductivity starts to be rebuilt at temperature 800-900°C; the difference between heat conductivity of samples before and after annealing ($\lambda_{irr+ann}$- λ_{irr}) at temperature 1200 °C lies within 19 ÷ 39 Vt / (m·K); ($\lambda_{irr+ann}$-λ_{irr}) decreases with increase fluence and irradiation temperature; $\lambda_{irr+ann}$ / λ_{irr} remains a constant, equal 2,3.

EVALUATION OF MECHANICAL PROPERTIES OF NUCLEAR REACTOR STRUCTURAL COMPONENTS WITH INNOVATIVE TESTING METHODS

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One of the most important nuclear power plant (NPP) management tasks is to ensure its safe operation. The most critical component in this case is the reactor pressure vessel (RPV), which is subjected to demanding operating conditions such as high pressure, high temperature and intensive neutron flux. These factors lead up to degradation of reactor vessel materials, which cause radiation hardening and embrittlement. Most of the NPPs have established the program of surveillance specimens for monitoring of RPV material properties changes in operational conditions. These programs involve mainly standard three-point bending specimen and cylindrical specimens for tension. Large sample sizes are associated with high radioactivity and higher consumption of archive materials, whose availability is often limited. One of the perspective ways how to evaluate the degradation of irradiated materials is the use of innovative semi-destructive test methods – ABIT (Automated Ball Indentation Test) or SPT (Small Punch Test).

Aim of presentation is to correlate results from conventional test methods with results from Automated Ball Indentation Test (ABIT). Both tests were done on 15KhMFA material in unirradiated and irradiated state. 15KhMFA is tempered bainitic steel used for the fabrication of RPV of WWER 440-type nuclear reactors. ABIT is fully computer controlled test, consisting in multiple indentation of the metal surface (scheme of indent is on Fig. 1. and schematic of applied force versus indentation depth is on Fig. 2.) Aim of the ABIT is to evaluate the localized strength characteristics of the metal. Because the indentation is carried out by a ball indenter, surface for indentation should be smooth and without sharp corners, from which could develop a crack. The development of guidelines for the evaluation of mechanical properties of structural steels of nuclear devices by the method ABIT was done by ÚJV Řež, a. s, together with the Czech Technical University in Prague, FNSPE. A number of tests of indentation have been carried in the past year in various structural materials of the WWER reactor in non irradiated state. Mechanical properties department in ÚJV Řež, a. s. held the final testing of irradiated material in semi-hot laboratories. Development of ABIT method is carried out with financial

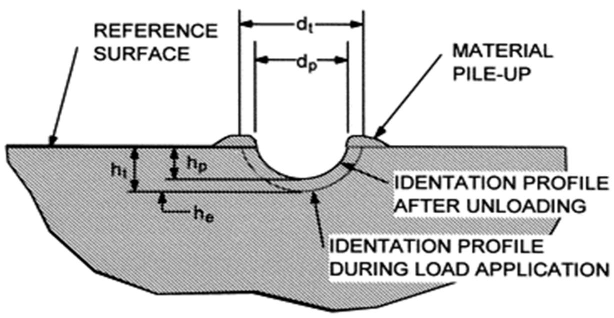

Fig. 1 - Instrumented Hardness Test method geometry during force application and after force removal (complete unloading)

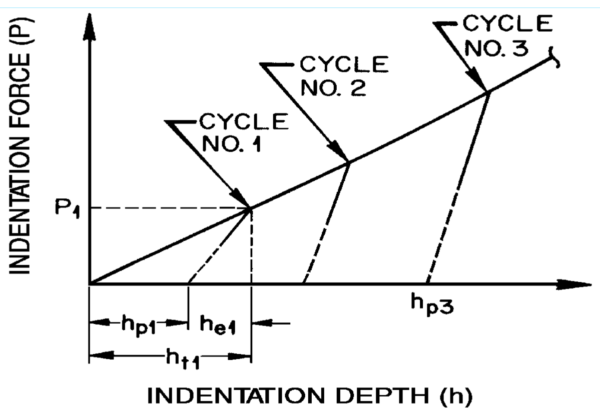

Fig. 2 - Schematic of applied force versus indentation depth of the ball indenter

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INFLUENCE OF PARAMETERS OF IRRADIATION WITH HEAVY IONS ON PHYSICAL AND MECHANICAL PROPERTIES OF THE REINFORCING THIN FILM COATING TiNbN

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Coatings based on nitrides of transition metals, due to high physical and mechanical properties - hardness, wear resistance and thermal stability, are promising structural materials for nuclear and thermonuclear power engineering. It is still a little studied the stability of the structure of such materials under irradiation; there are only a few works in this direction [1-3].

In this paper we studied especially nanohardness change Subsurface stratum of coverage TiNbN under the influence of Kr and Xe ions simulating the interaction of the nuclear fuel fission fragments with construction material, and physical surface sputtering under irradiation.

TiNbN coating thickness of ~800 nm were deposited on a stainless steel substrate 12X18H10T by magnetron sputtering of two magnetrons (Ti and Nb) content in the plasma-forming gas of nitrogen in the mixture to 35%.

Irradiation ions $^{84}Kr^{+14}$ and $^{132}He^{+18}$ samples with coatings carried out on low-energy accelerator channel DC-60. The ion energy was 20 keV per charge, i.e. the total energy of the ions Kr = 280 keV, ions Xe - 360 keV. Fluence irradiation was $1\cdot10^{15}$ - $1\cdot10^{17}$ ion×sm^{-2}, irradiation temperature did not exceed 150°C.

The sputtering coefficient was determined by measuring the thickness of the sprayed layer using the method of Rutherford backscattering on the nitrogen ions and protons. The study of the surface structure before and after irradiation was conducted by electron scanning microscopy and X-ray microanalysis and atomic force microscopy.

Studies have shown that sputtering coefficient of the surface coating TiNbN when irradiated with low-energy ions of argon and krypton lower than that of steel and is ~ 5 atom / ion, and identified relation The sputtering coefficient from fluence incident ions.

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INFLUENCE OF SHEAR UNDER PRESSURE ON STRUCTURE, PHASE COMPOSITION AND MECHANICAL PROPERTIES OF HIGH-NITROGEN AUSTENITIC STAINLESS STEEL

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A promising direction in creating economically alloyed high-strength and wear- and corrosion-resistant materials is connected with development of steels with enhanced nitrogen content, so-called high-nitrogen steels. Influence of effect of large plastic deformations through shear under pressure (SP) on the structure, phase composition, mechanical properties of high-nitrogen 08Kh22GA1,24 steel has been investigated. The steel was obtained by the casting method with counterpressure of nitrogen and was subjected to different heat treatments (quenching from 1180°C, aging at 450 and 550°C) that form an austenitic structure of the metallic matrix with chromium nitrides. After water-quenching from 1180°C (40-min holding) of the high-nitrogen steel, coarse undissolved primary nitrides Cr_2N are present in the austenitic structure. The nitrogen concentration in the γ-solid solution (0,67-0,74 wt. %) is markedly lower than the nitrogen content in the steel. Aging at the temperatures of 450 and 550°C for 0,5 h results in precipitation of uniformly distributed CrN nanoparticles with an FCC lattice that are isomorphically linked to the austenitic FCC matrix.

All three analytical methods used (transmission electron microscopy, X-ray diffraction analysis, and Mossbauer spectroscopy) fix: the appearance after the SP deformation at room temperature of nano- and submicrocrystalline structures; these structures contain austenite and strain-assisted martensite in an amount of 20 vol. %; deformation by SP results in the dispersion and deformation-induced partial dissolution of primary nitrides Cr_2N in quenched and aged steel and in the complete (after aging at 450°C) and partial (after aging at 550°C) dissolution of secondary nitrides CrN; the growth of the lattice parameter of austenite that corresponds to nitrogen saturation to 0,92–0,99 wt % is observed.

Using microhardness measurments by the restituted-indentation method with Vickers indented the effective (more than two fold) strengthening of the steel from the level of microhardness ~ 360 HV 0,025 after heat treatments to 830, 860, and 888 HV 0,025 after the SP deformation of the quenched state and states aged at 450 and 550°C, respectively. These results on strengthening were confirmed by the measurements of micromechanical properties of the nitrogen steel by the kinetic-microindentation method using Berckovich pyramid; the growth of indentation hardness was noted at the maximum load from H_{IT}=4,1–4,2 GPa in heat-treated states to 8,7 GPa in the quenched state and 9,8–9,9 GPa in aged states. Additional aging, as compared to quenching, yields a more effective strengthening upon deformation and more intense growth in the resistance of the steel to elastic-plastic deformations upon contact loading because of deformation-induced dissolution of finely dispersed secondary chromium nitrides.

Shear under pressure is effective way to strengthening, to dispersion of the austenitic structure, and deformation-induced dissolution of nitrides of high-nitrogen steel.

The investigation was supported by the RSF № 14-13-00908.

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IRRADIATION EFFECT ON 06Cr-18Ni-10Ti STEEL SUSCEPTIBILITY TO INTERGRANULAR CORROSION AND STRESS CORROSION CRACKING

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In-vessel internals of VVER-440 and VVER-1000 reactors containing an in-vessel core baffle, a barrel and a protective tube unit were designed as unchangeable structural elements with the same operating time as that of the reactor. The first VVER-440 production units are close to their specified operating time. It is a topical issue to find out if it is possible to prolong their operating time, in particular, to justify extending operating time for in-vessel internals. It is necessary to obtain data on the behavior of in-vessel internal materials under long-term irradiation.

All in-vessel internal elements of VVER-440 and VVER-1000 reactors are made of 08Cr-18Ni-10Ti austenitic chromium-nickel (ACN) steel and its welding joints. In its initial (unirradiated) state the steel is of high plasticity and corrosion resistance in oxygen-free water of the primary coolant. Basing on the data and low mechanical stress in-vessel internal elements were traditionally considered to be long-lived and not able to limit reactor facility life.

Materials science and laboratory investigations of physical and mechanical properties and service characteristics of ACN steels carried out for the last twenty years, and damages of in-vessel internals at foreign NPPs show that intense neutron irradiation of in-vessel internals induces ACN steel properties degradation (reduction in plasticity, cracking resistance and susceptibility to stress corrosion cracking), as well as significant internal stresses as a significant loading factor. Low properties of irradiated steel and high stresses can cause premature damage of in-vessel internal elements and loss of their function.

The mechanism significantly reducing stress corrosion cracking (SCC) resistance of the material is one of the main ACN steel damage mechanisms under neutron irradiation. Nowadays SCC mechanism for ACN steels has not been investigated properly. Therefore it is a topical issue to obtain some experimental data on the investigation of neutron irradiation effect on ACN steel resistance to SCC.

The paper gives the results of the investigation of 06Cr-18Ni-10Ti steel susceptibility to intergranular corrosion (IGC) and SCC after operation as external claddings for four vaporizing spent fuel assemblies of AMB reactors at a temperature of T=340-370°C to neutron fluence F=(2.01-8.05)$\cdot 10^{21}$ n/cm^2 (E>0.4 keV). 06Cr-18Ni-10Ti steel susceptibility to IGC has been defined by AMU, DU test methods according to GOST 6032-2003 standard and potentiodynamic reactivation according to GOST 9.914-91 standard. Susceptibility to SCC has been defined by accelerated testing method in boiling $MgCl_2$ solutions in the temperature range between 114 and 154 °C and at stresses of $0.5\cdot\sigma_{0.2}$, $0.75\cdot\sigma_{0.2}$, $\sigma_{0.2}$.

All three IGC test methods show that operated 06Cr-18Ni-10Ti steel is highly susceptible to IGC. The corrosion rate for irradiated steel samples in boiling 65% nitric acid is 200-300 times higher than that of unirradiated 12Cr-18Ni-10Ti steel. Accelerated SCC testing in boiling $MgCl_2$ solutions show that with increasing temperature, tensile stress and neutron fluence it takes less time to damage 06Cr-18Ni-10Ti steel samples. And the time till the steel damage is in quadratic inverse relation with neutron fluence.

INVESTIGATION OF CREEP IN AUSTENITE STEEL IRRADIATED IN BOR-60 AT TEMPERATURES 330-350^{O}C

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The work presents the results of investigation of the radiation-induced creep in gas-filled samples of intricate form irradiated in the reactor BOR-60 at the temperatures of irradiation 330-350oC to different damaging doses [1, 2].

The aim of the work was to experimentally determine the effect of the type of stressed state on the creep deformation in austenite steels X18H10T under neutron irradiation in the fast reactor BOR-60.

The effects of compression and tension on the creep in steel 08X18H10T were compared. The results can be used to verify models of the influence of different-type stresses on the radiation-induced creep.

Investigation of irradiated standard and coaxial gas-filled samples of the austenite steel 08X18H10T showed that with increasing the damaging dose, changes in the length and diameter of the gas-filled samples increase. The creep moduli calculated in this work for steel X18H10T agree well with those for the austenite X18H9-based steels.

The results of the present study are used in strength calculations выгородки of the reactor PWR-1000 and new designs PWR-1200.

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LOW ACTIVATION SNRUCTURAL MATERIALS FOR NUCLEAR REACTORS OF FISSION AND FUSION

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Design and creation of the large-scale nuclear and thermonuclear power engineering under conditions of the requirements of the expansion of capacity, reliability, safety and economics of the innovative reactors (fission, fusion, hybrid) and the realization of the full closed nuclear fuel cycle (FCNFC) and the radiation-equivalent (migration) disposal of radioactivity wastes (RAWs) after relative short (in historical scale) time period (100-300 years) after irradiation set requirements to structural materials (SMs) for the key reactor components. SMs must ensure normal and off-normal operating conditions, maximized the fuel use and reproduction, reduced nuclear waste production and increased ecology safety during operation and after shut down of reactors. Such conditions require special material science-based researches, qualification and industry fabrication of new high-performance SMs ensuring expansion of temperature, radiation and dose limits of their applications and minimizing of the time of a post-reactor cooling for the following processing (recycling) and the radiation-equivalent disposal of RAWs. The requirements for new materials are reaching technological limits.

The objective is to:

- create new nature-like technologies that do not cause damage to the environment and allow one to restore the disturbed balance between the biosphere and the technosphere.
- preserve the natural radiation balance of the Earth after a small (in the historical scale) period after extraction of raw uranium, operation and decommissioning of reactors.
- transfer the information and the guaranteed provision of radiation safety of nuclear installations (shut down reactors, disposal sites, dumps) in a thousand years' time.

Such requirements have been only satisfied by the low-activated (reduced activation) SMs (LASMs: ferritic-martensitic chromium steels, vanadium alloys, SiCf/SiC composite). LASMs will have provided the abilities of their re-use (recycling) after neutron irradiation in a time period of not more than 100-200 years (depending on neutron spectrum, radiation doses and element compositions).

LASMs and industrial technologies of their production are being developed (USA, Japan, Russia, France, Great Britain, Germany, China, India) for the cores of nuclear fission and fusion reactors with different types of coolants (liquid metals, liquid salts, helium, water) and nuclear fuels. To a large extent the scientific, material science and technological problems of selection, fabrication and further modifications of the LACMs have been resolved.

LASMs that are being developed in Russia (SC "VNIINM"), their properties, possibility and period of the radiochemical processing and perspective of applications are considered:

- Ferritic-martensitic 12% chromium steel EK-181 (RUSFER-EK181, Fe-12Cr-2W-V-Ta-B), industrial production.
- Vanadium alloys. The alloy V-4Ti-4Cr (VM-DPCh-9) was fabricated (experimental-industrial production). The alloys of the system V-Cr-W-Zr-C-O are under development as vanadium alloys with higher heat-strength and corrosion resistance (experimental production).

MAIN DEPENDENCIES AND INTERCONNECTION OF RADIATION PHENOMENA IN AUSTENITIC STEELS IRRADIATED TO HIGH DAMAGING DOSES

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During long-term operation of the reactor there is a need in the evaluation of the properties of materials irremovable elements and structures of the reactor, made usually of austenitic corrosion-resistant steels based IN. Long-term operation of various designs in difficult and harsh conditions, like prolonged active life, is not only one of the so-called "disease" and several related bouquet "diseases" that can accelerate the completion of the process operation of the elements.

Historically, in material science "youth" (1960-1970-ies) were mainly staged optimization experiments for the selection of the most radiation-resistant materials for reactor applications. Radiation effects were studied already in these developing new materials and therefore behind the scenes is always the aim was to compare the one or the other radiation phenomena for different materials.

Thus, the basic laws were studied in radiation phenomena: radiation swelling and creep, hardening and embrittlement, change of microstructure and phase stability. Radiation effects have been identified, worsening the radiation resistance of structural materials (reducing the service life of components and structures).

In the present study presents an analysis of dependencies of radiation phenomena and the current state of the new studies, paying attention primarily to the effect of duration of exposure (dose rate) on the properties and structure of irradiated steels.

The author discusses the relationship of radiation swelling and creep, and the influence of the microstructure on the physical and mechanical properties of the steels irradiated with neutrons.

NANOSTRUCTURING STRAIN-THERMAL TREATMENTS OF STAINLESS METASTABLE AUSTENITIC STEEL SURFACE

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Austenitic chromium-nickel steels are widely used in various industries owing to high corrosion resistance and manufacturability. Nanostructuring frictional treatment with a sliding indenter is an effective method for increasing the strength and tribological properties of thermally non-hardenable austenitic steels [1]. Austenitic steels could be subjected to heating during operation and processing. The work aims were investigation of thermal action influence on microhardness, phase composition and structure of the 12Kh18N10T steel subjected to frictional treatment and search of possibilities of austenitic steel hardening by combined strain-thermal treatments.

Transmission electron microscopy investigation established that frictional treatment by spherical synthetic diamond indenter results in formation in the surface layer of austenitic 12Kh18N10T steel fragmented submicrocrystalline (with crystallites larger than 100 nm) and nanocrystalline (with crystallites smaller than 100 nm) martensitic-austenitic structures. Amount of α'-strain-induced martensite on the steel surface attains 65 vol. % and the microhardness increases to HV0,025=690.

The influence of heating in the temperature range of 100-900°C on the structural-phase state and microhardness of 12Kh18N10T steel subjected to nanostructuring friction treatment was studied. Based on the results two regimes of combined strain-thermal treatments that include annealing treatment at 450 and 650°C (exposure 2 hours) after frictional treatment were suggested [2]. Annealing at 450°C provides saving in the structure 60 vol. % α'-strain-induced martensite and increasing surface hardness up to HV0,025=900 due to hardening of the martensitic-austenitic structures with nanoscale Cr23C6 carbides that precipitate from strain-induced martensite when aging. During combined treatment that includes frictional treatment and annealing at 650°C austenitic submicro- and nanocrystalline structure with hardness HV0,025=630 exceeding the initial hardness of the austenitic steel in the hardened state almost 3 times was formed on the steel surface.

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NEW INSIGHTS ON STRAIN HARDENING BEHAVIOR AND "TRAVELING WAVE" DEFORMATION MODES IN NEUTRON-IRRADIATED AUSTENITIC STEELS

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Digital Image Correlation (DIC) is an advanced test method for analysis of strain rate evolution and plastic strain distribution. The method's advantages and limitations are discussed with respect to LWR applications. Limited data exist for irradiated materials, however. This work analyzes a new DIC dataset (>30 tests) on austenitic steels irradiated at SNS to ~9 dpa for comparison with data from fast and light-water reactors. Strain hardening behavior associated with martensite formation is analyzed with special focus on small strain areas where deformation bands have been observed in many specimens, retrieving band parameters such as strain amplitude and propagation rate. Results on traveling deformation waves at small strains are compared with previous data on the high-strain-amplitude deformation bands in specimens irradiated in other reactors.

Previously, the spatial distribution of the traveling wave front was determined using magnetic probes of finite diameter and these studies gave the impression that the traveling wave "front" had a measurable thickness over which the transition occurred, but it was suspected that this result was a resolution limit problem imposed by the probe size. Using the EBSD technique, however, and imaging the wave front over a grain-to-grain dimension, it is clear that the wave front is very abrupt, with the martensitic transformation nearing completion before moving from one grain to the next adjacent grain.

The complexity of the deformation behavior and associated irradiation-assisted phase instability are discussed with emphasis on the possibility that this "second-order" phenomena may become first-order in importance at higher damage levels.

SCANNING ELECTRON MICROSCOPY INVESTIGATION OF IRRADIATION POROSITY FEATURES IN CLADDING TUBE

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One of the causes that limit life time of fuel pin of reactors on fast neutrons is shape changing caused by void swelling. The void swelling is accumulation of void under neutron irradiation. Irradiation porosity depends on such parameters of neutron irradiation as exploitations temperature and characteristics of neutron flux. Neutrons flux maximum in the center of active zone and monotone temperature changing through fuel pin length and width is feature of power reactors. Differences between irradiations parameters lead to space inhomogeneity of radiation porosity of cladding tube of fuel pin.

Investigations of space inhomogeneity of radiation porosity of cladding tube were studied by means of scanning electron microscope (SEM). Capability of modern SEMs are allow registering pores with size of 10 nanometers with possibility of study large surfaces [1]. Also, investigation of structural elements related with local inhomogeneity of porosity study was set by means of electron backscatter diffraction (EBSD).

Investigation carried out on transverse sections allowed to reveal significant volume allocation inhomogeneity in thickness of cladding tube. Depleted zone with width of 5-7 micrometers was observed on the all analyzed areas along height and around perimeter inner surface. In this zone maximum size of pore is no more than 30 nanometers. The average size pores decreased from inner to outer surface of cladding tube. The local inhomogeneity of porosity was observed on various elements of microstructure and deformation areas.

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STRUCTURE OF CLADDING MADE FROM ALLOY OF URANIUM WITH MOLYBDENUM AND ZIRCON AFTER EXPLOSIVE LOADING

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In the work, results are presented of the metallography examination of a thick-wall spherical cladding made from the alloy of uranium with molybdenum and zircon, which was subjected to explosive loading. Experimental data on the regularities of structure changes in the material resulted from the shock-wave action are given.

STUDY OF NANOSTRUCTURE EVOLUTION OF CHS-139 FERRITIC-MARTENSITIC STEEL UNDER Fe ION IRRADIATION

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Heat resistant ferritic martensitic steels are the most promising structural materials for new generation of fusion and fast breeder power plants. Well known examples of such steels developed in Russia are 12%-Cr steels Rusfer EK-181 and ChS-139 [1].

Mechanical properties degradation of structural materials is caused by reactor irradiation and high temperature. Whereas structure-phase state plays a key role in mechanical properties, information about behavior of the microstructure of materials under irradiation is necessary. The aim of the present work is investigation of evolution of the nanostructure of irradiated ChS-139 steel by atom probe tomography (APT). In this work, irradiation by iron ions beam was used. It allowed to simulate cascade formation of defects, consequently, to simulate influence of reactor irradiation on the fine structure of materials. Irradiation was performed at the Stand for Irradiation of Reactor MATerials (SIRMAT). APT samples were irradiated at room temperature by iron ions beam up to damage dose of ~9 and 18 dpa. It was shown with APT that ChS-139 steel in initial state contains high number density of nanoscale clusters (~10^{23} m^{-3}) enriched in chromium (Cr), vanadium (V), niobium (Nb), and nitrogen (N). It was shown that clusters change element composition and size under irradiation. The increase of cluster size under irradiation was accompanied by the decrease of V, Cr, Nb, and N concentrations in the clusters.

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STUDY OF ULTRAFINE AUSTENITE STAINLESS STEEL 18CR-10NI-TI AFTER IRRADIATION TO DIFFERENT DAMAGING DOSES IN REACTOR BOR-60

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In the contribution, results of studies of samples of austenite steel 18Cr-10Ni-Ti in the as-supplied state and after ECAP [1] prior and after irradiation in fast reactor BOR-60 (maximal damaging dose of 15 dpa) at the temperatures 320 and 450˚C are compared..

Equichanel angular pressing (ECAP) was employed to substantially decrease the average grain size in steel from 40-50 µm to 300-500 nm.

A preliminary investigation of structure peculiarities of nonirradiated steel after ECAP and irradiated at 320˚C was performed. The results testify to a mixed fragmentary character of the structure with a large degree of inhomogeneity.

The short-term mechanical properties and microstructure of steel 18Cr-10Ni-Ti were investigated in the state after ECAP and irradiation in the fast reactor BOR-60 (maximal damaging dose of 15 dpa) at the temperatures 320 and 450˚C

Results of [2] obtained after irradiation with different damaging doses at the temperatures, 350°C and 450°C make it possible to pick out several facts that are important for analyzing the influence of neutron irradiation on mechanical properties of stainless steels in the as ECAP state.

Among them are:

- under irradiation conditions specified in this work, it is experimentally found radiation strengthening of the steel in the as ECAP state, which depends on the temperatures;
- strengthening of steel in the as ECAP state diminishes with increasing the damaging dose, which is in part conditioned by radiation and thermal relaxation of elastic deformation stored in the process of ECA pressing;
- thermal stability of strengthening of steel 18Cr-10Ni-Ti in the as ECAP state enhances after irradiation. The enhanced radiation strengthening in the as ECAP state in comparison with the as supplied state is retained after irradiation up to the temperature 650°C;
- radiation induces the formation of particles of the α-phase at triple joints of grains with and average size of 50 nm;
- at T_{test}=550˚C total relative elongation of steel in the as ECAP state increases, the strengthening provided by the ECAP treatment being retained.

A conclusion on the necessity of continuation of studies with the account for the experimental results obtained is made.

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SWELLING, CREEP AND EMBRITTLEMENT OF D9 STAINLESS STEEL CLADDING AND DUCT IRRADIATED IN THREE FFTF DRIVER FUEL ASSEMBLIES TO HIGH NEUTRON EXPOSURES

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Most data sets on void swelling and irradiation creep of austenitic structural steels were derived in relatively small amounts, making it difficult to extract full parametric dependencies for development of predictive correlations of dimensional change. This paper presents a much larger data base derived from fuel cladding and ducts constructed from D9 steel, an improved titanium-modified variant of AISI 316 stainless steel.

This report focuses on the swelling, creep, length change, ovality and embrittlement behavior of 20% cold-worked D9 cladding and duct used in three mixed-oxide driver fuel subassemblies designated C1, D9-2 and D9-4 operating at rather different temperature histories, leading to significant differences in swelling. These 217-pin assemblies were irradiated in the FFTF fast reactor to maximum exposures of 16.3, 25.3 and 21.4 x 10^{22} n/cm^2 (E>0.1 MeV) or 73, 115 and 96 dpa, respectively. The fuel pin cladding reached swelling values of 21-28% in D9-4 and 37-38% in D9-2, with much of the in-core portion of the pins having attained the terminal swelling rate of ~1%/dpa. Since the D9-4 duct operated at lower temperatures than the D9-4 cladding, the swelling of the duct was relatively low, peaking at 6-7%. Due to the higher temperatures and lower dpa levels of the C1 assembly the cladding swelled the least of the three assemblies.

Void swelling was found to vary with dpa rate, irradiation temperature and small heat-to-heat differences in composition. The latter involved relatively small differences in phosphorus content, but produced significant differences in swelling. Compared to data sets derived from the smaller EBR-II fast reactor, it is shown that the temperature dependence of void swelling in the much larger FFTF is rather invariant over a large range of temperatures. The well-known "creep disappearance" phenomenon was observed to develop at moderate swelling levels. While no pin failures were observed during in-reactor operation, failure arising from severe void-induced embrittlement occurred in several D9-2 fuel pins and the D9-4 duct during post-irradiation handling.

TENDENCY TO INTERCRYSTALLINE CORROSION AND CORROSION-INDUCED CRACKING FOR 0.12C-18Cr-10Ni-Ti STAINLESS STEEL IRRADIATED WITH NEUTRONS AND ANNEALED AT 400-750°C

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Studies on the effect of neutron irradiation and temperature on microstructure and corrosion resistance of austenitic 0.12C-18Cr-10Ni-Ti stainless steel were performed. Objects of research were the samples cut from the ducts of spent fuel assemblies from BN-350 breeder reactor. Damage doses were 55.4, 55.7 and 58.9 dpa, and irradiation temperature did not exceed 400°C. Samples of cold-rolled 0.12C-18Cr-10Ni-Ti steel (austenized at 1050°C for 30 min) were irradiated with neutrons in WWR-K research reactor to fluences of $4 \cdot 10^{18}$ and $1.9 \cdot 10^{19}$ n/cm^2 (E>0.1 MeV). Austenized samples were annealed in the temperature range of 400-750°C (step 50°C, annealing time 3 hrs). Testing for intercrystalline corrosion was performed according to the state standard (GOST 6032-2003). Corrosion-induced cracking of irradiated and aged samples was investigated using constant load method in aggressive environment (30% $FeCl_3$) and without it. Forster ferroprobe was used to perform measurements of magnetic phase in the studied samples when corrosion tests completed.

Results of the investigations showed that austenitic stainless steel irradiated for a long period has a maximum tendency to intercrystalline corrosion. Transmission electron microscopy has confirmed that after 90° bending test intercrystalline corrosion has been mainly developed in the samples with a maximum magnetic phase. It could be assumed that in addition to dispersion of microstructural elements, magnetic α′-phase plays an important role to intercrystalline corrosion.

It was determined that an increase of annealing temperature of austenitic 0.12C-18Cr-10Ni-Ti stainless steel results in non-monotonous character of resistance to corrosion-induced cracking under the constant load and in an aggressive environment. Both aggressive environment and tension make the cracking mechanism complex, which is accompanied by appearance of numerous pitting cavities that transform to micro- and macro-cracks. Maximum amount of martensitic α-phase was developed in the samples tested in air and annealed at 650°C that was attributed to the process of sensibilization. It was concluded that a decrease of resistance to corrosion-induced cracking in chlorine environment is related to formation of carbides and martensitic α′-phase.

THE EFFECT OF IRRADIATION AND TEMPERATURE ON MICROSTRUCTURE, MECHANICAL PROPERTIES AND CORROSION RESISTANCE OF 0.12C-13Cr-2Mo-Nb-V-B STAINLESS STEEL

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Complex studies and analysis of experimental data were performed on the effect of irradiation and temperature on strength characteristics, plasticity and microstructure of the deformed 0.12C-13Cr-2Mo-Nb-V-B (EP-450) ferritic-martensitic stainless steel. It was shown that preliminary material treatment (variation of element composition and heat treatment), deformation temperature, irradiation parameters (neutrons and charged particles) influence processes of plastic flow as well as phase and structural transformations.

Optical microscopy was used to investigate microstructure of EP-450 steel, non-irradiated and irradiated with alpha-particles (50 MeV, U-150M) or neutrons (WWR-K). Thermo-mechanical treatment (1050°C / 30 min + 720°C / 1 hr) results in development of duplex structure containing ferrite (40%) and sorbite (60%) phases which ratio may vary under irradiation. A short-term irradiation with alpha-particles at 400°C or with neutrons (5.9×10^{20} n/cm^2) at <80°C usually does not lead to changes in volume fractions of ferrite and sorbite in the steel. Long-term irradiations to damage doze of ~40.3dpa at 300°C (BN-350), in contrary, significantly changes this ratio to an increase of ferrite (70% / 30%) in the steel due to dissolution of secondary carbides.

There were presented results of mechanical testing of steel samples irradiated with alpha-particles (He concentrations of 240 appm and 44 appm), and subsequently deformed with uniaxial tension at 20, 400 and 800°C. Volume doping with He leads to a decrease of strength characteristics in EP-450 at deformation temperature of 800°C compared to those for non-irradiated samples. In this case radiation-induced hardening was not observed presumably due to fast migration rate of He atoms in high-density grain boundaries.

Plasticity of the irradiated EP-450 steel has decreased when the samples were tested at 20 and 400°C, while experiments at 800°C showed a higher ductility compared to that for non-irradiated sample. Embrittlement at 20 and 400°C testing temperatures was attributed to presence of He at interfaces as well as at grain boundaries and sub-boundaries.

Metallography, density and microhardness measurements showed that additional neutron irradiation (5.9×10^{20} n/cm^2) of earlier irradiated with alpha-particles and aged samples resulted in significant changes of corrosion behavior and mechanical properties of the EP-450 steel. Additional irradiation of He-containing samples lead to an intensive intercrystalline corrosion, to a decrease in material density as well as to additional radiation-induced hardening that was accompanied by its more uniform distribution along the sample compared to that for the material implanted with He and aged.

THE EFFECT OF NEUTRON IRRADIATION AND SUB-ZERO TESTING TEMPERATURES ON MECHANICAL PROPERTIES AND PHASE γ→α TRANSFORMATIONS IN 18Cr-9Ni STEEL

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There were discussed results of mechanical testing and physical studies of 18Cr-9Ni type steel samples non-irradiated and irradiated with neutrons and deformed in tension at sub-zero temperatures.

In previous studies, the effect of the "wave" phase transformations in highly irradiated reactor steels was found [1,2] and it was shown that by varying such parameters as neutron irradiation, austenization and testing temperatures, it was possible to change post-irradiation plasticity of austenitic stainless steels. The current research continues studies in this direction. Heat treated samples (1050°C for 30 min), both non-irradiated and irradiated in the WWR-K reactor to neutron fluencies of 3.9×10^{18}, 1.9×10^{19} and 9.10^{19} n/cm^2 (E>0.1MeV) at ~80°C, were deformed in steps by uniaxial tensile testing (Instron-1195) at a strain rate of 0.5 mm/min in the temperature range from 20 to -100°C. In parallel with registration of stress-strain characteristics, data on formation and accumulation of deformation-induced ferromagnetic α′-phase were acquired. There were determined the effect of deformation temperature on strength and plasticity characteristics, as well as kinetic parameters of γ→α′ transformations. In particular, it was determined that a decrease in testing temperature to -100°C led to an increase of critical stresses for α′-phase development with a higher neutron fluence. At the same time, the volume fraction of α′-phase accumulated prior to ultimate stress decreases as damage dose increases. From experimental data, energy characteristics of deformation process were determine, and it was shown that mechanical work needed to initiate γ→α′ transformations in tension, both for non-irradiated and irradiated steel samples, increases with an increase of testing temperature (from -100°C to 20°C).

Analysis of the obtained results led to the conclusion that in addition to M_s и M_d temperatures, known from literature, it is suggested that M_t parameter could be used. The physical meaning of this parameter is when tension temperature, M_t, is reached, the intensity of γ→α transformation in non-irradiated and irradiated samples are becoming the same.

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THE INFLUENCE OF ALLOYING ELEMENTS (N, Mn, Cu, W) ON THE CORROSION AND MECHANICAL PROPERTIES OF NEUTRON-IRRADIATED AUSTENITIC AISI 316L STEEL

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The important goal of modern materials science is to create new structural materials with specified complex of physical and mechanical characteristics. The materials for fusion and fission reactors must not only provide continuous operation in stern environments (nuclear radiation, therm al treatment and corrosion environment) but also save the specified physical and mechanical properties.

For modern fission and fusion reactors structural materials with different mechanical and heat treatment are used. Cast austenitic steels are usually used for creation of complex designs. They are characterized by relatively low mechanical properties, coarse grain structure and the non-uniform distribution of elements in the material's matrix. Wherever possible to enhance the operation properties, steels are subjected to cold rolling followed by austenitization annealing. For 4th generation reactors, the special mechanical-thermal treatment was developed to produce materials with grain boundary engineering (GBE). They are characterized by improvement of corrosion resistance, reduced sink of impurities at the grain boundaries and sliding of grain boundaries [1-2].

Besides the thermo-mechanical treatment alloying is used to improve physical and mechanical properties of structural steels. In particular, nitrogen and manganese increase strength and stability of austenite. Alloying by nitrogen increases resistance of steels to local types of corrosion (pitting, knife, etc.). Copper also enhances the corrosion resistance of the steel. Tungsten increases the strength at high temperatures.

In this paper, a comparative study of the mechanical properties and resistance to pitting corrosion of the modified stainless steel AISI 316L, additionally alloyed with nitrogen, manganese, copper and tungsten were provided. Corrosion tests were performed in accordance with standard ASTM G48-03 (Method A) in 10% solution of ferric chloride ($FeCl_3 \cdot H_2O$). Investigated modifications of AISI 316L steel were cast, cold rolled and after the "Engineering of grain boundaries" (the part of the "special" boundaries, $\sum 3$, 9, 27 was ~75-80%). Part of the samples were irradiated with neutrons at the WWR-K reactor up to a maximum fluence of $5 \cdot 10^{18}$ n/cm^2.

Effect of alloying elements, thermo-mechanical treatment and neutron irradiation of steels on the mechanical properties and resistance to pitting corrosion is discussed for all investigated materials.

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TOMOGRAFIC ATOM PROBE STUDY OF NANOSACLED FEATURES IN STRUCTURAL MATERIALS OF NUCLEAR POWER PLANTS

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In modern approaches of nuclear material investigation microstructural peculiarities are of a great concern. The critical information can be derived from nano- and even atomic scales and should reflect not only structural alterations but also redistribution of chemical elements. These phenomena determine both stages of radiation damage and macroscopic changes such as swelling, embrittlement; which in some cases were driven by formation of structural nanoscale peculiarities. On the other hand, development of promising structural materials especially for reactor core requires formation of variety of nanoscale structural peculiarities that increase mechanical properties as well as radiation resistance. The most appropriate technique to investigate phase-structure peculiarities at atomic scale is tomographic atom probe.

ITEP has a considerable experience in atomic-scale investigation of structural material properties including after irradiation. At present in ITEP atom-probe investigations are carried out in the following directions: pressure vessel steels of operating and power plants; precipitation hardening ferritic/martensitic steels; oxide dispersion strengthened steels; radiation stability of nuclear structural materials in model experiments using heavy ion beams. The purpose of the present work is to give a survey on the nowadays investigations in ITEP.

Zr-2.5%Nb ALLOY STRUCTURAL EVOLUTION UNDER LONG-TERM NEUTRON IRRADIATION AT 40–80°C

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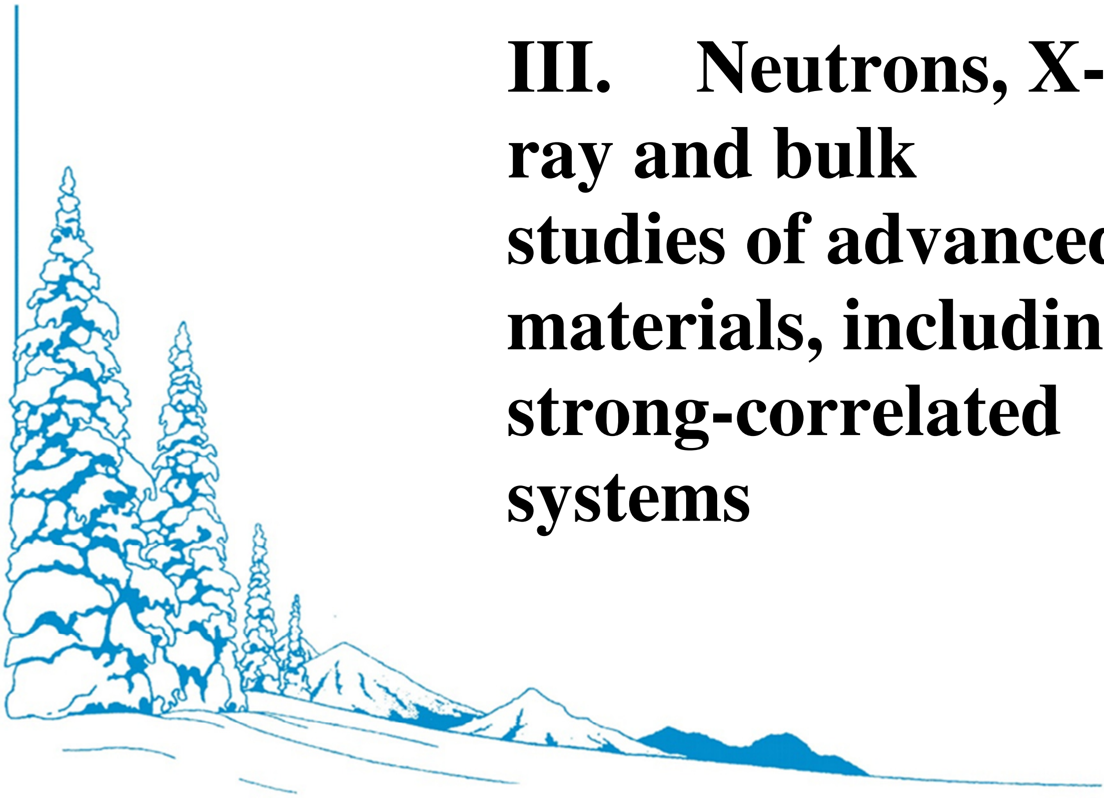
Zirconium alloys are widely used in nuclear industry as one of the main structural materials for thermal reactor cores. They are exposed to neutron irradiation at different temperatures. As a result material properties change, mostly due to structural evolution.

The results of the evolution microstructural analysis for Zr-2.5%Nb alloy after long-term irradiation in RBMK reactors depending on the gained neutron fluence (damage dose) are given.

The samples of control and protection system channels have been examined after 7-39 calendar years of operation at a temperature of 40–80°C exposed to neutron flux (E>1 MeV) with density of $2\cdot10^{12}$ cm^{-2}s^{-1}. Structural analysis using electron microscopy and X-ray diffraction analysis has been carried out.

It is shown that under irradiation the alloy grain structure almost does not change, radiation thermal annealing of initial dislocations occurs predominantly due to <**a**>-type dislocations, and the registered dislocations are <**c**>-component. Radiation defects in the form of clusters and <**a**>-type dislocation loops are developed. It is shown that under long-term neutron irradiation radiation-induced diffusion processes occur in the alloy causing Nb concentration reduction in β-Nb precipitates, and new Nb-based finely divided precipitates generate in matrix.



III. Neutrons, X-ray and bulk studies of advanced materials, including strong-correlated systems

The development of advanced technologies, including new generation nuclear techniques, make a strict requirement to structural and functional materials on the basis of which the element base for progressive computer, information and monitoring systems will be created. From this point of view, the perspective materials for it are materials based on d- and f-elements, having unique physical properties and known as systems with strong electron correlations. The spectroscopic investigations by neutron and X-ray scattering methods play the outstanding role in studying of physical properties of these materials. For this reason, in the Seminars' Programme is included reports, devoted to examination of perspective materials - new generation superconductors, frustrated magnets, valence-unstable systems, ferroelectrics, quantum magnets and hybrid nanostructures - by mean of inelastic neutron scattering, X-ray spectroscopy and measurements of microscopic parameters.

EFFECT OF SPIN REORIENTATION TRANSITION ON RARE-EARTH IN $YbFeO_3$: SPIN-1/2 ISING CHAIN IN TRANSVERSE AND LONGITUDINAL FIELD

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The low energy spin dynamics of Yb^{3+} in the orthoferrite $YbFeO_3$ have been studied at temperatures below and above the iron spin reorientation transition T_{SR} ~ 7 K using single crystal inelastic neutron scattering. Below T_{SR} we observe both sharp magnetic excitations and a broad continuum dispersing in only one direction, as predicted for spin-1/2 Ising chain in longitudinal magnetic field H_z which is large compared to the antiferromagnetic (AFM) exchange J. Above T_{SR} a continuum-like spectrum with dispersing low-energy onset emerges, a signature of independently propagating domain-wall quasiparticles (kinks) in a ferromagnetically polarized chain in transverse magnetic field. We establish that the fluctuations of Yb moments are mainly longitudinal and constrained parallel/perpendicular to the iron net moment below/above T_{SR}. The observed magnetic excitations are well described by a one-dimensional Ising-like AFM Hamiltonian with inclusion of a weak transverse Heisenberg term and a magnetic field H_z that fully polarizes all spins, $\langle S_n^Z \rangle = S$

EXOTIC MAGNETISM IN STRONGLY CORRELATED ELECTRON SYSTEMS

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Rare earth based strongly correlated electron systems (SCES) demonstrate a wide range of different types of a ground state. Its variety started from trivial paramagnetic states or long range magnetic ordering ones originating from crystal field splitting of f-electron multiplet competing with exchange interaction of local moments, and arrived at highly exotic ones. The latter, for instance, could be as Kondo-insulator with combination of charge-, spin-gap with valence instability; or long range magnetic ordered state in initially singlet ground state system; or some combination of long range magnetic order with superconductivity and valence instability; etc. Physical background for these features inherent to electron subsystem may be elucidated by detailed neutron scattering experiments, first of all by magnetic neutron scattering spectroscopy and diffraction. These methods provide microscopic information about the character of the ordered state and magnetic moment value as well as about spectral features of the dynamical magnetic susceptibility including the spin fluctuation characteristics of valence unstable compounds.

Specific features of such unusual ground states are analyzed on the base of the results of the extended experimental studies of CeT_2Al_{10} (T=Fe,Ru,Os), PrNi, $EuCu_2(Si,Ge)_2$. The report displays previous and recent results in the field under study for a number of representative rare earth intermetallic compounds. The number of the examples is presented, in particular: the systems with induced long range ordering for crystal field defined singlet ground state metals; Kondo-insulators with possibility for formation of long range magnetic order below metal to insulator transition; systems with coexistence of long range magnetic order with intermediate valence state or heavy fermion state.

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INVESTIGATION OF THE MAGNETOELECTRIC AND MAGNETOELASTIC PROPERTIES OF OXIBORATES SINGLECRYSTALS.

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It is still unclear which mechanism is responsible for the magnetoelectric effect at the microscopic level. The materials revealing the magnetoelectric effect exhibit the dependence of polarization on an applied magnetic field, i.e., the ME_H-effect, or the magnetization variation in an applied electric field, i.e., the ME_E-effect.

Among substances revealing the magnetoelectric effect is the borate family $RM_3(BO_3)_4$, where R is a rare-earth ion or Y and M is an Al, Fe, Ga, Sc, or Cr ion. Crystals in this family have the R32 space group, which determines the absence of the inversion center. The MO_6 octahedra sublattice forms a helical chain along the *c* axis with the exchange interaction of 3d elements; the rare-earth ions form RO_6 prisms and are isolated from one another by BO_3 triangles, i.e., there is no the R–O–R interaction. Both the BO_3 triangles and RO_6 prisms are coupled with three MO_6 chains.

In study by K.-C. Liang et al. [1], the authors reported both the giant ME_H magnetoelectric effect and magnetostriction in the $HoAl_3(BO_3)_4$ crystal. It is noteworthy that this material is not a multiferroic in the ordinary sense, since it is not magnetically ordered. However, the processes occurring at the microscopic level are still not fully understood. The magnetoelectric interaction, and in particular, the role of a rare-earth ion, needs further investigation.

The aim of this study was to investigate the ME_E-effect and permittivity in the $HoAl_3(BO_3)_4$ crystal in order to clarify the microscopic mechanism responsible for this effect. To test this model and to check the crystal field splitting when different 4f and 3d ions presented we prepared the direct magnetoelectric and magnetostriction measurements of the family of crystals $RM_3(BO_3)_4$, where R – Sm, La, Ho, Tb, and M – Al, Fe, Ga ions and their combinations.

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LOCALIZATION/DELOCALIZATION CROSSOVER IN THE VALENCE-UNSTABLE F-ELECTRON SYSTEMS

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Crossover between localized and delocalized (itinerant) f electron behavior constitutes one of the most interesting problem in physics of strongly correlated systems. Such a transition of the 5f electrons is the central event within the actinide series, where the 5f electrons behave in a localized fashion for the heavy actinides but in a more delocalized manner for the light actinides, with a nexus in the vicinity of Pu and Am. In the lanthanides, where the 4f orbitals are spatially less extended than the 5f in the actinides, the localization-delocalization transition occurs in the materials based on cerium (beginning of the rare-earths series), samarium (middle of RE series), and ytterbium (end of RE series) due to variation of temperature or pressure application, resulting, in some cases, in the structural phase transitions accompanied by volume collapse. Recently, significant progress has been achieved in the understanding the nature of localization/delocalization crossover in the systems with unstable f-electron shell, particularly owing to the inelastic neutron scattering experiments.

Intermediate-valence compound CeNi undergoes a pressure-induced structural phase transition with volume jump and as a such constitutes an attractive system to study pressure-driven f-electron delocalization in the systems with an unstable f-electron shell. Note, that Ce valence in the intermediate-valence CeNi differs distinctly from the integer value [1]. By the other words, 4f electrons fall within crossover region between localized and itinerant behavior even at ambient pressure. Therefore, one can expect the volume-collapse structural phase transition to shift the system further towards the itinerant (bonding) f electron behavior.

Recently, we have shown that the CeNi high-pressure phase belongs to the *Pnma* space group [2]. In the present work inelastic neutron scattering technique is employed to study dynamic magneto susceptibility of CeNi before and after structural transition. The results of these experiments show enhanced Ce 4f–Ni 3d hybridization due to the phase transition while the inelastic 4f magnetic form factor does not change and retains the value of the free Ce^{3+} ion. Bearing in mind recent theoretical results in this scientific area [3,4], we discuss the issue of physical meaning and quantitative characterization of the delocalization process in the systems with unstable f electron shell.

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MAGNETIC PHASE DIAGRAM OF $Y_{1-X}Tb_XMn_6Sn_6$ (X = 0, 0.175, 0.2, 0.225, 0.25) COMPOUNDS.

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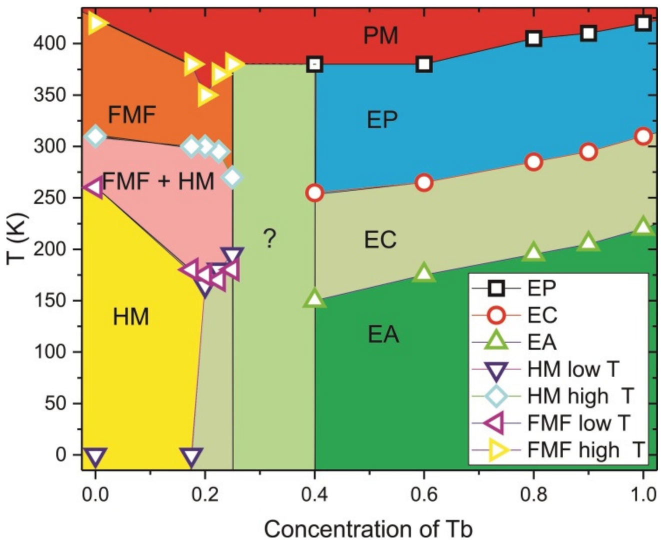
Over the last years, researchers have focused their attention on compounds, which possess a natural magnetic layered structure. A number of studies have been devoted to the RMn_6Sn_6 compounds with layered crystal structure, where R = rare earth ion [1-5]. The $Y_{1-x}Tb_xMn_6Sn_6$ compounds (x = 0, 0.175, 0.2, 0.225, 0.25) were studied by small angle neutron scattering (SANS) and paramagnetic neutron spin echo. The YMn_6Sn_6 compound is found to be a helimagnet in the whole temperature range below $T_N = 310$ K. Close to T_N an additional peak of a Lorenz shape was observed at $Q = 0$. The peak is thought to have originated from the ferromagnetic fluctuations of the magnetic Mn moment in the ab-plane of the hexagonal crystal structure. Compounds, in which Y is replaced by Tb, change their magnetic order with the increase of temperature: from easy cone ferromagnetic phase at low T through the helicoidal phase to the ferromagnetic fluctuation close to T_N. Temperature-concentration phase diagram of $Y_{1-x}Tb_xMn_6Sn_6$ is built on the basis of the obtained data.



The Magnetic phase diagram of $Y_{1-x}Tb_xMn_6Sn_6$ compounds. Data for concentrations higher than

$x = 0.25$ are taken from [3].

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MAGNETO- AND SPIN-DEPENDENT TRANSPORT PHENOMENA IN HYBRID STRUCTURES WITH A SCHOTTKY BARRIER

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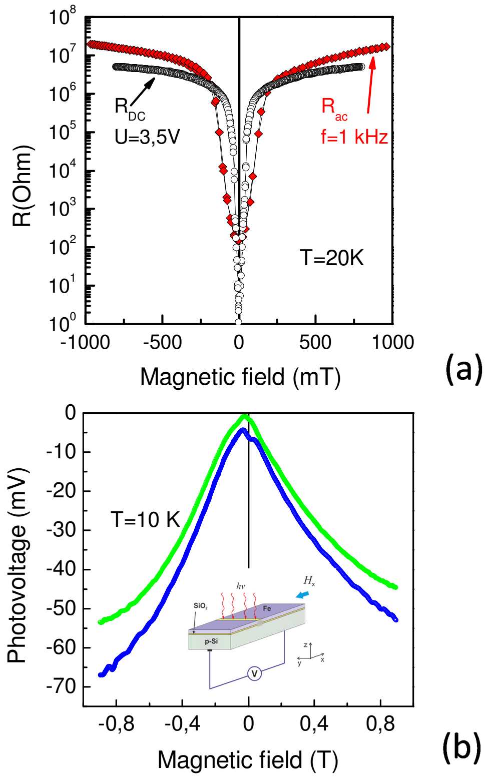

Figure 1. Magnetic field dependences of $Mn/SiO_2/p$-Si structure DC and AC resistance (a) and Fe/SiO_2/p-Si structure photovoltage at different laser power (b).

Magnetotransport phenomena in hybrid structures, which are compatible with CMOS technology, are an attractive field of investigation because of the interesting physical phenomena and promising application in memory devices, sensors, magnetic field-controlled logic, etc [1]. In this work we present some magnetotransport effects which were found in silicon-based hybrid structures.

The $Mn/SiO_2/p$-Si and Fe/SiO_2/p-Si structures were fabricated using ultrahigh vacuum thermal evaporation. Magnetotransport properties were measured using a KEITHLEY 2400 current/voltage source meter, KEITHLEY 2182A nanovoltmeter (dc) and an Agilent E4980A analyzer (frequency range from 20 Hz to 1MHz).

$Mn/SiO_2/p$-Si structure demonstrates gigantic magnetoimpedance (MI), dc magnetoresistance (MR) effects (Fig.1(a)). The effect of magnetic field attributed to suppression of impact ionization via two mechanisms leads to an increase in the carrier energy required for initiation of impact ionization. The first mechanism is related to displacement of acceptor levels toward higher energies relative to the top of the valence band and the other mechanism is associated with the Lorentz forces affecting carrier trajectories between scatterings events.

Strong influence of magnetic field on $Fe/SiO_2/p$-Si Schottky barrier structure lateral photovoltage is observed at low temperatures, below 12 K (Fig.1(b)). The origin of the magnetic field effect on the photovoltage in the structure is conditioned by a shift of acceptor levels and, as consequence, an alignment of the Schottky barrier. Since just the parameters of the Schottky barrier are responsible for a value and a sign of the lateral photovoltage, the magnetic field, thereby, controls the photovoltaic effect.

This work was supported by RFBR and Government of Krasnoyarsk Region (projects nos. 16-42-242036 and 16-42-243046).

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MAGNETOSTRICTION IN HEXAGONAL $HoMnO_3$ SINGLE CRYSTAL

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The typical example of hexagonal manganites is $HoMnO_3$, which magnetic phase diagram is well established. Following to [1], at temperature T_N = 72 K, $HoMnO_3$ ordered in noncollinear spin structure with magnetic $P6_3cm$ group symmetry. At the spin reorientation temperature T_{off} = 40 K, manganese moments rotate in a plane with the changing magnetic P63cm symmetry to $P6_3cm$, and transition temperature ~ to 4 K associated with rare-earth ordering.

In this study, single crystal of hexagonal manganite $HoMnO_3$ was synthesized by optical floating zone melting. The effect of magnetostriction was measured in a temperature range of 4.2 to 100 K at applied magnetic fields up to 14 T. The effect was measured along all axes in different crystallographic configurations (longitudinal and transverse magnetostriction).

The behavior of the magnetostriction effect showed a large number of features observed in different temperatures and field configurations, including nonmonotonically striction and change the sign of the effect. Moreover, the behavior of the magnetostriction effect in temperatures below the spin-flip transition of Mn correlates well with the magnetic phase diagram $HoMnO_3$.

However, since original compound attended 2 of the magnetic subsystem (4f and 3d elements), it was decided to synthesize a pattern of hexagonal substituted lanthanum manganite with replacement on non-magnetic ion in the rare-earth subsystem in order to determine the impact on the behavior of 4f subsystem magnetostrictive effect.

For this, the sample was synthesized with a nonmagnetic $YMnO_3$ 4f subsystem, on which the measurement of the magnetostriction effect were also been done. Measurement results showed that the value of the magnetostriction decreased by the order and lost all the features typical of $HoMnO_3$. It can be concluded that the main role in magnetostriction effect is the role of Ho ions.

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NMR STUDY OF KINETICS OF ISOTHERMAL PHASE TRANSFORMATIONS IN THE U-6Nb ALLOY

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Phase transformation in the rapidly quenched alloy U-6Nb (U: 6 wt% Nb) was for the first time investigated with the use of local NMR techniques at nuclei ^{93}Nb.

In the course of the phase transformation upon isothermal annealing at T_{ann} = 500°C, in the bulk of the alloy there takes place an increase in the amount of the Nb atoms with a local magnetic susceptibility that corresponds to U-Nb alloys with a higher concentration of Nb. The formation of structure precipitates enriched in Nb with a local magnetic susceptibility that is lower than that of the initial solid solution of the high-temperature γ-phase terminates after the 60 h annealing.

RECENT PROGRESS IN NEUTRON SCATTERING STUDIES OF COPPER- AND IRON-BASED SUPERCONDUCTORS

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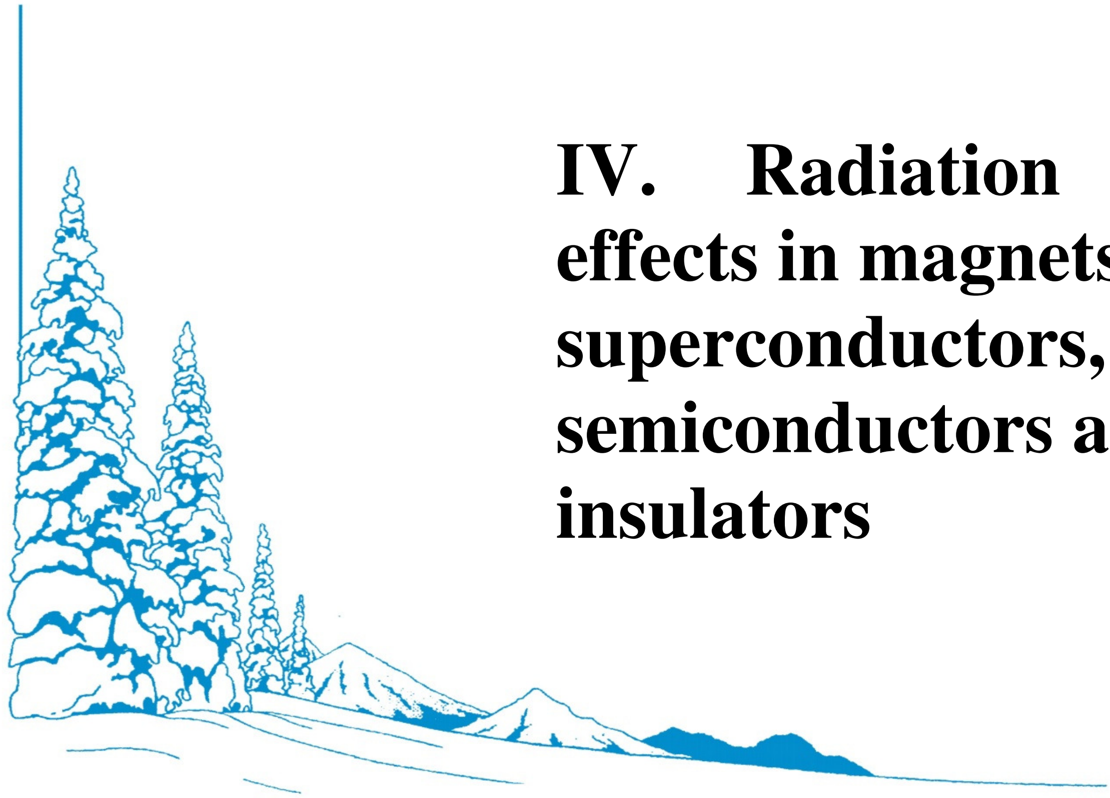
Spin excitation spectra are studied by inelastic neutron scattering in different families of superconductors and their parent compounds focusing at the “magnetic resonance” type of response. These excitations, first observed in YBCO family of the cuprate superconductors and then confirmed to be present in the other compounds including iron-based generations, attracted attention because it appeared when entering the superconducting state thus evoking a particular role of magnetic excitations in formation of superconductivity. The resonance is considered as a fingerprint of the “novel” type, called d-wave, of superconducting pairing contrary to “classical” s-wave pairing. In the report we outline the role in this research of neutron scattering spectroscopy at steady state neutron sources (nuclear reactors) with the help of three-axis spectrometers powered by “optical” focusing and measurement channel multiplexing as well as polarization analysis techniques.

We follow the evolution of the resonance and other magnetic excitations in various superconductors and relative compounds as a function of wave vector, temperature, magnetic field, doping with magnetic and non-magnetic impurities. The collected data are described within itinerant carrier models giving way to interpretation of the magnetic excitations in both normal and superconducting states.

In the case of cuprate superconductor the main attention in the recent experiments focused on the underdoped regime of the YBCO family with attention given to so called “pseudo-gap” state and anisotropy of the excitations in the mono-domain (detwinned) samples.

The iron based superconductors are represented by selenides family AFe_xSe_y (A = K, Rb) where a new resonance wave vector was discovered. The most recent research in the sulfurdoped derivative has permitted us to follow a specific transformation of the resonance excitation interpreted as an evidence for switching between s^{+-} and s^{++} types of pairing. In the other pnictides "122"-family $BaFe_2As_2$ with various dopings the anisotropy of magnetic response is emphasized in the experiments with uniaxial pressure applied *in situ* to the single crystal samples.



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

The subject of this Section is traditionally formulated with a view to introduce the Seminar attendees (mainly metal physicists) to the results of the latest research into radiation effects in superconductors, semiconductors and dielectrics (magnetic dielectrics including). In the case of the first two materials, their physical properties change significantly upon exposure even to rather low fluences of high-energy particles. Therefore, investigation of the causes of damage and the impairment of the physical and mechanical properties of the materials of this group has always been – and is today – a topical task. The Seminar Program includes papers on physics of radiation effects in semiconductors and insulators. The behavior of radiation defects and changes in the physical and mechanical properties of materials such as manganites $La_2SrMn_2O_7$, $LaMnO_3$, oxide CuO, Si, SmB_6, GaN, etc. are analyzed. The amorphization of silicon upon exposure to ion beams, the dielectric effect in HTSC ceramics, principles underlying the radiation modification of semiconductors and dielectrics, and the influence of radiation-induced disordering on semiconductor radiation detectors are discussed.

EFFECTS ON NEUTRON IRRADIATION OF $Bi_{0.85}La_{0.15}FeO_3$

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A prominent feature of $BiFeO_3$ is coexistence of ferroelectric (T_C=1123 K) and antiferromagnetic (T_N=643 K) states. This allows one to consider this material as promising for application in the recording devices, etc. Up to mow, many attempts have been undertaken to improve properties of $BiFeO_3$ via partial substitution of Bi and Fe atoms by other elements or irradiation with high-energy ions and electrons.

The sample under study was prepared by the method of solid reaction. Partial substitution of lanthanum for bismuth in $Bi_{0.85}La_{0.15}FeO_3$ made it possible to gain single-phase state. The sample was synthesized and kindly provided by our Portuguese colleagues. Methods of neutron diffraction, low-angle neutron scattering, and magnetic measurements were employed to investigate structural and magnetic state of $Bi_{0.85}La_{0.15}FeO_3$ irradiated in the reactor IBB-2M with fast neutrons (E>0,1 MeV) with a fluence of $5\times10^{20}cm^{-2}$.

The analysis of the neutron scattering patterns by the Rietveld method (FullProf program) showed that in the massive pressed sample after irradiation there formed two phases Bi_2O_3 and Fe_3O_4, the oxygen being deficient. This state has been retained for more than two years. Storing the irradiated and ground into powder sample in air for more than four months results in the restoration of the initial state. The magnetic measurements showed that in the massive sample, owing to precipitation of the Fe_3O_4 phase, a ferromagnetic state is formed with the coercitivity H_c=650 Oe.

The analysis of the results obtained allows an assumption to be made that the free path of oxygen atoms initially knocked out by neutrons (IKA) makes up about 350 nm, which exceeds by far, more than ten times, the free path of heavy IKA Bi, La, and Fe. In the process of irradiation, which lasted for 40 days and nights, part of the oxygen IKA went onto the grain boundaries, which resulted in the oxygen deficiency in the sample. It is this deficiency that plausibly causes the precipitation of the Bi_2O_3 and Fe_3O_4 phases. The storage in air of the irradiated sample with the developed surface (powder) resulted in the restoration of the oxygen content in the sample and its recovery to the initial state.

NEUTRON EXPOSURE INDUCED ELECTRICAL PROPERTIES AND LATTICE CONSTANTS MODIFICATION OF *wz*-GaN EPILAYERS GROWN ON (0001) Al_2O_3 SUBSTRATE

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The GaN/Al_2O_3 heterostructures are used widely in the technological aims today because ones give the opportunity to obtain the acceptable crystalline of the GaN structures quality. The effects of fast neutrons (E > 0.1 MeV) up to 1.75×10^{20} fn/cm^2 and fast plus thermal neutrons up to 3.5×10^{20} ftn/cm^2 irradiations on the electron properties and the crystal lattice parameters of the GaN(Si) and GaN(Mg) layers grown on the (0001)Al_2O_3 substrate have been studied. It was found that neutron irradiation converts the original n-GaN(Si) samples into the semi-insulating state with resistivity at about 1×10^{10} Ohm×cm at room temperature. At the same time the resistivity of the initial p-GaN(Mg) samples due to the radiation-induced defects (RIDs) raises higher than 1×10^{10} Ω×cm due to p- to n- type conductivity conversion as a result of the Fermi level shifting into the upper half of GaN gap, and then falls up to ~1×10^{10} Ω×cm as in the initial n-GaN samples. This transformation of GaN resistivity upon the neutron bombardment is the result of the charge carriers trapping by the acceptor type RIDs in initial n-type and by the donor-type RIDs in initial p-type samples. As the result of these effects the Fermi level in all investigated samples moves into the upper half of GaN forbidden gap and then pins below the bottom of the conduction band at the boundary position near E_c – 0.7 eV at room temperature that close to the intrinsic charge neutrality level position in the gallium nitride. The subsequent neutrons irradiation of these high-resistance samples cuts down the resistivity of the material up to ~1×10^{6} Ω×cm at the maximum neutron flux. for this work This “anomalous” decreasing of the resistivity in the “over-irradiated” GaN samples was observed earlier in some works for others neutron irradiated semiconductors, for example GaAs. This effect is associated with the hopping conduction of charge carriers over the states of radiation-induced defects in the heavily damaged material. In these GaN samples the ρ(*D*)-curves in large doses are virtually the same irrespective of the starting doping levels and of the initial samples conductivity type.

X-ray diffraction reveals the expansion of GaN *c*-lattice parameter upon the neutron bombardment up to the limit value at about 0.44% relatively to the initial value in the original samples and up to ~0.51% relative to the strain-free GaN while *a*-lattice parameter remains nearly unchanged. At the same time the *c*-lattice parameter expansion of the Al_2O_3 substrate achieves the value at about 0.11% only at the neutron irradiation, while *a*-parameter remains practically unchanged within the measurement accuracy.

The interpretation of the isochronal annealing data of the neutron irradiated n- and p-GaN samples suggests that donor-type and acceptor-type defects are annealed out in both materials. At the same time the electron properties of the heavily irradiated GaN samples indicates at the presence of the stable lattice defects after annealing near 1000°C. The thermal stability measurements of the neutron-induced RIDs reveal that $\Delta c/c_0$ expansion returns upon the heating up to 1000^0C to the original value with the main annealing stage near 400°C that indicates on the point defects annealing mainly.

PROBLEME OF RADIATION EFFECTS OF MATERIALS OF PEROVSKITE-BASED SOLAR CELLS

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The problem of radiation resistance, which is the most important attribute of the work of solar cells(SC) based on semiconductors, is divided into two aspects: 1) the degradation of the solar cell under the action of light of the operating range; 2) degradation of SC under the action of high-energy radiation. The first aspect is important for all work conditions, second aspect is actual at the operation in the space. Mechanisms realizing these two aspects of radiation physics are very different [1]. In the case of the organic-inorganic perovskite based solar cells, the processes of radiation degradation are the results of very specific types of processes, which are very different from other semiconductor solar cells (e.g., Si).

1. The degradation under action of light exposure. Physics features are associated here with the strong ionicity of the lattice and that the valence band is formed mainly from the orbital of I connected with the I^- ion state. The reaction $I^- + h\nu \rightarrow I^0$ occurs under the absorption of light, which eliminates the Madelung-Ewald well for I^- and promotes the I^0 release into interstitial position. This process goes in competition with the hole delocalization, so that the probability of degradation is: $\eta \sim \exp(-\Delta E_v^e/\omega_D h)$, where ΔE_v^e is the maximum width of the valence band, ω_D is the Debye frequency. This factor increases dramatically in the defect areas where ΔE_v^e is small.

2. The degradation under action of high-energy radiation. Here, the main feature of the material is the strong asymmetry of the masses of the atoms, which puts to the two-step process: first, the fast particle (electron) shifts the light atom from CH_3-NH_3 molecules, which then shifts under scattering the neighboring heavy atoms (eg, I^-). As a result of such formation of defects, the energy threshold of irradiating the particles is dramatically reduced. For example, the maximum possible transfer of energy to the atom is in the case of the fast electron with mass m_e and I^- atom with mass M_i: $E^{(2)}_{max}/E^{(1)}_{max} = 4M_i^2(m_e+M)^2/[(M_i+M)^2(m_e+M_i)^2 >> 1$,where M is the mass of light atoms. Thus, cross-section of the defect formation in the process of "particle - light atom - heavy atom" sharply dominates over "particle-heavy atom" processes. Note, that similar process have been discovered many years ago in germanium doped by hydrogen (see [1]).

3. Degradation of solar cells with fractal interfaces under ionization radiation.

Since the presence of fractal interface leads to its excessive area, the exposure by ionizing light (as such as by any type of ionizing radiation in general), taking into account the semiconductor nature of the perovskite, can lead to the different probabilities of defect formation and of the surface radiation-stimulated atomic diffusion in the regions with the different signs of the curvature. This, in turn, should eliminate the extra value of 13% of the photocurrent. Note, that the effect of the 13% increase of photocurrent have been discovered in [2]

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RADIATION-INDUCED CONDUCTIVITY OF POLYMERS: THEORETICAL MODEL AND ITS APPLICATIONS

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Appearing electric fields occurring in polymeric materials and fault currents occurring in ionising radiation domain can be the reason of complex technical systems failure. However, to date description of the radiation-induced electric conductivity of polymers is an important issue, which is largely due to differences in the structure of polymeric materials [1-5].

Radiation-induced conductivity both during irradiation and at the relaxation stage after cessation of irradiation is studied in this work. An analytical expression describing the decay of radiation-induced electric conductivity is derived within the Rose-Fowler-Vaisberg (RFV) model at low intensities of the radiation pulses. The analytical expression is compared with direct numerical computation. Convenient experimental techniques for determining the basic parameters of the RFV model (effective frequency factor, displacement of thermalized charge carriers prior to their capture in unit electric field, and dispersive parameter) are proposed based on the calculation results. The suggested method for determining parameters of the RFV model is checked using the available literary data for polystyrene and low-density polyethylene as an example. Along with an analysis of the low-signal mode we scrutinize also nonlinear effects associated with bimolecular recombination of charge carriers and filling the traps. The temperature dependence of the radiation-induced conductivity and its relation to molecular mobility in polymers are studied.

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THERMOELECTRIC PROPERTIES OF SOLID SOLUTIONS $(SnSt)_{1\text{-}X}(GdSe)_X$ γ-RAYS IRRADIATED

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Increase of materials radiation stability gained on the basis of compounds of type $A^{IV}B^{VI}$ is one of the topical issue of Semiconductor Physics. This led to interest in the ligation of these materials with rare earth elements, resulting in increased resistance to radiation exposure. We studied the influence of γ-irradiation on the main thermoelectric characteristics of $(SnSe)_{1\text{-}x}(GdSe)_x$ solid solutions.

It was studied the influence of gadolinium on the electrophysical properties of $(SnSe)_{1\text{-}x}(GdSe)_x$ ($x\leq2{,}00$ *mol%* GdSe) solid solutions. It has been established that the inversion with the conduction sign happens according to the content of gadolinium. With small content of gadolinium (up to ≈0,25 *mol%* GdSe) there is the intense spreading of charge carriers from phonons that results in the reducing of common thermal conductivity and mobility of carriers. It was found out that the studied samples are partially compensated semiconductor materials with the mixed type of conductivity.

The samples were gained by the method of directional crystallization. First of all before irradiation the next thermoelectric parameters were measured: thermal electromotive force (S); electrical conductivity (σ) and thermal conductivity (χ). Then it was measured the samples of γ-quanta with dose of D=0.6 *Qr/sec* during 30 hours (ε=9.0 *eV)* and then we again measured the above mentioned parameters. Some results are shown in the figure.

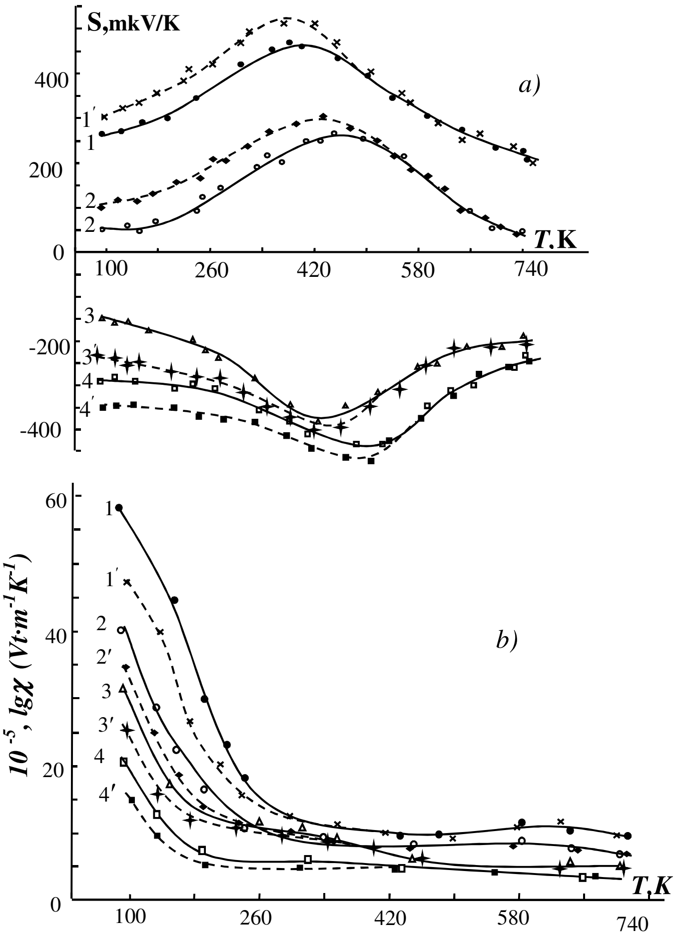
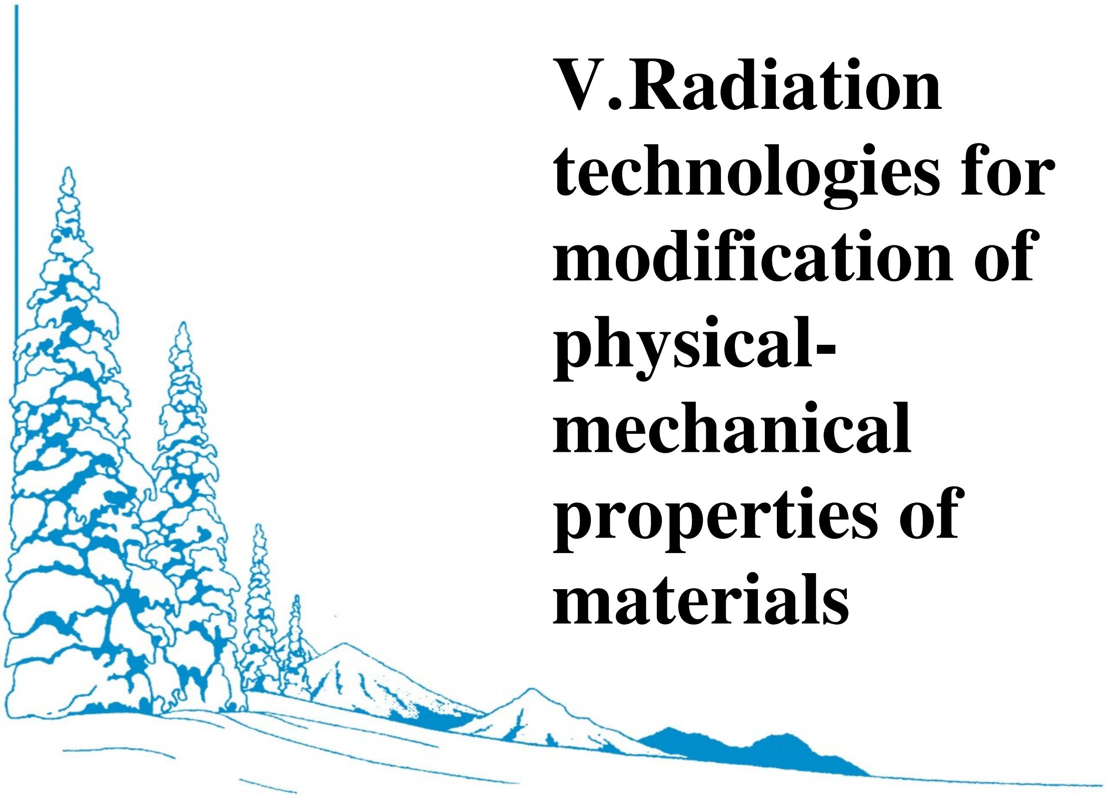


Figure 1. The temperature dependence of thermal electromotive force (b) in the system of alloy (SnSe)1-x(GdSe)x (the dashed line after irradiation)

The qualitative assessment showed us that after the irradiation of all studied samples, regardless the type of conductivity, the thermal electromotive force is increasing and the thermal conductivity is decreasing. The decrease of general thermal conductivity in all samples occurs due to the formation of a new inter specific subbarray of stannum and selenium. With the increasing temperature the relative change of thermal electromotive force and thermal conductivity is decreasing and this is apparently connected with a decrease in the rate of recombination between radiation and structural defects.



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

This section is introduced in the Seminar's Program in order to exchange information about the latest achievements in the field of radiation material science associated with the development of physical bases and the use of electron- and ion-beam and ion-plasma methods for modifying the structure and properties of materials at the macro-, micro-, meso- and nanoscale level. The section program includes presentations devoted to the consideration of the fundamental aspects of the impact of accelerated ion beams with matter, that are determined their corpuscular nature and are general for both continuous and pulsed ion beams.

The powerful pulsed beams of electrons, ions, plasma flows and laser irradiation ($P>10^7$ W/cm^2) cause instant melting and even evaporation of surface layer material. Modification of the properties at the same time is a result of the formation and propagation of powerful thermo-elastic waves. The combination of ion implantation with other methods, such as ion-beam mixing of films deposited previously on the surface of the target (Ion Mixing) or ion-assisted deposition of elements in vapor or plasma (Ion Beam Assisted Deposition) in order to increase the depth of exposure, which at normal conditions is only a percentage of a micron, leads to considerable complication and rise in price of the process. In connection with this, the intensively investigated recently long-range effects occur during ion bombardment, which allow significantly increasing the depth of the modified zone, becoming urgency, which is particularly important to develop methods for the modification of surface properties of construction materials.

The most promising is currently studying of nanoscale dynamic effects caused by corpuscular irradiation. Nanoscale regions of dense cascades of atomic displacements, warmed up for about 10^{-12} seconds to temperatures of 3000-5000 K and higher, are zones of explosive energy release and the source of the post-cascade solitary shock waves, which can rebuild the metastable environment. The rate of energy release is comparable to that for a nuclear explosion. Radiation-dynamic effects, which are not taken into account in the classical radiation physics of condensed matter, play an important role also under neutron irradiation and self-irradiation of fissile materials. They should be considered in connection with the nuclear safety issue in the development of new materials for use in the internals of nuclear power plants, as well as materials for use in outer space.

ANALYSIS OF THE MICROSTRUCTURE OF TITANIUM ALLOYS SUBJECTED TO ION BEAM TREATMENT (Ar^+, E=30 keV)

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The effect of argon ions with an energy of 30 keV on the structure and properties of the samples (2.5-3 mm thick) of Gr2 and Ti6Al4V titanium alloys being in different initial states were studied in order to investigate the radiation-dynamic effects under ion irradiation and their possible use for the modification of the structure and properties of the titanium alloys.

The samples were irradiated with Ar^+ ions in a continuous mode using an ILM-1 ion implanter, changing the exposure parameters: at ion energy E = 30 keV, ion current density j = 200-500 μA/cm^2, and fluence of $F = 10^{16}$-$2{\cdot}10^{18}$ см$^{-2}$. In the course of irradiation, the sample temperature was controlled with the help of a thin chromel-alumel thermocouple connected with an Advantech Adam 4000 automated system designed for digital signal registration.

It was found that the initial microstructure, which is recrystallized equiaxed grains, retained after irradiation of the annealed alloys under selected conditions; the hardness of the irradiated samples was comparable with that of the initial samples. The effect of ion irradiation using the used modes on the structure and properties of the deformed samples depends on the alloy composition. Thus, in the case of the irradiation of Ti6Al4V alloy samples, the initial fine fiber structure was retained and the hardness remained the same. Irradiation of the deformed Gr2 alloy samples with the initial fine fiber structure reduces its hardness, which is associated with the recrystallization in the entire volume of samples, resulting in the formation of fine equiaxed grains of 5-10 μm in size. Such radiation-induced annealing during ion bombardment occurs during heating of the samples (without holding) to a temperature that is lower by 150-180°C than the conventional annealing temperature of these alloys (680°C) and for a shorter time (9 min instead of 35 min). Thus, the possibility of rapid radiation annealing of the titanium Gr2 alloy with beams of accelerated ions of inert gas at low temperatures was shown.

This work was supported by the Russian Scientific Foundation, project no. 15-19-10054.

ANALYSIS OF THE ROLE OF NANOSIZED DYNAMIC EFFECTS IN THE INITIATION PROCESSES OF LONG-RANGE TYPE UNDER IRRADIATION OF Fe + 8.16 ат % Mn SUPERSATURATED SOLID SOLUTION WITH IONS OF VARIOUS ATOMIC MASSES (Ar^+, Xe^+)

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The atom redistribution and the characteristics of α(bcc) → γ(fcc) structure phase transformation in the volume of the foils of Fe+8.16 at % Mn alloy (30 μm thick) during Ar^+ ion irradiation (E = 20 keV, j = 50-100 μA/cm^2, a projected ion range of <0.003 μm) were studied.

The Cowley parameter of short-range atomic order, the number and composition of the α and γ phases formed during α → γ transition were calculated. The parameters of the hyperfine electric and magnetic interaction of ^{57}Fe nuclei, which illustrate the change in the electronic structure of iron atoms depending on the alloy state, were determined in the various nearest neighborhood of atoms.

The supersaturated (metastable at room temperature) Fe+8.16 at % Mn solid solution decomposition was found to become more intensive as the atomic weight of implanted ions increases. This is the case of both pre-precipitation stage with the formation of short-range atomic order and the stage of the structural α → γ phase transformation.

The comparison of the results obtained for the exposure to the beams of Ar^+ and Xe^+ ions of different masses with previously studied data [1] obtained in the case of light beam exposure of the hardened Fe+8.16 at % Mn alloy (under the same heat conditions) indicates the existence of a nonthermal component in the effect of accelerated ion beams, the role of which increases with the atomic ion mass. The latter is associated with greater energy release density for more massive ions.

This work was supported by the Russian Scientific Foundation, project no. 15-19-10054.

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CHANGE IN THE RELIEF AND PHASE COMPOSITION OF THE $Fe_{72.5}Cu_1Nb_2Mo_{1.5}Si_{14}B_9$ METASTABLE ALLOY UPON NANOCRYSTALLIZATION INDUCED BY ION IRRADIATION

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A number of applications of soft magnetic materials in modern engineering is steadily grow with a need to develop new and effective techniques to control various properties of electrical alloys. Several works [1–3] indicate the enhancement of the atomic and magnetic structures of soft magnetic materials after exposure to accelerated ion beams.

The aim of this work was to study the effect of 30-keV Ar^+ ions on soft magnetic metastable amorphous ribbons prepared by ultrarapid melt quenching of the $Fe_{72.5}Cu_1Nb_2Mo_{1.5}Si_{14}B_9$ alloy.

Ribbons 25 μm thick were irradiated with continuous Ar^+ ion beams (E = 30 keV, j = 300 μA/cm^2, $D = 3.75 \cdot 10^{15}$ cm^{-2}) using a PULSAR-1M ion source based on a glow discharge with a hollow cold cathode [4]. On-line heating of the samples was controlled by a thermocouple. Initial and irradiated samples were annealed in air for an hour in the temperature range 730–840 K.

Structural and phase transformations induced by irradiation and occurring during heat treatment were investigated by X-ray diffraction analysis (on both irradiated and nonirradiated sides) and atomic force microscopy using the change in the surface relief during the transformation from an amorphous state into multiphase noncrystalline one. X-ray diffraction patterns were taken on a D8 Discover diffractometer (Bruker, Germany) in copper radiation (Cu $K_{\alpha1,2}$). The sample surface was examined using a CMM-2000 scanning probe microscope [5] in the atomic-force microscopy mode.

It was found that the Ar^{+} ion irradiation causing short-term heating to 620 K (lower by 150 K than thermal limit of crystallization) results in the complete crystallization of the amorphous alloy (over the entire ribbon thickness) with precipitation of α-Fe(Si) solid solution crystals which are close to $Fe_{80}Si_{20}$ in composition, Fe_3Si stable phase, and metastable hexagonal phase.

Atomic force microscopy demonstrates the transformation of the weakly visible relief of an amorphous structure in a clearly pronounced irradiation-induced grained structure. The grained structure is formed on both irradiated and nonirradiated surface, indicating the crystallization process over the entire volume of the investigated samples, which is also supported by X-ray diffraction analysis.

This work was supported by the Russian Scientific Foundation, project no. 15-19-10054.

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COMPUTER SIMULATION OF ION IMPLANTATION IN THE IRON BASED METAL SYSTEMS

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Ion implantation is widely used in various fields of science as a method of modifying the mechanical properties of the surface layer of a solid, but some questions still remain poorly understood. Study of the formation and accumulation of radiation defects, behavior of interstitial atoms, the effect of surface segregation and the impact of short incoherent sources of elastic waves remain relevant. Their study is a difficult task, since at the room temperature of the radiation defects annealed and the physical state of the material during and after irradiation are different. Therefore, the most interesting results are obtained directly during ion implantation and immediately after its completion. This is possible by computer simulations of ion implantation.

Simulation is performed using the software package LAMMPS [1] and the embedded atom potentials [2, 3] for iron based systems. This makes it possible within the framework of classical MD more accurately describe the nature of the interaction, properties and structure of metals and alloys in comparison with pair interatomic potentials. This provides good quantitative agreement with a wide variety of experimental data and ab initio calculations, including the lattice constant for different temperatures, elastic modulus, the energy of point defects, the melting temperature, energy of the bcc-fcc transfer, density and the structure factor of the liquid phase. The time step was chosen for a variety of energy ion implantation and was 10^{-16} seconds.

In this work, using software LAMMPS package created FeNi system that contains not more than 60000 atoms. We chose a few of Ni atoms to simulate the ion implantation process that is assigned to the speed corresponding to radiation of 10-30 keV energy. Further carried out the system stabilization by relaxation at room temperature. To analyze the structure under study were built radial distribution functions at different times. In the simulation it was found that the formation of various defects in the modeled structure of the sample. Also, there is surface segregation. Calculate the width of the modified layer.

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FRACTAL SURFACE PROPERTIES OF RADIATION-MODIFIED POLYMER MATERIALS

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As a rule, radiation modification of polymer materials is aimed at changing the surface properties of materials [1]. Roughness is one of the main characteristics of the material surface [2], therefore it is essential to study radiation-induced changes of surface roughness of polymers. Currently for analysis of the surface microstructure changes in materials increasingly used the fractal approach [2].

The purpose of this survey consisted in the feasibility of applying a fractal approach to study the possibility of application of fractal approach to explore patterns of change: i) the surface micro-geometry of the Polyethylene Terephthalate (PET) films irradiated by a flux of accelerated xenon ions (or nuclear filters (NF)) and further treated by ozone; ii) the surface roughness of the gamma-irradiated polytetrafluoroethylene (PTFE) powder particles.

i) The changes of the surface microstructure of Xe-irradiated PET films (or nuclear filters (NF)) subjected to the gas and the liquid-phase ozonolysis have been studied by scanning electron (SEM) and atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS) and water wettability. Correlation between the change of the surface fractal dimension value (D_s) and NF surface properties has been found. Direction of modification of the NF surface properties determined by the processing mode: surface hydrophobization is taking place in case of gas-phase ozonolysis; on the contrary, surface hydrofilization occurs during liquid-phase treatment. It is concluded that the nature of detected changes of the NF surface properties is determined by the surface roughness.

ii) The radiation-induced changes of surface roughness of PTFE powder particles (grade F-4

PN 90, GOST 10007-80), gamma-*irradiated* (^{60}Co) in the range of absorbed doses from 10 to 1000 kGy at a dose rate of 15±3 G/s have been studied by means transmission electron microscopy and low-temperature nitrogen adsorption. Correlation between surface roughness changes of the gamma-irradiated PTFE powder particles and D_s value with increasing of the absorbed dose has been observed. It is assumed that the nature of detected correlation is determined by competition between the processes of crystallization and radiation degradation of PTFE.

The present study was conducted with the support of the Ministry of education and science of the Russian Federation (Subsidy to conduct applied scientific researches from October 20, 2014, No. 14.576.21.0053; unique identifier of applied research RFMEFI57614X0053) and the Russian Fund of Basic Researches (project No. 14-07-00025).

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NANOWIRES OF IRON GROUP METALS: FABRICATION BY MATRIX SYNTHESIS TECHNIQUE AND INVESTIGATION OF STRUCTURE AND MAGNETIC PROPERTIES

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Nanowires (NW) of iron group metal alloys (Fe-Ni, Fe-Co) were obtained using matrix synthesis technique based on polymer track matrixes [1]. The problem of suitable matrix for synthesis was discussed- the commercial filtration matrixes [2] are not good for template (matrix) synthesis. The galvanic process was investigated and it was found that it consists of different stages. Deposition of metal inside the pores has non-linear character due to diffusion limitation. The specific features of the next part (formation and growing of the “caps’) were also studied. Electron microscopy, X-rays analysis, Mössbauer spectroscopy and magnetic hysteresis were applied to investigate the dependence of structure and magnetic properties of the NW on electrodeposition conditions. It was found that the composition of two-component NWs differs from the composition of electrolyte and different at different parts of NW. Mössbauer spectroscopy gave possibility to estimate hyperfine parameters for Fe-Co NWs. For Fe-Ni NWs it was supposed that the spectra could be presented as superposition of at least three magnetic sextets with hyperfine parameters B_{hf} 27-33 T. It was shown that Fe-Co samples have “hard magnetic” properties (coercivity more than1000 Oe), while Fe-Ni samples have “soft magnetic” parameters (coercivity less than 100 Oe). The dependence of these parameters on the synthesis conditions was demonstrated.

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RADIATION STABILITY OF METAL NANOWIRES

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The aim of this work is to investigate the radiation stability of pure nickel and iron–nickel $Fe_{0.56}Ni_{0.44}$ alloy nanowires fabricated by matrix synthesis using polymer track membranes and Ar^+ and Xe^+ -beam irradiation. It is known that the stability of nanowires must be different from the stability of corresponding bulk material [1]. The dependence of the stability of nanowires on their diameter, fluence, and type of implanted ions is investigated. As a result, the study showed that under both Ar^+ and Xe^+ ion irradiation conditions (E = 20 keV, j = 300 μA/cm^2, fluences of 10^{16}-10^{18} cm^{-2}), NWs are deformed and melted even upon slight general (not local) beam heating (to 150°C). The effect of Xe^+ ion irradiation is more pronounced. The conclusion about the low radiation stability of the NWs under used Ar^+ and Xe^+ ion irradiation conditions can be drawn. As an explanation for the observed effect of melting of NW arrays at decreased temperatures we propose to consider the formation of thermal spikes under ion irradiation. The assumption that the thermalized regions of dense cascades of atomic displacements (thermal spikes) play an important role in the nanowire structure change is made. These regions are nanosized zones of explosive energy release and heated to several thousands of degrees.

We thank V.V. Artemov (Institute of Crystallography of RAS) for the electron microscopy studies.

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STRUCTURE-PHASE FEATURES TO A DEPTH OF NITRIDED LAYER OF AUSTENITIC ALLOYS SUBJECTED TO FRICTION STIR PROCESSING AFTER ION-PLASMA SPUTTERING

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As a method for surface modification to improve the functional properties of steels and alloys are widely used ion-plasma (SP) coating and, in particular, nitriding. In nitrided ion-plasma method of austenitic alloys Fe-12Cr-30Ni and Fe-15Cr-38Ni using dry sliding friction and shear pressure in the anvils of Bridgman implemented an increase in the depth (5 to 20 μm) with gradient of concentration and the phase composition of the surface. The basis of the processing based on the phase of cyclic deformation-induced transitions "dissolution-release" nitrides of chromium. The result of nitriding at 500 C, 1 h in the surface layer of the alloy formed by the solution of nitrogen in the matrix of Fe-Cr-Ni-N and particulate chromium nitrides CrN and Fe4N iron. Subsequent dry sliding friction or shearing under pressure lead to the nanostructuring, the deformation dissolution of iron nitrides and chromium, as well as mechanical alloying of surface and internal, not susceptible to nitriding, layers of alloy. In addition, in the deformed matrix of austenite formed secondary chromium nitrides Cr2N. Additional annealing at 600 C, 2 h. there is additional release of nitrogen austenitic Fe-Cr-Ni-N solid solution with tendency to formation of nitride Cr2N and increase volume (depth) is changed according to the composition and the structure of the matrix alloy. The reverse sequence, namely, the preliminary friction effects and the subsequent nitriding of the surface do not give a noticeable increase in the depth of the nitrided layer. This is due the accelerated migration of nonequilibrium grain boundaries in the nanostructured surface friction, leading to complete recrystallization for a time much shorter than the time of nitriding for 1 h. the at 500 C. the Result of fast recrystallization is little effect of the rapid diffusion in nanostructured friction surface.

The work is executed at financial support of RFBR (project № 15-08-07947) and grant of UB RAS (No. 15-9-12-45).

STUDY OF THE EFFECT OF ION IMPLANTATION OF ARGON IONS ON THE CORROSION RESISTANCE OF HIGH-CHROMIUM STEEL 30Ch13

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Chromium steels are widely used in various fields of technology. However, their significant drawback is the susceptibility to local corrosion. Therefore, there remains the question of finding new methods of improving the corrosion resistance of high-alloyed steels. The aim of our work was to study the effect of implantation of argon ions on the physic-chemical structure and corrosion behavior of high-chromium steel.

The object of the research is steel of grade 30X13. Previously there was heat treatment of steel – annealing in a protective atmosphere at a temperature of 900°C with air cooling. Then carried out the mechanical processing of samples grinding and polishing paste GOI to roughness of R_a=0.02 μm (13th class of roughness). After polishing, the samples were subjected to irradiation by argon ions with energy of 30 Kev and the following doses: 10^{16} ion/cm^2 (sample No. 1), 5*10^{16} ion/cm^2 (sample No. 3), 10^{17} ion/cm^2 (sample No. 5). Processing was carried out on the original ion-beam installation PION – 1M ultra-high vacuum on the basis of fasting USU–4. Surface topography of samples as the original (without irradiation) and after ion implantation were examined by AFM on the device SOLVER-P47PRO. The microhardness measurements were carried out on the device PMT-3M with a load of 10 g and aged 8 C. the Chemical structure of the sample surface was studied by XPS on the device ES-2401 with layer-by-layer etching with argon ions to a depth of 20 nm. Polarization measurements were performed in a potentiometric mode on the potentiostat P-30. As corrosive media were selected borate buffer solution with pH=7.4 with the addition of 0.01 M K_2SO_4.

As a result of researches it is established that the physical and chemical structure of samples and their corrosion behavior change irregularly with increase in irradiation dose. The microhardness of the initial sample coincides with the microhardness of sample No. 3 within measurement errors, while the hardness of samples No. 1 and No. 5 was lower by ~49%. XPS data indicate that after ion implantation increases the concentration of carbon and oxygen and the change in the chemical state of all elements in the deeper layers of the material compared to non-irradiated sample. On anodic polarization curves maximum currents observed for sample No. 5, the minimum for sample No. 3, the values for the original sample and sample No. 1 occupies an intermediate position. The results of AFM show that corrosive destruction of the surface of the original sample passed more intense than the samples after ion implantation. Also in the image of the AFM significantly, which changed the nature of corrosion damage. The source model is a uniform deep pitting, and the surface of the samples after ion implantation has been allegedly pitting. Depth of ulcers about 20 nm, they are located Islands on the sample surface.

The proposed mechanism of the processes explains the observed phenomena.

SURFACE SEGREGATION AND CHANGES IN THE STRUCTURE IN AMORPHOUS MATERIALS UNDER ION IRRADIATION

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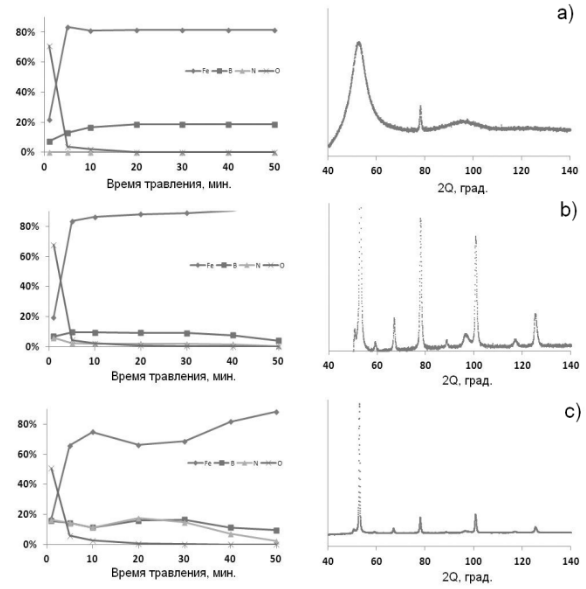
One of the important fundamental and applied research trends is the question concerning the thermal stability of the amorphous alloys. In this connection it is useful to analyze the structure and segregation processes, especially at the early stages of crystallization, since the crystallization of amorphous alloys proceeds through a sequence of metastable states, and the properties of the alloy are changed drastically, so we can speak of two different materials with the same chemical composition. This raises the problem how to control the crystallization process in order to use it as a method of creating the new materials. The work concerns the investigation of structural and compositional evolution laws with respect to the surface layers of amorphous ion-beam treated iron-based alloys. It has been shown that structural changes of the amorphous phase and the crystals at the surface of the amorphous alloy depend not only on the exposure parameters - the dose and the energy of ions, but also on the type of the implanted ions.

Result of ion bombardment is the breakdown of the amorphous phase with the allocation of a set of metastable phases, the speed and number of new phases depends on parameters of irradiation and the type of the irradiated ions. In this case it is important that the heating-up temperature of the target practically does not depend on the type of ions, and is determined by the current density and the energy of the primary atoms. Crystallization in ion implantation takes place at lower temperatures than in the case of thermal crystallization. From this we can conclude that the decisive role in the processes of diffusion and phase formation play the microscopic mechanisms of the atomic-atom collisions cascades development. Comparing the results of X-ray analysis and compositional analysis data of the surficial region, it can be assumed that there is active formation of metastable phases at the surface layers as a result of radiation, and the composition of the phases varies depending on irradiation parameters.



The distribution of the alloy components $Fe_{82}B_{18}$ in the surface layer after irradiation by ions of nitrogen: a) initial; b) D = 10^{16} ion/cm^2; c) D = 10^{17} ion/cm^2

THE CHEMICAL COMPOSITION OF THE SURFACE LAYERS OF TITANIUM FOIL WITH A DEPOSITED LAYER OF ALUMINUM, AFTER MIXING BY ARGON IONS

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Methods of ion-beam and ion-plasma processing, having a number of fundamental advantages compared to traditional methods of chemical-thermal treatment, received active development in the field of modification of surface layers of metals and alloys with the aim of improving their strength properties [1, 2]. In addition to the classical advantages of ion treatment (the possibility of exceeding the solubility limit, control of the depth of impurity, the possibility of selective processing of parts of details, etc.) in the last decade managed to add completely new methods of influencing on the near-surface layers of materials [3, 4]. In particular, by forming on the surface of the target, one or more layers of other materials nanometer-scale thicknesses, and their subsequent ion processing of high-energy particles, able to form new compounds and phases in the surface layers. The thus obtained surface layers can acquire a different from the "parent" tensile strength, yield strength, impact strength, fracture toughness, corrosion resistance, and wear resistance [5]. Additionally, the combination of the coating process with the ion treatment allows you to vary the thickness of the modified layer, which then allows you to change its physical, mechanical and performance properties in a range of values[6].

The aim of this work was to study the influence of irradiation by argon ions on the formation of the composition and structure of the surface layers of commercial titanium VT1-0 sputtered Al layer.

A study by XPS showed that the mixing is accompanied by the formation of compounds of titanium with aluminum Ti-Al. Revealed the formation of bonds Ti-C, after the deposition of a film of aluminum, and after ion-beam mixing. Identified the sequence of formation of bonds of Al-O to Ti-O with increasing depth of the surface layer, after the deposition of a film of aluminum, and after ion-beam mixing.

The work was supported by the fundamental research program of UrB RAS, project No. 15-17-2-50

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THE FORMATION OF NANOSIZED LAYERS ON THE COPPER-NICKEL ALLOY SURFACE BY IMPLANTATION O^+ IONS

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Formation of chemical and phase compositions, atomic and local atomic structures of surface layers of metallic materials, including nanoscale, with improved mechanical and exploitation properties by different physical or chemical methods, in particular by ion implantation, to be one of the directions of modern science and technology [1-2]. The processes of forming these layers, the structural mechanisms for their implementation and the nature of change of various properties of metals and alloys by ion irradiation still remain unclear despite the research in this field.

The aim of this work is a comparative study of the formation of the composition and chemical structure of nanosized surface layers of copper-nickel $Cu_{50}Ni_{50}$ alloy by implantation O^+, Ar^+ ions and sequential implantation Ar^+ and O^+ ions in the pulse-periodic regimes. The choice of copper-nickel alloy was determined to view as a model alloy. The copper-nickel alloys find wide application in various branches of modern industry, particularly, in shipbuilding [3]. The implanted ions were selected to be the elements chemical and inert nature, respectively.

The accumulation of oxygen atoms in the nanoscale surface layers of copper-nickel alloy after implantation O^+ ions has been identified in the paper. The accumulation of oxygen atoms accompany by the simultaneous segregation of nickel atoms and formation of NiO nickel oxide. The implantation by Ar^+ ions lead to the enrichment near-surface layers of copper atoms and the depletion of nickel atoms. It has been shown that segregated to the near-surface layers of copper atoms under the conditions of implantation Ar^+ ions prevent the accumulation of oxygen atoms in near-surface layers by a subsequent implantation O^+ ions, what is determined by a weak chemical activity of the oxygen atoms to the copper atoms.

This study was supported by the grant of RFBR (№ 16-43-180765).

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THE INFLUENCE OF THE FOCUSED PULSE LASER RADIATIONS ON THE PHYSICAL-CHEMICAL STRUCTURE AND MICROHARDNESS AMORPHOUS $F_{E}S_{I6}B_{16}$ ALLOY

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Amorphous metal alloys thanks to the properties draw attention of researchers long ago. Interest in them is connected with their possibility of a unique combination of such properties as magnetic, electric, mechanical, strength, etc. unattainable for crystal materials. It does them perspective in use in many industries [1,2]. But at the same time it should be noted that the amorphous condition is a nonequilibrium condition. Under the influence of temperatures or long-term storage in them there can be a disintegration of an amorphous phase to loss of properties. Therefore the research of behavior of such materials under thermal impact is of scientific and practical interest. To one of methods of such thermal impact can serve laser handling of materials. Laser handling provides local impact on material in case of which it is possible regulating to achieve operating modes of the laser machine such conditions of impact of the laser which will allow to change only structure and properties of a blanket of material and not to mention its inside layers. It in turn gives the chance of creation of materials with the specific modified superficial properties [3-5]. It is important to note that laser impact is urgent for handling of fragile materials and materials of small thickness (tapes, foils or thin plates). However it is necessary to consider that such impact is high-energy that in case of the pulse mode for a short period in case of energy absorption various processes may happen material: high-speed heating, current and evaporation of material, hardening of a surface, phase transitions, etc. For an amorphous condition of material it can lead to redistribution of elements of system or to partial or complete crystallization of alloy or final fracture of the irradiated object. Therefore, studying the happening processes in amorphous alloy under the influence of the laser, it will be possible to determine the modes of handling and mechanisms of forming of the necessary properties of the studied alloy required for conditions of its operation.

In work results of a research of influence of pulse laser radiation on change of topography, structure, structure and microhardness of amorphous metal $FeSi_6B_{16}$ alloy are provided.

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VI. Facilities and techniques of experiment

The Seminar Program traditionally includes a methodological section. Its purpose is to acquaint the attendees with the latest methodological developments in the sphere of radiation physics and radiation material science, and inform them about new radiation sources and application of the new methods for condensed matter investigation.

ATOM PROBE TOMOGRAPHY DATA PROCESSING METHODS DEVELOPMENT FOR NANOSCALE STRUCTURAL PHASE FEATURES CHARACTERIZATION

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The modern development of the perspective materials means a control over structural phase features on the nanoscale. Atom probe tomography (APT) is the most dynamic developing method for the analysis on the atomic scales. This method based on the process of material evaporation, atom by atom and detecting all of them by the position sensitive detector which is the mass-spectrometer in the same time. Therefore APT can construct the 3D atom maps and identify chemical nature almost of all atoms contained in the material. Further analysis of the atom map can detect and characterize features of the structural phase state in the material.

The task of searching and describe of studying features can be solved by methods of statistic process of the atom probe data, such as cluster analysis, pair-correlation method, frequency distribution analysis, linear and radial concentration profiles and proxygramm. The results obtained during the processing of data can to describe the amount, chemical composition and dimensions of features, and build concentration profile of interfaces.

In this paper the main trend of development of atom probe data processing methods, which are used in the ITEPh is described. Originally, the first set of tools was enough for the characterization of clusters and large interphase boundaries in a small volume of data (~10×10×500 nm^3) collected atom probe ECOTAP in the mid-2000s. Solution of such task was performed by analysis of homogeneous of the solid solution with frequency distribution method, pair-correlation method and using by the basic algorithm of the cluster searching. Atom probe prototype with laser evaporation APPLE-3D designed in ITEP in 2015 has increased the amount of data acquisition in the several tens of times, which led to a significant increase in the amount of species, size and complexity of the research objects. Thus, there was the task of improving the analytical tools to describe the more complex nanoscale features in materials. This paper presents the realized and planned to realization data processing methods, such as nearest neighbor algorithm envelop and erosion, which specifying the form of clusters, and construction of iso-surfaces and proxygramm. Features of application of different atom probe data processing methods will be demonstrated by the example a large number of experiments on the study of nanostructured multicomponent alloys.

COMPRESSIBILITY AND PHASE TRANSITION IN E635 ZIRCONIUM ALLOY UNDER STATIC LOADING

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E635 zirconium alloy (Zr – Nb 1% - Sn 1.2% - Fe 0.35%, % wt) is a promising material for fuel-element jackets. Calculations of the material behavior under high pressures and temperatures, as well as prediction of its behavior in severe operating conditions and probable emergency environments shall consider the α-ω phase transition.

This paper presents results of diffraction measurements on E635 zirconium alloy within the normal and 11 GPa pressure at the room temperature. Measurements were taken in the Mo-Kα radiation using the X-ray diffractometer with the *Imaging Plate* two-axis detector. The *Boehler-Almax* diamond anvil cell was used for the sample compaction.

The experiment demonstrated that in the alloy, α-, and ω-modifications of zirconium coexist in different volumetric proportions in the pressure range from 6.9±0.3 up to 10.9±0.3 GPa (Fig.1).

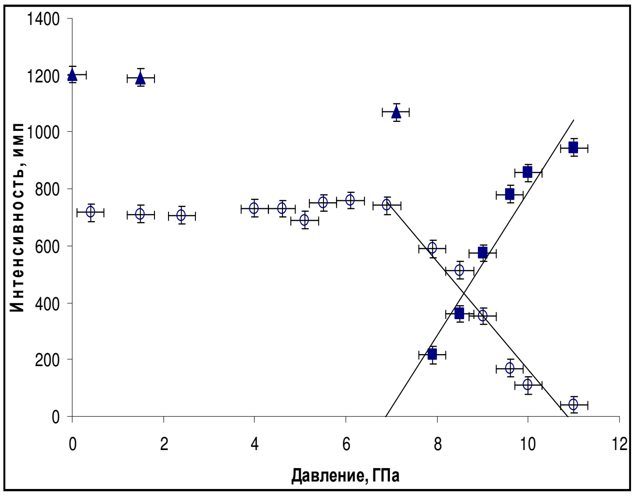

Fig.1. Intensity of Zr α-, and ω-phase peaks with the pressure increase (α – circle, ω-square) and decrease (ω – triangle).

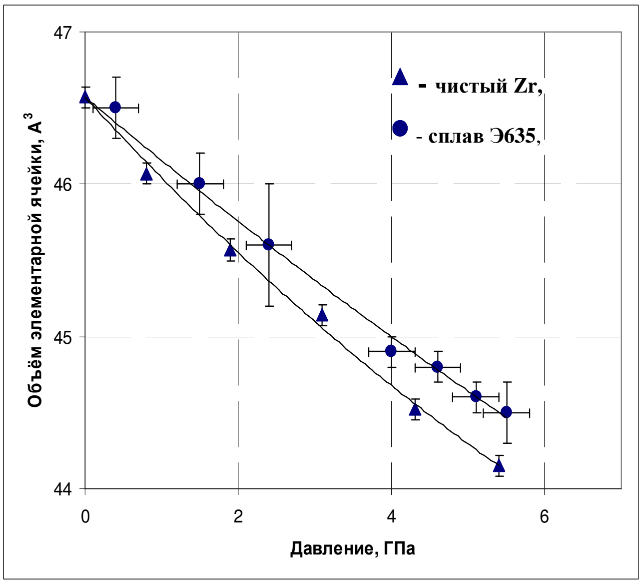

Fig.2. Volume of the α-phase elementary cell in E635 alloy versus pressure (circles).

In E635 alloy, pressure that initiates the α→ω phase transition under the static volumetric compression turns out to be higher compared to pure zirconium. When pressure drops to the normal one, no reverse ω→α transition is observed to take place in E635 alloy just like in pure zirconium.

Parameters of the ω-phase lattice under normal pressure are determined. During the α→ω transition, loss of volume per one atom is 1%. In E635 alloy, the isothermal bulk modulus uder normal conditions for the α-phase is approximately by 15% greater than that obtained for pure zirconium.

DESIGN OF ATOM PROBE TOMOGRAPHY WITH LASER EVAPORATION FOR STEEL AND ALLOY NANO-SCALE RESEARCH.

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The advanced development of perspective materials and devices increasingly required the controlling the state of material on nanometer scale. The atom-probe tomography is quite new and rapidly developing method of materials research on the nano- and even atomic scale, with reconstructing the arrangement of atoms in the bulk of the material at simultaneous determining their chemical nature. This method is based on atom-by-atom specimen “disassembling” and projection magnification, previously used in the field ion microscopy and time of flight mass spectrometry applied to each vaporized ion.

Currently atom probe tomography, along with pulse-field evaporation specimen ions become widespread laser evaporation. Application of lasers in atomic-probe tomography allows to study not only metals, but also semiconductors and dielectrics. With the introduction of new types of detection systems and geometries of the evaporation of ions, it was possible to increase significantly the volume of the useful data.

This paper presents the results of the development, assembling and launch Atom Probe-tomography Prototype with femtosecond Laser evaporation and a position-sensitive detector base on delay lines for tomographic (3D) analysis of the materials chemical composition (hereinafter APPLE 3D). Application of laser evaporation can significantly extend the range of the materials from steel to glass. The ability to resolve of the probe is 1-2 Å in depth and lateral resolution of about 3 Å. Maximum mass resolution at half maximum of the peak is 1000. In this paper we illustrate the steps of development installation, as well as the demonstration the ability to study materials with nano- and micro-features.

DETERMINATION OF PHOTOSTIMULATION PARAMETERS AND TESTING OF HIGH-DOSE PTTL-METHOD USING TLD-500K DETECTORS

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Currently, wide application of high-power ionizing radiation sources entails intensive development of the high-dose dosimetry. When registering the thermoluminescence (TL) signal from a heavily irradiated detector, the thermoluminescence-curve peaks containing information on the absorbed dose in the material are registered in the high-temperature (up to 700°C) range. Deep traps existing in the detector material are responsible for these peaks. Within the above range, we observe effects that interfere with the qualitative measurement of the signal from the detector, i.e. thermal background, destruction of the detector’s original structure, etc. This is the problem that should be resolved through improvement of the existing TL-signal registration methods. A possible approach is application of the phototransfer thermoluminescence method (PTTL-method).

This paper aims to determine the effective photostimulation parameters and to test the high-dose PTTL-method using TLD-500K detectors.

This paper investigates standard TLD-500K thermoluminescent detectors based on nominally pure anion-defected α-Al_2O_3 monocrystals. The samples were exposed to doses from the ^{60}Co gamma-radiation source in the range from 100 Gy to 20 kGy. Blue light-emitting diods (λ=470 nm) were used for photostimulation. The experimental facility of the department “Physical methods and non-destructive testing instrumentation” at the Ural Federal University, Yekaterinburg, was used for PTTL-measurements.

In the case of luminescence photostimulation, it is necessary to take into account the ratio between two simultaneous and competing processes, i.e. charges transition from deep traps of the material into shallower ones and simultaneous empting of the traps under exposure to light. As a result, the effective photoluminescence modes for the irradiated TLD-500K detectors were determined, i.e. current through the light-emitting diods (300 mA) and stimulation time (15 seconds). With these parameters, PTTL of the irradiated samples has two peaks in the field of not-too-high temperatures (200 and 300^{o}C, respectively).

For both PTTL-peaks, dose characteristics are observed to be close to the linear ones. Thus, our experiments demonstrated the PTTL-method to be promising for high-dose measurements using TLD-500K detectors.

DIFFUSE X-RAY SCATTERING ON HEXAGONAL LATTICE OF COBALT

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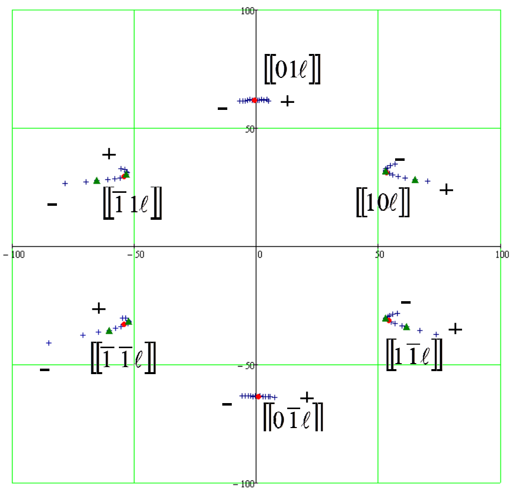
The theory relying on the coherently oscillating macro-objects existing in ideal single-crystals allowed patterns of diffuse scattering on bcc single-crystals of pure metals to be calculated [1,2]. These patterns are noted to give good description of observed distributions [2,3]. Phase transition from bcc to hcp structure is observed to take place with the temperature decrease, though a group of coherently oscillating planes stays on in the low-temperature lattice and this causes a set of luminous rods going through the nodes of the reciprocal lattice to arise in the reciprocal space.

Mono-Laue measurements with a rotating sample (Fig. 1) experimentally confirm existence, in the reciprocal space of the hexagonal lattice of cobalt, of luminous rods induced by coherently oscillating planes being parallel to the base plane. Intensity distribution along a rod between nodes of the reciprocal lattice is obtained (Fig. 2). Along the entire rod, the intensity is recorded to be essentially higher than the background and also to monotonously decrease with the distance from the reciprocal lattice nodes. Intensity maxima width is recorded to be different near the reciprocal lattice nodes due to the different brightness of reciprocal lattice nodes. Brightness depends on the geometrical structure factor of an appropriate set of planes in the straight space. Geometrical structure factors are noted to strongly influence intensity in an experiment and thus they shall be taken into account.



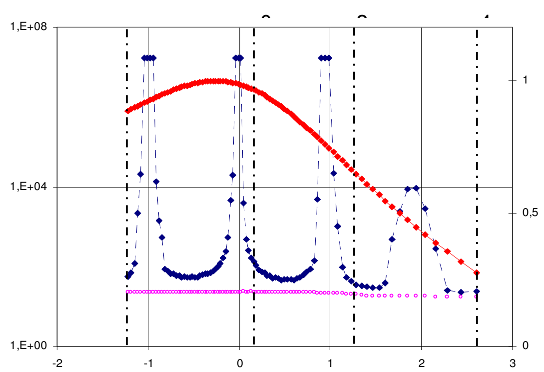


Figure 1. Motion of reflexes on the detector during the sample rotation.

Figure 2. Intensity variation along the rod $[[10\ell]]$.

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POSSIBILITIES OF NEUTRON DIFFRACTION STUDIES OF REACTOR STRUCTURAL MATERIALS AT THE NEUTRON MATERIAL SCIENCE COMPLEX OF THE IMP UB RAS AT THE IVV-2M RESEARCH REACTOR

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The Institute of Metal Physics UB RAS has designed The Neutron Material Science Complex (NMSC) at the research nuclear reactor IVV-2M, which is now on the list of class-1 Unique Scientific Installations in Russia. Nowadays, NMSC is the only Russian scientific center where high radioactive materials are studied by the neutron diffraction methods, including industrial functional materials. In particular, in recent years we have carried out systematic studies of radiation-induced phenomena in austenitic steels used as a basic material for production of fuel pin claddings for fast reactors. Neutron diffraction methods are quite high-effective tool to trace evolution of the materials microstructure under neutron irradiation, including phase composition of micro-precipitations, texture, grain size, state of their boundaries, etc. At the NMSC, the neutron diffraction methods are supplemented by the possibilities to also carry out the X-Ray structure analysis of samples and study of their magnetic properties. In the nearest future, we'll put into operation a Mossbauer spectrometer.

It should be noted that studies of materials of the real pin claddings after their exploitation in the fast reactor are the matter of especial interest. In Zarechny-city there exists a unique combination of facilities for such an activity. First, in the nearest neighborhood with the Beloyarsk Nuclear Power Plant (BNPP) the Institute of Nuclear Materials (INM) is situated which is equipped for preparation of samples from the fuel pins after their exploitation in BN-reactors and also for studies of their physic-mechanical properties and electron microscopic studies. Second, our Neutron Material Science Complex is situated and functions on the INM territory. Experience of long-term cooperation of BNPP, INP and IMP UB RAS and consolidation of their facilities allow one to provide systematic complex studies of the radiation-induced effects in the materials of the pin claddings of the BNPP fast reactors.

In recent years, we have already obtained new data on the processes occurring in the real reactor steels under neutron irradiation and in the model alloys depending on their content, doping and production technology. There have been revealed the existence of competition processes evolving in the microstructure of these materials and the influence of the irradiation conditions on them.

Besides, we have gained significant experience of studying radiation defects and influence of neutron irradiation on the properties of different superconductors and magnets.

Detailed review of our activity see at the IMP UB RAS site:

http://imp.uran.ru/?q=ru/content/neytronnyy-materialovedcheskiy-kompleks-instituta-fiziki-metallov-uro-ran-na

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REEXAMINATION OF ION IRRADIATION AS A CREDIBLE TOOL TO SIMULATE NEUTRON-INDUCED VOID SWELLING

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Unavailability of high-flux test reactors requires that ion irradiation serve as a surrogate for investigating factors that lead to swelling resistance of improved alloys. Most current studies are directed toward lower-swelling ferritic-martensitic alloys and their ODS variants. The credibility of using charged particle simulation requires that the impact of all neutron-atypical features of ion irradiation be identified, understood and minimized.

In order to demonstrate that ion irradiation is a credible tool, it is required that self-ion irradiation reproduce major aspects of neutron-induced swelling dependencies (compositional, fabricational, flux-spectral) observed in neutron tests. Ion irradiation should also reproduce the swelling behavior (bilinear, steady-state after incubation), but should especially reproduce the well-established post-transient swelling rates of 1%/dpa for fcc iron-base and 0.2%/dpa for bcc iron-base alloys.

While recent studies show very clearly the bilinear swelling behavior of ferritic-martensitic alloys with a post-transient swelling rate of 0.2%/dpa, most studies on austenitic alloy were conducted in the 1970s-1990s, but these did not show the expected 1%/dpa for fcc iron-base alloys. Many earlier studies, especially for simple metals and fcc iron-base alloys, are reexamined in light of recently attained insights and current calculational practices. The results of this reexamination are very encouraging, attesting to the credible use of ion simulation for void swelling.

It is shown that dpa calculational codes (EDEP, BRICE, IONDOSE, early versions of TRIM) used in earlier studies overestimated energy deposition rates by ~20 -35%, leading to artificially high dpa levels and an incorrect visualization of swelling vs. depth. When these earlier data sets are reevaluated using the SRIM code, the 1%/dpa is indeed routinely observed. Additionally, injected-interstitial suppression of void nucleation, not clearly observed in these earlier studies, is equally strong in both bcc and fcc iron-base alloys. Previous theoretical treatments did not predict this latter result.

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