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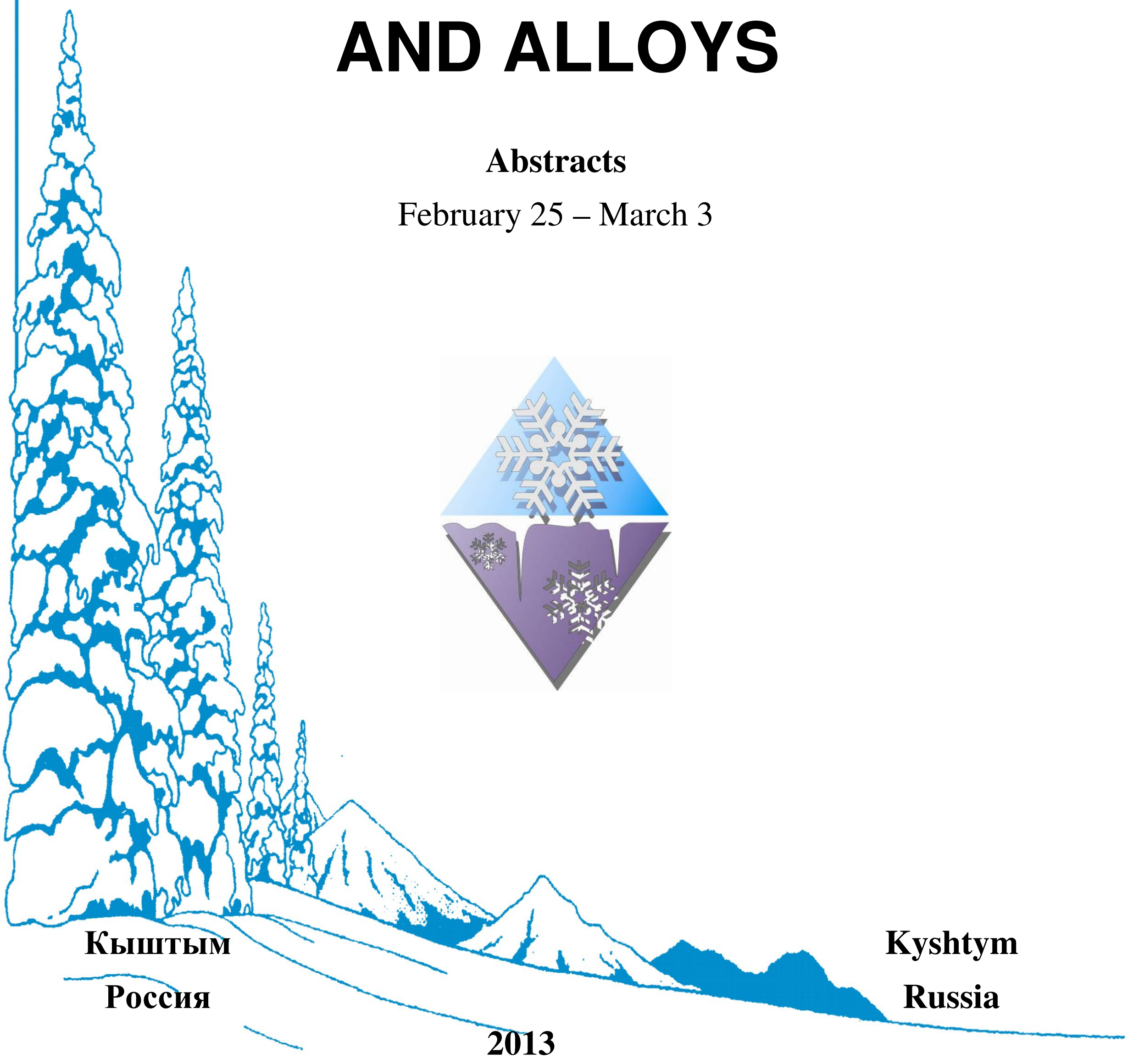
RADIATION DAMAGE PHYSICS OF METALS AND ALLOYS

Abstracts

February 25 – March 3



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Compiled by
Denis Perminov

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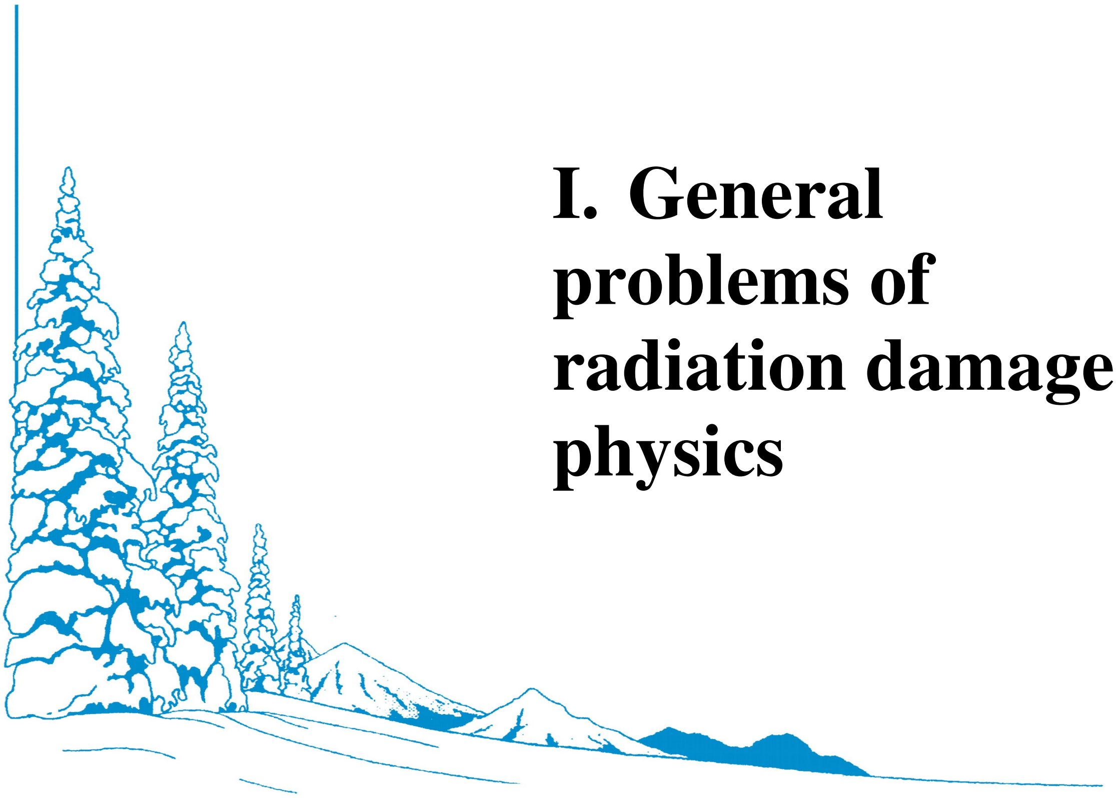
I. General problems of radiation damage physics



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.

RADIATION-INDUCED PROCESSES IN Fe-Ni-Ti ALLOYS WITH DIFFERENT MICROSTRUCTURES DURING ELECTRON AND NEUTRON IRRADIATION

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Investigations of thermal and radiation aging of austenitic stainless steels and precipitation-hardening model alloys is important because of the precipitates depend many macroscopic characteristics, such as mechanical properties, radiation vacancy swelling, etc. The alloy Fe-35Ni-3Ti, model alloys for austenitic stainless steels, in the quenched state is a supersaturated solid solution and aging it stands ordered γ'- phase, similar in composition to Ni_3Ti, which has a lattice parameter close to the matrix and coherently related. This makes it difficult to study using standard techniques in the early stages of the formation of the new phase when the size of the precipitates is not more than a few nanometers.

It presents the results of the study of radiation-induced structural and phase changes in the Fe-34,7at.% Ni-2,6at.% Ti, prepared by vacuum induction melting of pure components, by methods of residual resistivity, electron microscopy, X-ray diffraction and scanning tunneling microscopy. Alloys for research were taken in a state quenched from 1373 K in water, in a plastically deformed state, in a state that has only dislocation sinks by annealing at 573 K after deformation and in the aged state at 923 K after quenching condition. Alloy samples were irradiated (5MeV) to a fluence of $5{\cdot}10^{18}$ cm^{-2} and fast neutrons (E> 0.1 MeV) to a fluence of 10^{20} cm^{-2} at temperatures 300-340 K and annealed in irradiated and unirradiated states at different temperatures in the atmosphere of purified helium.

In these alloys with different initial microstructure during electron irradiation and at low fluence neutron irradiation to $5x10^{18}$cm^{-2} the process of intermetallic precipitates formation prevalent type Ni_3Ti. At higher neutron fluence up to $5x10^{19}$ cm^{-2} and above, disperse γ'-particles Ni_3Ti, dissolve in displacement cascades, and grow as competing processes, the balance between them depends on the temperature and the intensity of neutron irradiation. Under electron irradiation at 300 K as in the quenched and in the aged alloy is formed precipitates from 2 to 5 nm, with a concentration at $2x10^{17}$ cm^{-3}. With isochronous annealing of irradiated alloys are fine precipitates coalesced from 500 K. At 1000 K, as in quenched and in aged alloys it is presented only large precipitates size of 12-15 nm and a density over $5x10^{16}$cm^{-3}. The formation of intermetallic precipitates is confirmed radiation hardening. It is discussed the effect of the dislocation microstructure and vacancy clusters in radiation-induced structural phase processes

The work was done within RAS Program (project № 0120106436), with partial support of Russian Foundation for Basic Research (grant № 11-03-00018 and grant № 11-02-00224) and Ural Division of RAS (grant № 12-23-2031)

RADIATION AND THERMAL INDUCED PROCESSES IN THE Fe-Ni-Si ALLOYS WITH DIFFERENT MICROSTRUCTURES

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It presents the results of the study of structural and phase changes by the residual electrical resistivity under the deformation and electron (5Mev) irradiation in invar alloy Fe - 34,7at. % Ni (Fe-Ni), and Fe - 32,1at. %Ni - 5,7 at. %Si (Fe-Ni-Si), prepared by vacuum induction melting of the pure components. Alloys for research were taken in a state quenched from 1373 K in water, in a plastically deformed state (ε ~ 40%), in a state that has only dislocation sinks by annealing at 573 K after deformation as well as in the aged at 723-823 K after quenching condition. Since even quenching by a water-cooled drum in this alloy can not get the state of the silicon completely in solid solution, in this paper, it is understood that all of the experiments is only part of silicon in solid solution, while the other part of the silicon is in the form second phases of the Ni_3Si.

It is shown that the plastic deformation of the quenched alloy, lead to decreases the in electrical resistivity below the initial level. It is associated with the dissolution of the particles of intermetallic precipitates, which remained after quenching. Irradiation near room temperature, on the contrary, leads to an increase in electrical resistivity due to the migration of point defects formed during irradiation and, consequently, to the decomposition of solid solution with the formation and growth of intermetallic precipitates. In addition, the deformation and the irradiation above 240 K, leeds to the formation of vacancy clusters. Upon annealing in the 350-500 K, as well as for other invar alloys based on Fe-Ni, the dissociation of vacancy clusters formed by irradiation as well as formed by the deformation occurs, which leads to the continuation of a solid solution decomposition with the formation and growth of intermetallic precipitates.

The presence of the dislocation microstructure reduces the decomposition of solid solution by reducing the length of the migration of point defects. Thermal diffusion starts above 600 K and provides the further decomposition of the solid solution ap to 700 K. Above of this temperature, the reverse is true - the dissolution of intermetallic compounds in accordance with the equilibrium phase diagram.

The work was done within RAS Program (project № 0120106436), with partial support of Russian Foundation for Basic Research (grant № 11-03-00018)

EFFECT OF INTERSTITIAL IMPURITIES ON THE EVOLUTION OF VACANCY-TYPE DEFECTS IN NEUTRON-IRRADIATED NICKEL

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Ni-base alloys have been proposed for various in-core applications in Generation IV reactor system, because of their superior high temperature strength and corrosion properties. However, irradiation damage data for these alloys either limited or non-existent. The displacement damage in metals takes place in the form of cascades during irradiation with neutrons [1]. Vacancy clusters and self-interstitial atom (SIA) clusters are directly formed in displacement cascades.

Residual interstitial impurities could be one of the responsible factors which control a formation of the primary and secondary vacancy clusters under neutron-irradiation [2].

It is well known that positrons are a sensitive probe of vacancy-type defects, with sensitivity starting from the atomic size to large vacancy clusters and nanovoids, whereas they are insensitive to interstitial atoms and their small agglomerates.

In the present work, in order to investigate the effect of impurities on vacancy defect evolution in nickel, specimens with high (5N) and technical (3N) purity were neutron-irradiated at ~ 330 K in the IVV-2M reactor (Russia) to fluencies in the range of $1x10^{21} – 1x10^{23}$ n/m^2 ($E >$ 0.1 MeV) corresponding to displacement dose levels in the range of about 0.0001 – 0.01 dpa and subsequently stepwise annealed to about 900 K. The specimens of Ni with different purities were characterized both in as-irradiated state as well as after post-irradiation annealing by positron annihilation spectroscopy. The formation of three-dimensional vacancy clusters (3D-VCs) in cascades was observed under neutron irradiation [3]. The density and size of 3D-VCs depended not only on dose level, but also on purity. The population of 3D-VCs in the technical Ni is lower than that in the high-purity Ni. 3D-VCs collapse into secondary-type clusters (stacking fault tetrahedra (SFTs), and vacancy loops) during stepwise annealing at 350 – 450 K (stage III in Ni). The suppression of secondary cluster formation in 3N Ni is attributed to an effective vacancy interaction with impurity carbon atoms, which based on a relatively large vacancy-carbon atom binding energy (0.32 - 0.35 eV). The trapping of vacancies released at the collapse of 3D-VCs by the interstitial impurity atoms dominates at low irradiation dose level (10^{-4} dpa). Thus, we found that carbon impurity atoms have strong effects both on the primary vacancy-type defect aggregation, and on the secondary vacancy clusters and complexes formation.

This study was done within RAS Program (Project No. 01.2.006 13394) with partial support of Russian Foundation for Basic Research (Project No 11-02-00224-a), Ural Branch RAS (Project No. 11-2-21 YaTs) and The Ministry of education and science of the Russian Federation (Contract No. 16.518.11.7032).

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EFFECT OF Si ATOM CONCENTRATION ON FORMATION OF VACANCY COMPLEXES IN ELECTRON-IRRADIATED Fe-Cr ALLOYS

Anatoly P. Druzhkov and Alexander L. Nikolaev
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Understanding the effect of solute atoms on microstructural evolution is important for developing nuclear reactor materials. Solute atoms may capture mobile point defects thus affecting their migration, recombination and clustering. Therefore, the binding energy is one of the key parameters, which determines the effect of solute atoms on microstructural evolution.

A traditional simplified approach to accounting for the effect of solutes is the following. The interaction between point defects and solute atoms is investigated in a course of annealing after low temperature irradiation in model systems doped with 100-500 at ppm of solute. The obtained values of binding energy are used then in model calculations of radiation damage in commercial steels, which are doped with solutes at a level of 1 at %. It is assumed by default in this scheme that a value of binding energy obtained at 100-500 at ppm of solute stays the same if a doping level is increased up to ~10000 at ppm (~1 at %). The aim of our study was to understand to what extent this assumption stays valid.

We have investigated the effect of Si addition in the range of 0.2-1.5 at % in Fe-16Cr alloy on accumulation of point defects after irradiation with 5 MeV electrons at room temperature by means of positron annihilation. Basing on the available data it may be expected that Si atoms in a concentration about 500 at ppm have a very weak effect on accumulation of defects because these atoms do not capture defects at room temperature. On the contrary to the assumption above we have found a clear effect of Si concentration on accumulation of defects. The effect of Si addition on accumulation of defects is weak at 0.2 at % Si and very strong at 1.5 at % Si.

Kinetics of post-irradiation annealing of defects of similar samples irradiated to different fluence (high and low) has been also investigated. Annealing curves of Fe-16Cr-0.2Si demonstrate a shift about 150 K when changing fluence by an order of magnitude similar to that observed in the non-doped alloy. This shift is reduced to 25-50 K in Fe-16Cr-0.75Si and Fe-16Cr-1.5Si.

The changes in kinetics of accumulation and post-irradiation annealing of defects indicate that a new type of defect traps appears at Si concentration near 1 at %, which does not manifest itself at low Si concentrations. Thus, a simple extrapolation of data on binding energy obtained at low solute concentrations to a case of high concentrations may be erroneous.

RADIATION DEFECTS IN BERILLIUM AND ZIRCONIUM

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This report presents the results of the modeling of radiation defects in beryllium and zirconium - two *hcp* metals, which play an important role in both mordern and in the future fission and fusion facilities. The combination of *ab initio* and molecular dynamics simulation shows that the behavior of interstitials in both materials qualitatively very similar, although they differ in details. In particular, the same configuration of the ground state and qualitatively similar mechanisms of diffusion with strongly pronounced anisotropy of the diffusion coefficient mainly along the basal planes. In both materials, not only the ground state, but also some other well-known for the hcp lattice metastable interstitial, even though their energetical preference and stability in Be and Zr are noticeably different. Comparison of *ab initio* results with published to the date data (existing only for zirconium) demonstrates that a lot of the old concepts for interstitial atom behavior in Zr should be put under serious revision.

THEORY OF RADIATION GROWTH OF HCP METALS

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Models of radiation growth have developed up to date are all based on the assumption that the primary damage produced via neutron irradiation takes place in the form of single point defects. These models do not account for the most important feature of cascade damage: intra-cascade clustering of self-interstitial atoms (SIAs) and their one-dimensional diffusion. During the last twenty years, a 'Production Bias Model' (PBM) has been developed, which shows that the damage accumulation in BCC and FCC metals crucially depends on cascade properties. Since the cascade properties in hcp, e.g. zirconium, are found to be similar to those in cubic crystals one may expect that the PBM can provide a realistic framework for the hcp metals as well. An objective for the work is to present such a model in application radiation growth of Zr alloys.

INFLUENCE OF IRRADIATION ON THERMOELECTRICAL PROPERTIES OF TIN SELENIDE ALLOYED WITH Pr AND Er

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To study the influence of irradiation on the thermoelectrical properties of $SnSe$ alloyed with $\Pr$ and Er in equal concentrations there were produced single crystals $Sn_{0,99}\Pr_{0,01}Se$ and $Sn_{0,99}Er_{0,01}Se$. First, thermoelectrical parameters, namely, thermo emf. (α), resistivity (ρ), and heat conductivity (χ), were measured prior to irradiation. Then, both samples were cut in halves. One half was irradiated with intense integral electron flows (*E*= 1.2MeV), whereas the other, with γ-quanta with a dose of *D*=0.6 G/ s during 30 hours ($\varepsilon = 9.0$ keV), and the above parameters were measured again.

Samples alloyed with erbium 0.01% in content (n_{300} – 4.5 ×10^{16} cm^{-3}) had an n-type conductivity. Upon transition from $SnSe$ to alloyed samples the value of thermo emf decreases and the conductivity changes its sign from *p*- to n-type (Fig. 1). Qualitative estimates show that at $T = 80K$, the thermo emf (α) in $SnSe$ decreases by 4,7%and in $Sn_{0,99}\Pr_{0,01}Se$, by 23%. On the contrary, in the samples with erbium presenting the n-type conductivity the thermo emf increases by 50%. With increasing the temperature, the relative change of the thermo emf decreases and at $T = 300K$, becomes equal to 2.4% for the 1st sample, 4% for the 2nd sample, and 19% for the 3rd one.

After irradiation with intense integral flows of electrons (E=1.2 MeV), the resistivity of $Sn_{0,99}Er_{0,01}Se$ at $T = 80K$ decreases by 46%. With increasing temperature, the difference $\Delta\rho$ prior and after irradiation decreases and at $T = 300K$ becomes equal to 14.6%. The course of conductivity changes $\sigma(T)$ after irradiation notably differs from the conductivity behavior for the nonirradiated samples $\sigma_0(T)$ and at $T = 95K$ the $\sigma(T)$ dependence reaches saturation. It changes slowly on growing temperature, which is evidently related to a decrease of the rate of recombination between radiation and structure defects. The same experiments were carried out for $Sn_{0,99}\mathrm{Pr}_{0,01}Se$ as well. After irradiation with fast flows of electrons, the electrical resistivity in these samples, on the contrary, increases by 37% at T=80K and by 13% at T=300K, which is likely to result from the compensation of charge carriers. After irradiation, in the samples $SnSe$ the total heat conductivity decreases by 3.5%, in the samples with Pr, 4%, and with Er, 6% (Fig. 2). The decrease of the total heat conductivity in all samples is caused by the formation in the sublattices of tin and selenium of new interstitial defects.

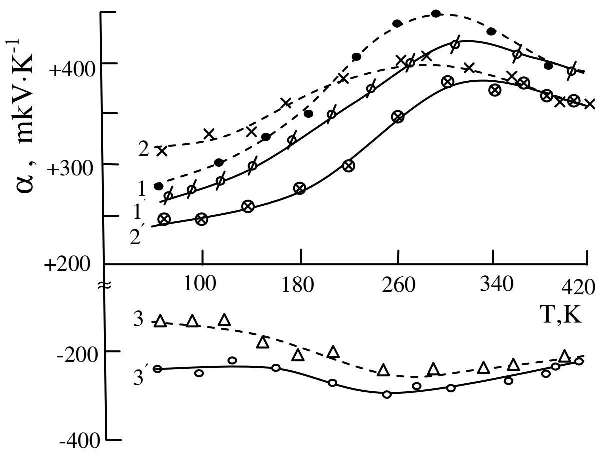

Fig.1. Themperature dependences of thermo emf 1-SnSe, 2- $Sn_{0,99}Pr_{0,01}Se$, 3 - $Sn_{0,99}Er_{0,01}Se$(solid lines, after irradiation)

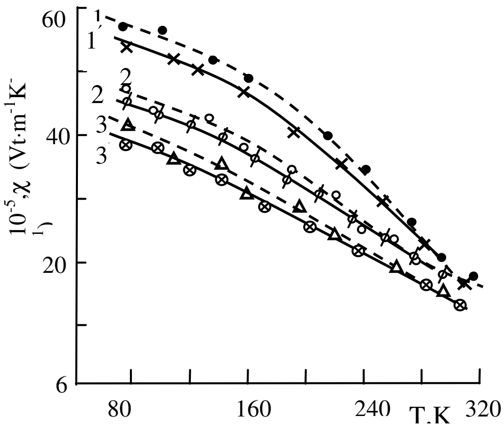

Fig.2.Temperature dependences of heat conductivity of samples: 1- SnSe, 2- $Sn_{0,99}Pr_{0,01}Se$, 3- $Sn_{0,99}Er_{0,01}Se$ (solid lines, after irradiation)

INFLUENCE OF γ IRRADIATION ON THERMOEMF AND THERMAL PROPERTIES OF ALLOY SYSTEM $Tb_xSn_{1-x}Se$

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Irradiation of solid solutions with rare earth elements (REE), including tin selenide alloyed with Tb, has been poorly studied so far. REEs in $SnSe$ give rise to the formation of radiation defects, significantly improve mechanism of conductivity and thermal properties, as well as increase hardness. Therefore, these solid solutions can be used as structural and thermoelectrical materials in thermal generators and different optical and magnetooptical memory devices. The effect of γ-irradiation on thermo emf and thermal properties of single crystals of solid solutions $Tb_xSn_{1-x}Se$ produced by the method of directional crystallization has been studied. Qualitative estimates show that after irradiation at $T = 80\ K$ the thermo emf. (α) in $Sn_{0,99}Tb_{0,01}Se$ decreases by 15%, whereas in the samples $Sn_{0,95}Tb_{0,05}Se$, on contrary, it increases by 20% and with increasing temperature, the relative change of thermo-emf decreases.

Figures 1 and 2 show temperature dependences of the heat conductivity and thermal resistance prior and after irradiation of the samples $Sn_{0,99}Tb_{0,01}Se$ и $Sn_{0,95}Tb_{0,05}Se$. With increasing content of Tb, the heat conductivity decreases. The total heat conductivity decreases after irradiation. For all samples, the thermal resistance is linearly dependent on temperature, which indicates that the thermal resistance is mainly due to phonon-phonon interaction. After irradiation the phonon part of heat conductivity decreases whereas the electronic one, increases.

It is supposed that upon irradiation of samples, terbium atoms are localized in vacancy pores between the crystal-lattice sites, thus resulting in a self-compensation with the formation of Frenkel defects. takes place. This leads to a decrease in the concentration of charge carriers; however, the activation energy does not change. At a large content of Tb in $SnSe$, the amount of charge carriers changes are poorly pronounced. However, upon irradiation with γ-quanta, the radiation defects formed become partially compensated when interacting with the structure defects.

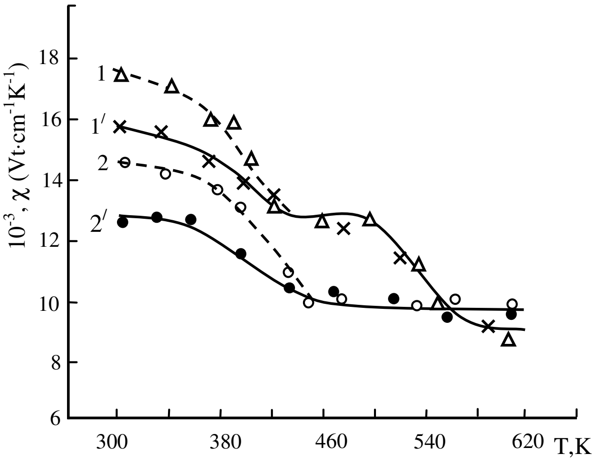

Fig1. Temperature dependence of the heat conductivity: 1-$Sn_{0,99}Tb_{0,01}Se$, 2- $Sn_{0,95}Tb_{0,05}Se$. 1/ and 2/-after irradiation

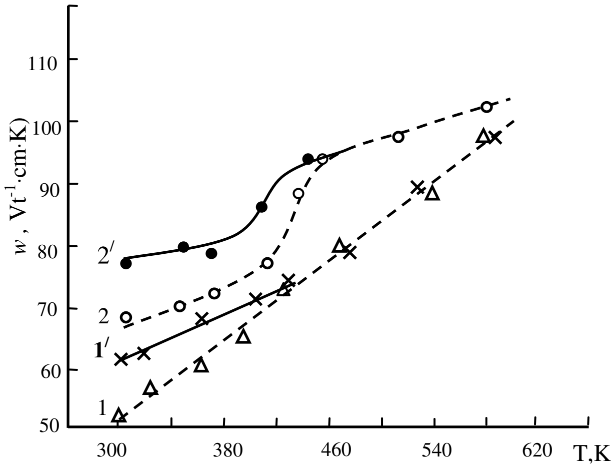

Fig2. Temperature dependence of the thermal resistance: 1-$Sn_{0,99}Tb_{0,01}Se$, 2- $Sn_{0,95}Tb_{0,05}Se$. 1/ and 2/-after irradiation

INTERACTIONS AND CLUSTERING OF POINT DEFECTS IN METALS

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Computational *ab initio* studies provide useful information about the driving forces and atomistic mechanisms of point defect clustering in metallic materials, thereby enabling predictive modeling of structure evolution in materials under irradiation or heat treatment [1,2]. This is exemplified by two case studies of point defect interactions and clustering presented here.

The first study is concerned with the interactions between vacancies and impurities of hydrogen and oxygen in the copper metal, to form embryos of gas-filled pores. Stable and metastable atomic configurations in the ternary Cu-O-H system [3] are of interest in connection with catalytic applications of copper metal and its oxides [4], as well as with the Swedish plan of spent nuclear fuel disposal in a deep geological repository using copper canisters [5]. We have investigated the structures and energies of hydrogen and oxygen impurity interaction with a monovacancy in copper metal using *ab initio* calculations with the Quantum Espresso code [6]. A strong tendency for hydrogen accumulation (up to six H atoms per vacancy) is found [7].

The second study deals with atomic diffusion in refractory ceramic materials TiC and ZrC. Phase separation of a mixed carbide (Ti,Zr)C into TiC-rich and ZrC-rich fractions (via spinodal mechanism) can be used in order to achieve great mechanical hardness of the material. Phase separation is a diffusion-controlled process and, therefore, detailed knowledge about the diffusion of metal atoms is important. It has been studied in this work employing the projectoraugmented-wave method [8] as implemented in the Vienna ab initio simulation package (VASP) [9]. The mechanism of metal atom self-diffusion in the sub-stoichiometric carbides is shown to involve clusters of one metal vacancy and up to six carbon vacancies [10]. Such vacancy clusters are strongly bound and can propagate through the lattice.

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DESCRIPTION OF BULK DIFFUSION IN MOLYBDENUM AND URANIUM BASED ON ATOMISTIC SIMULATIONS

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The diffusivities of point defects are important parameters in kinetic models for description of the irradiated fuel behavior and fission products release. However there is large uncertainty in the experimental estimates of the corresponding values. The present work describes an attempt to evaluate the diffusivities of basic point defects in pure Mo and gamma-U from the atomistic simulations, namely by means of molecular dynamics (MD) with the interatomic potentials [1,2] recently constructed by a force matching method to optimally reproduce per-atom forces (together with total energies and stresses) computed by density functional theory (DFT) for a fine-tuned set of reference structures.

Diffusion coefficients of vacancies, self-interstitial atoms (SIA) and SIA-clusters (including dislocation loops) in Mo are evaluated as a function of temperature. The contribution of vacancies predominates in a self-diffusion of Mo at thermal equilibrium due to a small vacancy formation energy (compared to other defects), as in most of bcc metals. That is the reason diffusivity of SIA cannot be accessed directly in the experiments. Both classical MD and DFT-MD simulations demonstrate long segments of nearly 1D motion of SIA. The activation energy of the 1D diffusion is an extremely small (~ 0.02 eV) due to a small energy barrier between dumbbell and crowdion configurations along <111> direction. However it is shown that neither of these configurations do not correspond to the global minimum. According to our DFT calculations, the latter is approx. 0.1 eV lower, which agrees very well with the estimate (0.11

eV) from the resistivity recovery measurements following electron irradiation [3]. Migration energy of SIA clusters in Mo is nearly independent on the size and quite close to the migration energy of a single interstitial.

The potential [2] predicts that the formation energy of a self-interstitial atom is substantially lower than of vacancy for a gamma phase of pure U in a good agreement with the DFT calculations. It implies large concentration of interstitials in a thermal equilibrium and anomalous (unusual for most bcc metals) self-diffusion well-known from the experiments [4,5]. Contrary to SIA diffusion in Mo, 1D mobility in gamma-U is hardly observed: it can be noteworthy just at temperatures lower than ~ 800 K or under compression. The mechanisms of point-defects migration for the structures of U-Mo alloys are quite close to a one observed in pure gamma-U.

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ATOMISTIC STUDY OF SUBSTITUTIONAL ELEMENTS SEGREGATION ON GRAIN BOUNDARIES

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Segregations of solute atoms at grain boundaries (GBs) have a significant impact both on the phase stability, and the physical and mechanical properties of alloys. Although the thermodynamic principles of segregations formation have been known for a long time, the microscopic mechanism of this phenomenon remains a subject of debates. In particular, it is not clear what factors determine the increased tendency of certain elements to the segregation on GBs, the fraction of segregating impurity, width of segregation. Traditional approaches consider the dimensional mismatch of ionic radii as the root cause of the dissolved element interaction with GB (strain interaction). At the same time an important role in the formation of segregation on GBs should play a chemical interaction, which depends on the electronic structure of the impurity.

To clarify the microscopic mechanism of segregation on GBs two methods were used of different levels of scale, including: 1) the calculation of the total energy and the crystallite structure containing special GB and dissolved atoms by methods of density functional theory (PAW-VASP); 2) molecular dynamics simulations of large polycrystals with different types of GBs and solute atoms at finite temperatures (many-body interatomic potentials were used obtained in the framework of "embedded-atom"). Calculations were made for GBs in Al with the addition of Mg, Si or Ti.

First-principles calculations show that the interaction with the special GB is short (concentrated in the boundary layer of 0.5 nm), and reduces the energy when placed on GB as Mg and Si, but the mechanism of interaction with the boundary of these elements is different. In the case of Mg, with the least number of electrons and more than Al atomic radius, interaction with GB is mainly of deformation character, while the interaction of Si c GB (having more electrons than Al) is determined by the formation of a covalent chemical bond in GB center. Ti atom in the lattice behaves as an impurity with smaller than Al radius, that is the main reason for the increase of energy when placed on a special Ti GB - an area with low atomic density. The results of MD simulations of segregation in Al polycrystal showed that the deformation mechanism dominates in the interaction of Mg and Ti and nonequilibrium GBs and GBs of common type. Such boundaries, in which the atomic coordination is broken in the adjacent region of ~ 2 nm, have an increased tendency to segregation of alloying elements with an ionic radius large compared to the matrix atoms. The results reveal the mechanism of segregations formation and explain the observed features of the GBs enrichment in alloys subjected to severe plastic deformation.

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STUDYING OF SUPRA-ATOMIC STRUCTURE OF ALUMINIUM ALLOY CAB-1, IRRADIATED WITH FAST NEUTRONS UP TO HIGH FLUENCES BY SMALL-ANGLE NEUTRON SCATTERING METHODS

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Modern nuclear technologies need the advanced methods for investigation and examination of physics-chemistry properties of substance. The nondestructive small-angle neutron scattering technique creates new opportunities for studies of irradiated metals and alloys, composites, nanostructures and other materials. One of important problems it is the study of an ageing process of the reactor materials in the strong neutron and gamma fields.

Aluminum alloys CAB-1 were used widely in atomic machine-building. In the WWR-M nuclear reactor of B.P. Konstantinov Petersburg Nuclear Physics Institute, the aluminum-based CAB-1 (Al–Mg–Si) alloy is the basis structural material of the reactor core elements and fuel element shells. The WWR-M reactor built and started up in 1959 operates up to the present time owing to high functional properties of materials, first, aluminum alloys used.

The samples of CAB-1 alloys were irradiated in the SM-3 reactor (Dimitrovgrad, Russia) with γ-rays and fast neutrons (E_n >0.8 MeV) at a maximum fluencies of $2.78 \cdot 10^{22}$ and $3.48 \cdot 10^{22}$ neutron/cm^2 at a temperature not higher then 70^{o}C.

The supra-atomic structure of the initial and irradiated alloys (Al-Mg-Si) samples was studied on a MEMBRANA-2 difractometer using small-angle neutron scattering. In the initial and irradiated samples, there are defects, namely, pores with a characteristic radius < 20 nm and 40–50 nm (Fig). The irradiation decreases the volume fraction of coarse scattering regions with the radius 40–50 nm, along with this, increases the fraction of the scattering regions with the radius < 20 nm, This effect is explained by fragmentation of the coarse regions.

Results of neutron investigations are correlated with data of mechanical tests of irradiation samples and modification of their elemental composition.

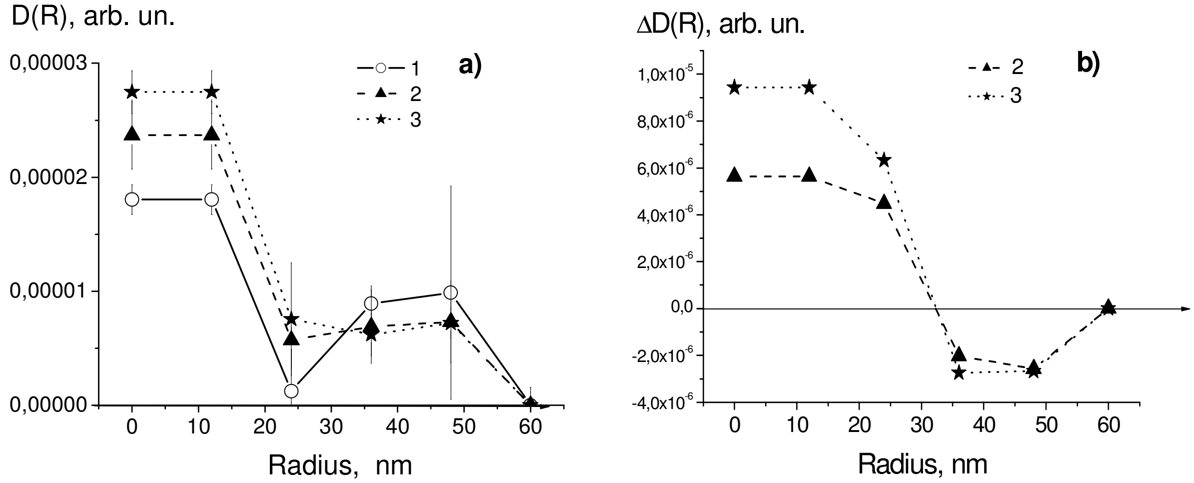

Fig. Volume fractions *D*(*R*) of particles in the (a) initial and (b) irradiated samples of the CAB-1 alloy and (b) difference between the volume fractions Δ*D*(*R*) of particles in the irradiated and initial samples: 1 – initial sample, 2 – maximum fluency $2.78 \cdot 10^{22}$ n/cm^2, 3 – maximum fluency $3.48 \cdot 10^{22}$ n/cm^2.

ANALYSIS OF TEMPERATURE-DOSE DEPENDENCES OF CRITICAL PARAMETERS OF γ→α MARTENSITIC TRANSFORMATIONS IN STAINLESS STEELS IRRADIATED WITH NEUTRONS

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Mechanical, magnetic and energy characteristics of plastic deformation for 12Cr18Ni10Ti and 08Cr16Ni11Mo3 reactor steels both non-irradiated and irradiated with neutrons in the temperature interval of 20-100 ºC were determined. Temperature relationships of true critical stresses and strains at which α-phase originates and its amount accumulated to the failure point were determined.

Experimentally the values of latent energy required for γ→α-transformations in austenised steel samples at low-temperature deformation were determined.

It was shown that mechanical work, required for failure of steel samples, decreases with an increase of irradiation damage dose (0.001-56 dpa).

ON SOLUBILITY OF CHROMIUM IN α-IRON AT LOW TEMPERATURES

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The iron-rich Fe-Cr alloys form a basis of the conventional stainless steels, which are widely used in industry due to their excellent mechanical and chemical properties. However, Cr solubility in α-iron is limited. Because of this limitation, high-Cr alloys and steels demonstrate a tendency to the phase separation into Fe-rich (α-phase) and Cr-rich (α′-phase) fractions leading to the embrittlement (found first during ageing at 475 C and named as 475 C embrittlement), which degrades seriously the mechanical properties of the alloys and ferritic steels.

To understand behaviour of the alloys with respect to the phase separation a solubility limit has to be known, at first. However, it is not known exactly being a subject of the intense discussion. A solubility limit at low temperatures where atomic mobility is virtually frozen is of a special interest because it cannot be determined directly by common experimental means.

We pay attention to the fact that nucleation of α′-precipitates may occur only if neighbouring of a Cr atom with other Cr ones is energetically preferable. In terms of the short-range order (SRO), this means that precipitating Fe-Cr alloys should demonstrate a tendency to short-range clustering. On the other hand, an inversion of a type of SRO from short-range ordering to short-range clustering is known to occur near 10 at % Cr above 700 K. Thus, a concentration, at which the inversion of the SRO type takes place, indicates directly the highest Cr concentration, below which a tendency of Cr atoms to neighbouring with Fe and avoiding Cr ones (i.e. short-range ordering) is incompatible with a tendency to nucleation of Cr clusters (precipitates). In other words, a Cr concentration, at which the inversion occurs, is a lower estimate of the solubility limit.

It is known that resistivity recovery (RR) in concentrated alloys irradiated with electrons at low temperatures is affected by the SRO formation enhanced by long-range migration of irradiation-induced defects. Comparison of RR curves of the similar samples irradiated to different initial defect concentrations allows revealing as a fact of the SRO formation as a sign of the SRO-induced contribution to resistivity [1]. It is known that a sign of the SRO-induced contribution to resistivity (i.e. whether the SRO formation increases or decreases residual resistivity of the alloy) is unambiguously related with a type of SRO in Fe-Cr [2].

Therefore, we refer to RR data obtained in five Fe-Cr alloys (4-16 at % Cr) irradiated with 5 MeV electrons at low temperatures. It is found that the lowest temperature, starting which a type of SRO can be determined in all our alloys basing on RR data, is near 300 K.

As a result, a tendency to short-range ordering is observed in alloys with 8.7 at % Cr and below while alloys with a Cr concentration of 10.8 at % Cr and above clearly demonstrate a tendency to short-range clustering. Basing on these data we conclude that a solubility limit near 300 K is positioned between 8.7-10.8 at % Cr. The similar result was obtained earlier for Cr solubility at 773 K [3].

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RADIATION-ENHANCED GRAIN BOUNDARY DIFFUSION IN IRON, IRON BASE ALLOYS AND STAINLESS STEELS

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The procedure and results of radiation-enhanced grain boundary diffusion (REGBD) characteristic prognostication in α- and γ-Fe, γ-Fe-Ni alloys and austenitic alloys and stainless steels: Fe-17Cr-11Ni-2,3Mo(SS316), Fe-17Cr-12Ni(SS305), Fe-20Cr-25Ni/Nb are presented. The generalized temperature dependence of grain boundary diffusion (GBD) coefficients for outlined above metals and alloys is obtained by statistic handling of more than one hundred the most plausible experimental literature data and is used as a data base for REGBD coefficients calculations. The resulting temperature dependence can be expressed as:

$$D_{GB} = (20{,}15 \pm^{4,13}_{3,41}) \exp\left[-\frac{(25{,}28 \pm 0{,}99)T_m}{RT}\right], cm^2/s \qquad \textbf{(1)}$$

where T_m – the melting temperature of phase.

All original data by coefficients GBD was used considering the grain boundary width δ=5·10^{-8} cm. The used up values for calculate T_m phases iron and alloys are in the form (in K): α-Fe: 1600; γ-Fe: 1800; γ-Fe+40Ni: 1720; Fe-20Cr-25Ni: 1705; SS305, 316: 1745.

Coefficients REGBD are calculated designed with the help previously developed procedure [1]: D_{REGBD}=R·D_{gb}, where R is the coefficient radiation-enhanced diffusion process. It is hypothesized in the report that value R for volume diffusion agrees within the limits of experimental accuracy [2]. For design D_{REGBD} in this report were used values R for radiation-enhanced volume diffusion in α-Fe, Ni and Fe-Cr-Ni alloys. The temperature dependence of R, obtained by statistical processing of experimental data is presented in from:

$$D \cong (2{,}75 \pm^{2,99}_{1,43}) 10^{-8} \exp\left[\frac{(22{,}89 \pm 0{,}17)T_m}{RT}\right] \qquad \textbf{(2)}$$

Here, the temperature dependence of D_{REGBD} appears as in form (and in figure):

$$D_{REGBD} = (5{,}48 \pm^{1,90}_{1,41}) 10^{-7} \exp\left[-\frac{(2{,}49 \pm 0{,}12)T_m}{RT}\right], cm^2/s \qquad \textbf{(3)}$$

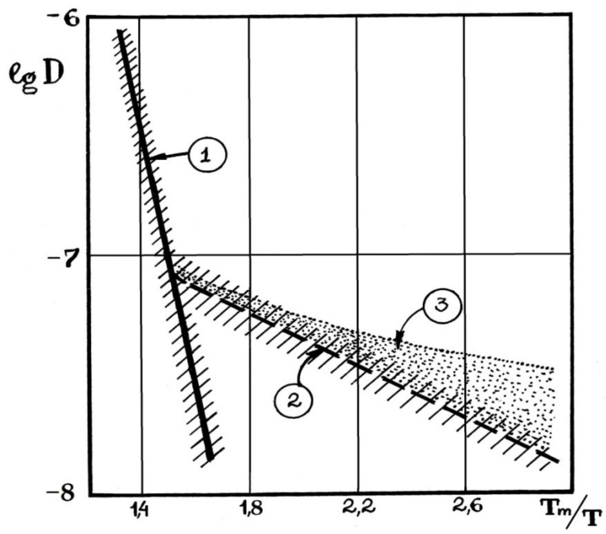

Figure 1. The temperature dependences of D_{GB} (1), D_{REGBD} (2) and D^{imp}_{REGBD} (3) for $E^b_{vI} = 0{,}1-0{,}3$ eV and $C_I \cong 10^{-3}$ in iron base alloys and steels.

Reasoning from this expression values energy migration (E^v_m) and formation (E^v_f) vacancies in grain boundary for α-Fe, γ-Fe and iron base alloy are estimated. The results are compared with those obtained previously for volume RED in α-Fe, Ni and iron base alloys.

Estimates $D^{imp}_{REGBD} \cong R \cdot R^{imp}_{REGBD} \cdot D_{GB}$ for values $E^b_{vI} = 0{,}1-0{,}3$ eV and $C_I \cong 10^{-3}$, obtained in the form of non-linear temperature dependence (see figure). The mechanisms of GBD and REGBD are discussed.

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ATOMISTIC MODELING OF RADIATON DEFECTS AND GRAIN BOUNDARIES INTERACTION IN MOLIBDENUM

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Radiation-nduced defects significantly affect metal characteristics. It can cause steel embrittlement and radiation-swelling of fuel rods. Though, understanding of defects diffusion mechanisms can lead to a breakthrough in the field of creating irradiation-resistant materials.

Molibdenum was chosen as a subject of this research because it is used both as irradiation-resistant construction material and as a component of metal fuel rods.

Different ways to control formation and growing of irradiation defects clusters are being discussed in the literature. One of the ways is based on particular properties of impurities on grain boundaries [1].

In this work we calculated grain boundary formation energy as a function of misorientation angle. After analyzing the results we chose several structures, for which diffusion mechanisms were investigated.

Symmetric tilt GB was created by rotation two coherent grains around <001> in the opposite directions. We use two-dimensional periodic boundary conditions. Third dimension was excluded to avoid GB interaction with its periodical replica and other effects, for example, GB migration. So we decided to fix free surfaces of each grain.

We used the embedded atom method potential [2] for describing atoms interaction. Molecular dynamics calculations were established using the LAMMPS package.

On the first step the bycrystal was relaxed to zero stresses and required temperature. This way we created a range of grain boundaries, each of them corresponds to its own misorientation angle. GB formation energies were found. Though, we calculated the dependence consistent which with the data for iron [3]. Based on the dependence, several the most stable structures were chosen.

On the second step, a self-interstitial atom was placed on each of the boundaries. And all of them were investigated on diffusion mechanisms with Parallel Replica Dynamics method. Though, we showed that pipe diffusion is the prevalent for low misorientation angles. With increasing the angle, the probability of interstitial “jumping” between two dislocation cores also increases. But calculations for bigger angles, especially which are close to 90 degrees, showed relatively high diffusion activity of defect within dislocation core, but almost no mass transfer.

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FUNDAMENTAL PROCESSES UNDER ACTION OF RADIATION ON SEMICONDUCTOR NANOSTRUCTURES

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Modern trends of the conversion of solar and thermal energy, based on solid-state electronics, show the shift onto the use of low-dimensional systems. This concerns both the photoconversion [1] and thermoelectricity [2]. The absence of the knowledge of the mechanism of radiation stability of the photo- and thermoelements in the extreme conditions of radiation is in the way of their practical use. In this area the researches on the theory of the micromechanisms of radiation action on the low-dimensional systems are behind (the exception is, apparently, the paper [3]). In this regard, the systematic research of radiation degradation of low-dimensional photo- and thermoelectric converters is very important. The amount of studies performed in the field of microscopic models of radiation nanophysics is rather limited and, with the exception of carbon nanostructures, they are non-systematic. The purpose of the present work is to initiate a systematic approach to build the theoretical models of radiation nanophysics with the account for fundamental properties of nano-objects. We choose at this stage to consider two basic phenomena (Frenkel pair formation and amorphization) modified by only one nanoproperty, i.e. the presence of an interface. We develop a mathematical framework to describe the modification on the nanoscale. From the general expression for the modified radiation phenomena, we find that any radiation effect can be modified at least by 48 ways. This predicts a very rich future of radiation nanophysics both in the fundamental and applied aspects. The developed theoretical concepts are applied to the study of radiation stability of photo- and thermoelectric converters.

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FEATURES OF NANOSCALE INTERMETALLIC-PHASE FORMATION IN ALLOY SYSTEM Al–Li–Mg–Cu–Zr–Mn UNDER ION IRRADIATION

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Irradiation-induced changes in the phase composition of the cold-worked alloy 1441 of an Al–Li–Mg–Cu–Zr–Mn system have been analyzed using transmission electron microscopy.

Samples were irradiated by continuous Ar^+ ion beams using an ILM-1 facility for ion beam treatment, equipped with a PULSAR-1M ion source based on a glow discharge with a cold hollow cathode. The ion current density was 150 μA/cm^2; the ion energy, 20 keV; the radiation dose was varied from $1{\cdot}10^{15}$ to $1{\cdot}10^{17}$ cm^{-2}. The temperature of the samples under irradiation was constantly monitored using a chromel-alumel thermocouple. At relatively low doses ($D \leq 10^{16}$ cm^{-2}) the maximum temperature of the samples did not exceed 40-60° C and at higher doses it did not exceed 260-370° C.

It was shown that under Ar^+ ion irradiation with an energy of 20 keV there was observed dissolution of β' (Al_3Zr) and δ' (Al_3Li) phases in the whole volume of the samples 1 mm thick and a decrease in size and partial dissolution of intermetallic compounds Al_8Fe_2Si of crystallization origin. In addition, supersaturated solid solution decomposition was initiated by irradiation in the alloy, which was followed by the formation of fine nano-sized particles of hardening θ' (Al_2Cu) and S_1 (Al_2LiMg) phases. The degree of the solid solution decomposition increases with the increasing radiation dose. It should be noted that the particles of these phases have not been detected in the alloy 1441 after deformation and annealing. These particles are formed near the irradiated surface (at a distance of 150 m away from it) when the dose reaches $5.6{\cdot}10^{16}$ cm^{-2} and in the entire volume of the sample with a thickness of 1 mm when the dose is 10^{17} cm^{-2}. Al_2LiMg-phase particles 50-100 nm in size uniformly precipitate in the grain volumes rather than along their boundaries under Ar^+ ion irradiation of the alloy 1441, as is often the case in quenching of aluminum-lithium alloys. The presence of nano-sized particles of hardening θ' (Al_2Cu) and S_1 (Al_2LiMg) phases in the grain volumes explains a significant hardening of the alloy while retaining a sufficiently high level of plasticity found after high-dose-irradiation of the cold-worked alloy 1441.

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MODELING OF RADIATION-INDUCED SEGREGATION IN ALLOYS UNDER NONUNIFORM IRRADIATION

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Radiation-induced segregation (RIS) during spatially uniform irradiation leads to significant changes in alloy composition near main microstructural features acting as point defect sinks, namely grain boundaries, free surfaces, dislocations, precipitates and voids. As a consequence RIS often strongly affects various radiation damage phenomena in alloys. Additionally, RIS should also operate in the alloy matrix (even in the absence of microstructural sinks) in regions of high non-uniformity of point defect (PD) generation rate. A currently relevant example of such non-uniformity exists in ion simulation studies where there reveals a strongly localized region of maximum PD generation rate.

Numerical methods are being developed in this study for modeling of non-steady-state RIS along the projected range under ion irradiation accounting for a very non-uniform profile of PD generation rate and accumulation of implanted ions. Modeling is performed of RIS in fcc Fe-Cr-Ni and bcc Fe-Cr-Si alloys under irradiation with 7 MeV Ni^{+2} and 1.8 MeV Cr^{+3} ions.

The major difficulty in modeling of the RIS process, especially in bcc alloys, originates from incomplete knowledge of diffusional characteristics (i.e. diffusivity coefficients, correlation factors) of alloy components and PDs in concentrated complex alloys and their dependence on alloy composition. That is why some specific simplifications are usually used in computing RIS.

Such typical simplifications involve the neglect of correlation effects and an assumption that the migration energy is independent of local alloy composition.

In this work we propose a self-consistent approach based on molecular dynamics simulations to compute diffusional characteristics necessary for the assessment of RIS in concentrated alloys. As an example, the interstitial mechanism of RIS in Fe-Cr alloys is considered. Calculations have been performed in the temperature range 600-1000 K in alloys with Cr contents of 5-25 at.%, a range relevant for ferritic/martensitic steels. Available experimental data on RIS in bcc Fe-Cr alloys and ferritic/martensitic steels are discussed.

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PRIMARY RADIATION DAMAGE IN MATERIALS UNDER REACTOR IRRADIATION

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Displacements per atom (dpa) provides a convenient correlation parameter for an analysis and forecasting of radiation-induced phenomena in reactor structural materials. The use of dpa allows to compare results of irradiation of materials in different neutron energy spectra and with different types of particles (neutrons, ions, fast electrons). Calculations of energy spectra of primary knocked atoms (PKA) and “effective” dpa, which are introduced to take into account the point defect recombination during the relaxation stage of a displacement cascade, are of both scientific and practical interests.

In this work the results of calculating fast neutron fluxes with different threshold energies, dose rates and "effective" dpa for a number of pure metals and structural materials in cores of Russian thermal (WWER-440, -1000) and fast (BN-600, -800, -1200) and also test (BR-10, BOR-60, MBIR) reactors are presented. Energy spectra and mean PKA energy are calculated for the metals in all reactors. Effect of neutron spectrum on damage dose is studied. The characteristics of dose can be used for an analysis of radiation-induced phenomena in structural materials, and also for the development of physical models of these phenomena.

Limitations and uncertainties in the standard dpa formulation (the NRT-dpa) are discussed. An IAEA initiative on the development of improved parameters for correlating damage from irradiation facilities with very different particle types and energy spectra, including fission and fusion reactors, charged particle accelerators, and spallation irradiation facilities is presented.

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THE DOSE DEPENDENCE OF VACANCY DEFECT EVOLUTION IN NEUTRON-IRRADIATED PURE NICKEL

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It is well established that materials upon irradiation exhibit embrittlement and swelling that can often be traced to the atomic scale processes of defect accumulation. Defects (self-interstitial atoms (SIAs) and vacancies) are produced; they diffuse and aggregate that leads to SIAs and vacancy clusters. Depending on the crystal lattice, the defects may be arranged as three-dimensional clusters (nanovoids) or, if the point defects cluster in a planar way, dislocation loops.

In the face-centre cubic (fcc) metals, the agglomeration of vacancies may result in the formation of vacancy type dislocation loops (V-loops) and stacking fault tetrahedra (SFTs). However, it is less well understood how SFTs form. In [1] it is postulated that nanovoids collapse into Frank loops (a disk of vacancies in {1 1 1} plane) which then dissociate into SFTs. Whereas, it has been indicated in [2] that voids can thermally transform directly to SFTs without passing through a Frank loop.

In the present work we have investigated the effect of neutron irradiation dose level on the vacancy defect accumulation and post-irradiation annealing in pure nickel. In order to investigate the dose dependence of vacancy defect evolution in nickel, specimens of high-purity Ni were neutron-irradiated at ~ 330 K in the IVV-2M reactor (Russia) to fluencies in the range of $1x10^{21}$ – $1x10^{23}$ n/m^2 (E > 0.1 MeV) corresponding to displacement dose levels in the range of about 0.0001 – 0.01 dpa and subsequently stepwise annealed to about 900 K. Ni was characterized both in as-irradiated state as well as after post-irradiation annealing by positron annihilation spectroscopy. The formation of three-dimensional vacancy clusters (3D-VCs) in cascades was observed under neutron irradiation [3], the concentration of 3D-VCs increases with increasing dose level. 3D-VCs collapse into secondary-type clusters (stacking fault tetrahedra (SFTs), and vacancy loops) during stepwise annealing at 350 – 450 K. It is shown that the thermal stability of SFTs grow with increasing dose level, probably, it is due to growth of the average SFT size during annealing. The results of annealing experiments on electron-irradiated Ni at 300 K were carried out, for comparison. In the report, the positron response to the SFT-like structures is briefly discussed also.

This study was done within RAS Program (Project No. 01.2.006 13394) with partial support of Russian Foundation for Basic Research (Project No 11-02-00224-a and No 13-02-00321-a), Ural Branch RAS (Project No. 11-2-21 YaTs) and The Ministry of education and science of the Russian Federation (Contract No. 14.518.11.7020).

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ACCUMULATION OF IMPLANTED DEUTERIUM IN Fe AND Fe-Cr ALLOYS

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Ferritic stainless steels possess a combination of properties that are required for materials of fuel elements of fast –neutron reactors. Model materials for studying the behavior of these steels under irradiation are BCC-alloys Fe-Cr. Of interest is the behavior of hydrogen in these alloys under conditions of radiation damage.

For investigation, iron alloys with 0. 8, 10.8, and 16 mass % Cr were used. The alloys were prepared of powder carbonyl iron and electrolytic chromium. In the iron the main impurities were (in ppm): C ~ 170, N ~ 70, Ni ~100, and Cr ~ 2, whereas in chromium, C ~ 200, N ~ 200, Al ~ 80, Fe ~ 60.

Similarly to the conventional practice for the ferritic –martensitic steels, the model alloys were treated in two steps. First, they were heated to 1070 K (in the ferritic region) and held at this temperature for 4 hours in a vacuum of 10^{-4} Pa. Then, they were annealed at 730 K for 4 hours and cooled in air. The grain size amounted to 100-200 μm.

The method of nuclear reactions (reaction D(d,p)T, deuterium energy 700 keV) was employed to study the trapping of deuterium depending on the dose of implantation and sample composition. The diameter of implanting (measuring) beam of deuterium ions was 1 μm, the temperature of implantation, 300 K.

In the course of experiment the average concentration of the implanted deuterium in the irradiated volume of the samples under study was measured. It is established that the efficiency trapping of deuterium in the irradiated iron is significantly higher than in Fe-Cr alloys. The lowest efficiency corresponds to the alloy with 8 mass % Cr. The efficiencies of trapping of deuterium in the alloys with 10.8 and 16 mass % Cr virtually coincide in the range of implantation doses $(1\text{-}18)\times10^{16}$ cm^{-2}.

The results obtained are discussed taking into account the data gained earlier in works [1-3 and others] on the structure of alloys Fe-Cr prior and after irradiation.

The work was performed according to the Plan of RAS (theme "Impulse", project №. 0120106436), Plan of the Presidium of Ural Branch, RAS (JFI-M №12-M-23-2031) with a partial support of the Russian Foundation for Basic Research (project № 11-02-00224).

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DISLOCATION SINKS EFFICIENCY UNDER DIFFERENT TEMPERATURES AND APPLIED LOADS IN BCC (Fe, V) AND FCC (Cu) CRYSTALS

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Simulation of self-point defects (SPDs) diffusion in elastic fields of dislocations in different slip systems under different applied loads at $T = 293 - 1000$ K was performed by object kinetic Monte Carlo method for bcc (Fe, V) and fcc (Cu) crystals. Elastic interaction of self-point defects (SPDs) considered as elastic dipoles (vacancy and self-interstitial atom in stable and saddle-point configurations) [1, 2] with dislocation and external stress fields was calculated by means of the anisotropic theory of elasticity.

Dependences of dislocation sink efficiencies and linear (no interaction) sink efficiencies on the value of external loads (up to 200 MPa) of different types were calculated for bcc (Fe, V) and fcc (Cu) crystals. Comparison of the obtained dependences with Saralidze's analytical solution for linear sinks [3] was made. Saralidze's solution describes the linear sink efficiency for SPDs up to 1% at $|\sigma/T| \leq 0.34$ MPa/K, where σ is the largest component of the tensor of the external stresses. Saralidze's solution for linear sinks describes calculated values for dislocation sink efficiencies, divided by the dislocation sink efficiency in the absence of external stress, up to 1% at $|\sigma/T| \leq 0.27$ MPa/K.

Bcc lattice symmetry leads to the facts that: (1) the diagonal components of the stress tensor in the crystallographic coordinate system do not affect the dislocation sink efficiency, and (2) the sink efficiency of dislocations oriented along <100> crystallographic directions is independent of any type of loads.

Obtained results allow one to evaluate the climbing rate of edge dislocations and, as a consequence, the deformation (creep, swelling, etc.) rates of crystals under combined effect of irradiation, external loads and temperatures. Several particular cases have been considered for bcc (Fe, V) and fcc (Cu) crystals.

The present work was funded by the Ministry of education and science of the Russian Federation (contracts #14.740.11.0162). The results of the work were obtained using computational resources of MCC NRC "Kurchatov Institute" (http://computing.kiae.ru/).

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SOME PROBLEMS OF KINETIC THEORY FOR RADIATION-ENHANCED GRAIN-BOUNDARY DIFFUSION IN POLYCRYSTAL MATERIALS WITH IMPURITIES

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The systematical analysis of the description possibility for radiation defects (RD) annealing processes in systems with grain boundaries (GB) taking into account influence of vacancy and interstitial impurity complexes resulting inside GB on acceleration of radiation-enhanced grain-boundary diffusion (RGBD) is carried out. The incorrectness of notions about predominantly vacancy mechanism of grain-boundary diffusion (GBD) is shown. The evidence of the possibilities for vacancy-interstitialcy mechanisms of GBD are presented [1], in particular analysis of compensation effects of GBD and REGBD processes demonstrated of collective mechanisms diffusion processes possibility likewise of mechanisms in disordered systems. In considered model is taken that vacancies and interstitials are mobile. The possibility reducing of generalized system of kinetic equation to classic equations for pure metals introducing the effective coefficient of recombination velocity is confirmed [2, 3]. The solution and analysis of kinetical equations annealing system for stationary and quasi-stationary processes are presented. The expressions for concentrations of radiation defects and complexes, for REGBD coefficients with impurity complexes influence and for coefficients of impurity acceleration REGBD are obtained. The simple expression for coefficient of impurity acceleration REGBD for close meanings of binding energies arbitrary complexes R_{REGBD}^{imp} is presented:

$$R_{REGBD}^{imp} \cong \sqrt{1 + zC_I \exp\frac{E_k^b}{kT}},$$

where C_I – impurity concentration; E_k^b – binding energy of complex. The presented results used for estimation of REGBD coefficients in iron, alloys steels [4].

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SIMULATION OF PULSED LASER IRRADIATION OF AMORPHOUS Fe BASED MATERIALS.

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Amorphous materials attract attention of researchers in view of widely spread spheres of their practical application. Amorphous state of a surface layer is characterized by a high hardness, corrosion resistance, and other specific properties of the material. A purposeful action on the material surface with the aim to gain the required combination of properties is one of the topical problems of modern science.

This work deals with the behavior of the amorphous $Fe_{80}B_{20}$ alloy upon irradiation of its surface with a picoseconds laser pulse.

Despite the lack of theoretical model for the process of crystallization of amorphous alloys after the laser irradiation, in some researches on physics there are put forward assumptions on the emergence of a supersonic wave upon absorption of the quantum flow by the amorphous-alloy surface. However, up-to-date, the mechanism of appearance of such waves has not been studied in full detail, and the hypotheses suggested, as a rule, have been verified only qualitatively.

With the use of the program package LAMMPS, amorphous state of $Fe_{80}B_{20}$ was obtained by heating and rapid quenching of a model crystallite. With the help of program package MDOMP, simulation of shock waves that arise in the process of irradiation of the amorphous alloy with a laser pulse was performed. Mechanisms of the appearance in the system under simulation of shock waves due to gradients of temperatures and internal stresses have been analyzed. The speed of propagation of the shock wave in the sample was estimated. The impact of shock wave on the redistribution of components of the amorphous alloy has been revealed. Regularities of changes in the structure and elemental composition of the surface alloy after irradiation are discussed.

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MD SIMULATION OF GRAIN BOUNDARY SEGREGATIONS IN Fe-Ni ALLOY

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Segregation of alloying elements at the grain boundaries (GBs) have a significant impact on the structural and phase stability, mechanical properties of polycrystalline alloys. In the intensive external action (intensive deformation, irradiation), along with the thermodynamic factors (energy gain), an essential role is played also by the kinetic mechanisms of segregation, which is due to the flow of non-equilibrium point defects at GBs.

In order to determine the thermodynamic stimuli of segregation formation on GBs in iron-based alloys we performed molecular dynamics simulations of polycrystalline fcc alloy $Fe_{0.7}Ni_{0.3}$. We used the EAM-potentials [1] which are well proven to describe the cohesive properties and polymorphic transformation in Fe-Ni system. Simulation was carried out for a sufficiently large polycrystal containing a few grains with tilt boundaries of different types: small-angle GB, unsymmetrical boundary Σ5 (misorientation axis [001], misorientation angle $\Theta = 53.13^{\circ}$), and common type boundary (axis [001], $\Theta = 41^{\circ}$). Since the energy of the alloying element in an alloy depends on the local environment, the energy of its interaction with the boundary was calculated by averaging over the set of configurations in which the central Ni atom was located at a given distance from the GB.

The simulation results showed that Ni atoms interact weakly with the GBs of considered types (segregation energy is less than 0.1 eV), because they have the ionic radius and the electronic structure close to that of the matrix Fe atoms. Thus, the Ni atoms in the alloy $Fe_{0.7}Ni_{0.3}$ have no their own incentives for segregation to sinks of point defects, which are mainly GBs. Therefore, the main cause of segregation in the Fe-Ni base alloy should be considered non-equilibrium flows of point defects at GBs (see, e.g. [2]) under the action of irradiation or intensive plastic deformation.

The work was supported by the Presidium of Ural Branch of the Russian Academy of Sciences (project 12-P-2-1043) and RFBR (projects 10-03-00113 and 11-02-00224).

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MODELING OF CHROMIUM NANOCLUSTERS GROWTH UNDER NEUTRON IRRADIATION

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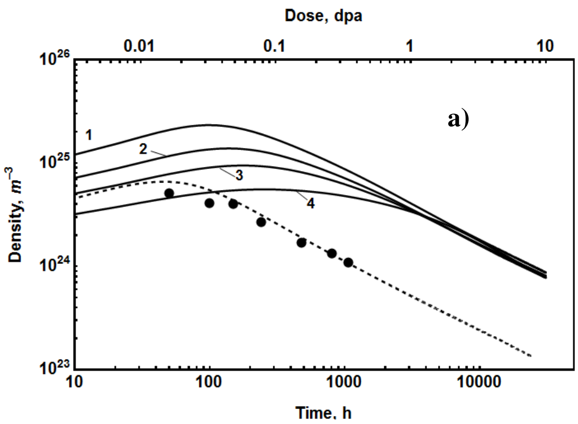
In this work we have performed the simulation of nanoclusters growth in iron-chromium based alloys in conditions of neutron irradiation at temperature T=300C. The developed model was based on the two assumptions: 1) nanosized clusters consist of both iron and chromium atoms and cluster's composition depends on their size and temperature [1]; 2) the chromium atoms diffusion coefficient under irradiation is proportional to vacancy concentration.

Kinetics of nanosized clusters growth was considered by means of the model developed in [1]. The main parameters of the model are: the radiation-enhanced diffusion coefficient and nucleation rate under irradiation. These parameters were varied to satisfy the experimental data for Fe-12at%Cr alloy at T=300C and damage dose 0.6dpa [2] (see fig.). The obtained value of radiation-enhanced diffusion coefficient is $1.4\times10^{-19} cm^2/s$, that is seven order of magnitude greater then corresponding thermal value at T=300C ($2.2\times10^{-26} cm^2/s$ [4]) and quite close to the diffusion coefficient at T=500C ($7.0\times10^{-19} cm^2/s$ [4]). The calculation of the diffusion coefficient based on the analysis of generation and recombination of radiation defects gives the same estimation of the radiation enhancement of the diffusion under irradiation.



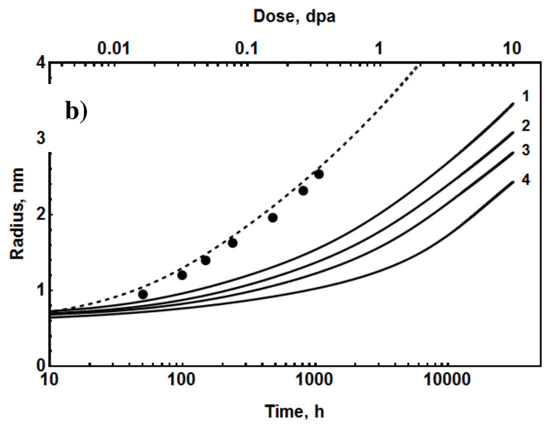


Fig. The depandance of the clusters concentration (a) and average radius on the ageing duarationa or damage dose. Dashed lines (modeling) and dots (experiment [3]) for Fe-20at.%Cr at thermal ageing (T=500C). Solid lines are the result of modeling of the different iron-chromium based alloys alloys under irradiation (dose rate 0.9 10^{-7} *dpa/s*) at T=300C: 1 - 20at%Cr, 2 - 16at%Cr, 3 - 14at%Cr, 4 - 12at%Cr.

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DISLOCATION LOOPS IN Fe-BASED ALLOYS: FEATURES LEARNED FROM ATOMISTIC MODELLING

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Body Centered Cubic (BCC) Fe-based alloys such as ferritic steels are common structural materials for nuclear application, hence the importance of understanding of radiation damage in these materials. The primary defects composing microstructure of neutron irradiated BCC Fe-based alloys are dislocation loops of ½<111> and <100> type, depending on temperature and composition of the material as revealed by transmission electron microscopy (TEM). The formation, growth and diffusion of dislocation loops will determine the global evolution of microstructure as well as hardening associated with the retardation of dislocations interacting with the loops.

This presentation gives an overview of the efforts done over last decade dedicated to the understanding of properties of dislocation loops as products of collision cascades, diffusing objects, sinks for point defects, sites for heterogeneous precipitation, interacting objects and obstacles to dislocation motion. The focus is made on the results obtained using atomistic simulations in pure Fe, Fe-C, Fe-Cu-Ni-Mn and Fe-Cr alloys. The latter two alloys exhibit composition of solutes close to the well established commercial reactor pressure vessel (RPV) and high-Cr (i.e. T91, EUROFER, F82H) steels.

INTERACTION BETWEEN ATOMIC DISPLACEMENT CASCADES AND CHROMIUM-RICH PRECIPITATES IN Fe-9%Cr ALLOY: MD SIMULATION

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Present work is devoted to modeling cascades of atomic displacements in the Fe-9at.% Cr binary alloy with Cr-rich clusters. Simulation was carried out using molecular dynamics (MD) technique at the crystallite initial temperature of 300 K. The spherical precipitates with a diameter of 1 to 5 nm, containing 95at.% of randomly distributed Cr were considered. Cascades were simulated for the two energies of the primary knock-on atom (PKA): 15 and 20 keV. Simulation was carried out using a n-body interatomic potential A. Caro et al. [1].

We modified used potential for a more accurate description of interactions at short interatomic distances, which is important for modeling radiation damage. It was also shown that the modified potential provides a reasonable agreement with ab-initio calculations of formation energies of defect structures containing Cr atoms in the matrix of the bcc Fe obtained by P. Olsson et al. [2].

The parameters of the primary radiation damage with and without Cr-rich precipitates were calculated. It was concluded that the precipitate with diameter of 5 nm causes the growth of surviving defects number in cascades with energy of 15 keV up to ≈25%. A slight increase of Cr fraction in self-interstitial atoms (SIAs) was observed for cascades of both energies initiated on short (up to 5.1 nm) distances from the precipitate with diameter of 5 nm. Precipitate with diameter of 1 nm did not significantly affect on the primary radiation damage. Our estimations for PKA energy of 20 keV and a precipitate diameter of 5 are in good agreement with results obtained early by K. Vörtler et al. [3].

The main result of this study is revelation that Cr-rich precipitates tend to dissolve in displacement cascades. However large precipitates (with the diameter of 3-5nm) exhibit only slight modifications and can be considered stable. On the contrary, the composition and size of small (1 nm) precipitates changes considerably. Sometimes they complete dissolve in cascade. Considerable decrease of Cr fraction can occur in medium 2 nm precipitates without their total dissolution. We believe that these effects should be taken into account when considering the process of α-α' phase separation under cascade-producing irradiation.

The work is supported by the Russian ministry of science and education in frame of state assignment in 2012-2014, the Program Research and Scientific-Pedagogical Brainpower of Innovated Russia in 2009–2013, and RFBR grant – project 12-08-97076.

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SIMULATION OF ATOMIC DISPLACEMENT CASCADES NEAR TWIN GRAIN BOUNDARY IN FECR ALLOY

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Due to the rapid development of computer systems the use of computer simulations is expanding in those scientific areas where experimental investigations and direct measurements are difficult and sometimes are impossible. The study of material properties at the nano- and micro-scale is one of the areas. Atomistic simulations by means of Monte Carlo method, molecular dynamics, and Ab Initio calculations are widely used there.

An atomic model of extended twin grain boundaries (GB) in metals with bcc structure was considered in the present study. The energy properties of such boundaries was studied in α-iron, chromium, vanadium and Fe-10 at.% Cr binary alloy. Interatomic potentials used here were taken from papers [1-4]. Obtained quantitative assessments of the GB's specific energy for a temperature of 300 K lie in a relatively narrow range from 0.054 to 0.087 eV/$Å^2$. The width of the intergranular region was evaluated in range of 1-2 nm.

The simulation of atomic displacement cascades with energy of 10 keV in bi-crystals of α-Fe and Fe-10 at.% Cr alloy containing Σ5 (310) [001] GB was performed. The initial temperature of the modelled system was 300 K. The mean numbers of surviving defects were estimated for different PKA directions and distances between PKA and GB. These estimates were compared with the results obtained for the single crystal α-Fe. The following features of GB's influence on radiation damage were revealed. The average number of produced SIAs was estimated 1.5-2 times as lower in comparison with the case of a single crystal for cascades initiated at relatively short distances from the GB. When cascade area sides with intergranular region at ballistic stage, an increase in the number of "surviving" vacancies on factor of 2-2.5 was observed. Both cases are explained by intense absorption of formed SIAs by intergranular region. Vacancy transition into intergranular region is significantly lower because of their low (compared to the SIAs) mobility.

The work is supported by the Russian ministry of science and education in frame of state assignment in 2012-2014, the Program Research and Scientific-Pedagogical Brainpower of Innovated Russia in 2009–2013, and RFBR grant – project 12-08-97076.

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ATOMISTIC MODELING OF RECOMBINATION AND CLUSTERING KINETICS OF RADIATION DEFECTS

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In order to predict the evolution of defects and increasing of materials damage kinetic rate theory is applied [1], which includes the description of microscopic processes such as recombination, clustering of point defects, voids and bubbles formation, and dislocation nucleation and growth.

This work is devoted to the description of the recombination and clustering of self interstitial atoms (SIA) and vacancies based on molecular dynamics simulation. Uranium dioxide and molybdenum are considered. The interaction between Mo atoms is described by embedded atom method potential [2]. The interaction between ions in UO_2 is described as in [3]. Two MD models of crystal lattice with defects are considered: only SIAs, SIAs with vacancies [4]. In the first model the clustering of SIA is observed as a result of diffusion and attraction. In the second model the recombination predominates over the clustering. In order to simplify the analysis the second model consists only equal number of SIA and vacancies or the number of vacancies is much larger than number of SIA.

The dependences of concentration of SIA, vacancies and clusters on time are obtained. The comparison of results obtained is carried out with analytical solution of the dependence of the concentration from kinetic rate theory. The comparison shows that the reactions of recombination and clustering can be described as the second order reactions. The rate constants in the dependence on temperature are calculated. The values calculated are in a good agreement with theoretical predictions of diffusion controlled reactions.

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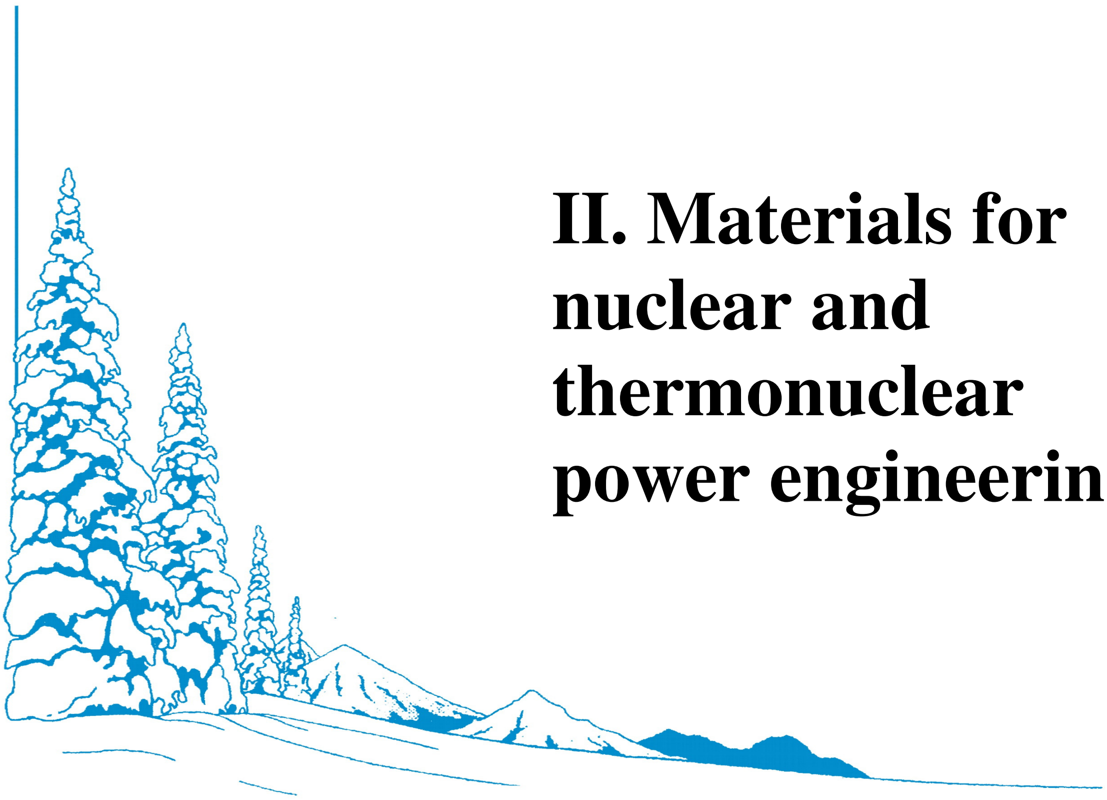

II. Materials for nuclear and thermonuclear power engineering

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).

ATOM PROBE TOMOGRAPHY OF NANOSCALED PRECIPITATES IN 13%Cr ODS STEELS WITH DIFFERENT CONTENT OF TITANIUM

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Structural materials for nuclear fission and fusion power reactors of a new generation must stand for more severe radiation damages at higher temperatures (~ 700ºC). One of possible materials for such applications is ferrite-martensite steels dispersion-hardened with oxides (ODS). Such materials are expected to be able to work up to a damaging dose higher then 140dpa. The specific feature of the ODS steels is a large number of nano-scaled oxide inclusions, which, being the pinning center for dislocations and sinks for point defects, play an essential role in strengthening of the material.

Currently, works on the development of dispersion-hardened steel of the further are intensively performed. The most notable difference is an enhanced content of chromium (higher than 12%), as well as special requirements to the fine structure. Such requirements are traceable, on the one hand, to the need for increased corrosion resistance, which can be gained via increasing the chromium content in the matrix steel. On the other hand, these materials must have the average size of disperse inclusions of about several nanometers (1-3), the total fracton of the inserted oxides being fixed. To achieve such parameters, additional alloying of steels with titanium is employed, which favors the process of refinement of the oxides inserted upon mechanical alloying. Optimal mechanical properties of steels dispersion-hardened with ittium oxides are gained at a titanium concentration from the range 0 – 0.5%. In this work effect of titanium concentration on the nano-scaled state of 13,5%Cr ODS ssteel was studied using the methods of atom probe tomography.

CURRENT ADVANCES IN DEVELOPMENT OF RADIATION-RESISTANT NANOSTRUCTURED MATERIALS (ALLOYED STEELS AND SILICON CARBIDE)

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Nowadays, nanostructure-based approach to the problems of material science is still increasingly employed in researches. Within such approach, capacities of different nanotechnologies are employed which make it possible to create nanostructures with a small (1-2 to ~100 nm) size of main structure components (grains, phase inclusions, layers, and voids). That this approach provides ways to produce various structural and functional materials with a high level of physico-chemical and physico-mechanical properties has been paid attention of both scientists and engineers [1]. As applied to the problem of creation of new radiation-resistant materials, the presence of a significant amount of interfaces (grain boundaries and triple joints), which function as sinks for removing radiation defects, can result in increasing the radiation resistance of nanomaterials , compared to conventional coarse-grained analogs. Therefore, the problem of radiation resistance of nanomaterials is currently of great interest. Information on the nature of radiation processes in nanoobjects is scarce in comparison with that for conventional coarse-grained materials, and studying the properties of radiation defects in nanomaterials has been launched relatively recently. [1-3].

In the presentation, current advances in the development of nanomaterials based on alloyed steels and silicon carbide are described in detail; the influence of irradiation at high-energy-ion accelerators, as well as with neutrons in the reactor experiments has been analyzed. The results of microscopic approaches and simulation by the methods of molecular dynamics are reported. Special attention is paid to an anomalous grain growth, which turns off possible advantages of nanomaterials as radiation-resistant objects.

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INFLUENCE OF HIGH- TEMPERATURE IRRADIATION ON STRUCTURE AND PROPERTIES OF MOLYBDENUM ALLOYS

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Molybdenum is a refractory material and Mo - based alloys are able to withstand rather high mechanical loads under high temperatures. That is why they are advanced materials for application in nuclear engineering. However, the data on a neutron irradiation influence on the structure and properties of Mo alloys at temperatures higher than 1000 °C practically are not available.

Three Mo alloys were investigated, i.e. Mo of commercial grade, Mo alloyed with Zr (0.2 wt.%) and Mo alloyed with Ti (0.4 wt.%). The specimens of these alloys were irradiated in the reactor IVV -2M to fluence $5*10^{20}$ neutron/cm^2 within a temperature range of 1000 to 1250 °C.

The comparative study of the specimens in the initial condition and after irradiation was conducted by using metallography, transmission electron microscopy and micro hardness measurements. As a result, several regularities of deformation and damage after mechanical rupture tests at 1200 °C were revealed.

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METALLOGRAPHIC STUDY OF LONGITUDINAL SECTION OF CONTAINMENT MADE OF U-1,5% Mo-1% Zr ALLOY AFTER EXPLOSIVE LOADING

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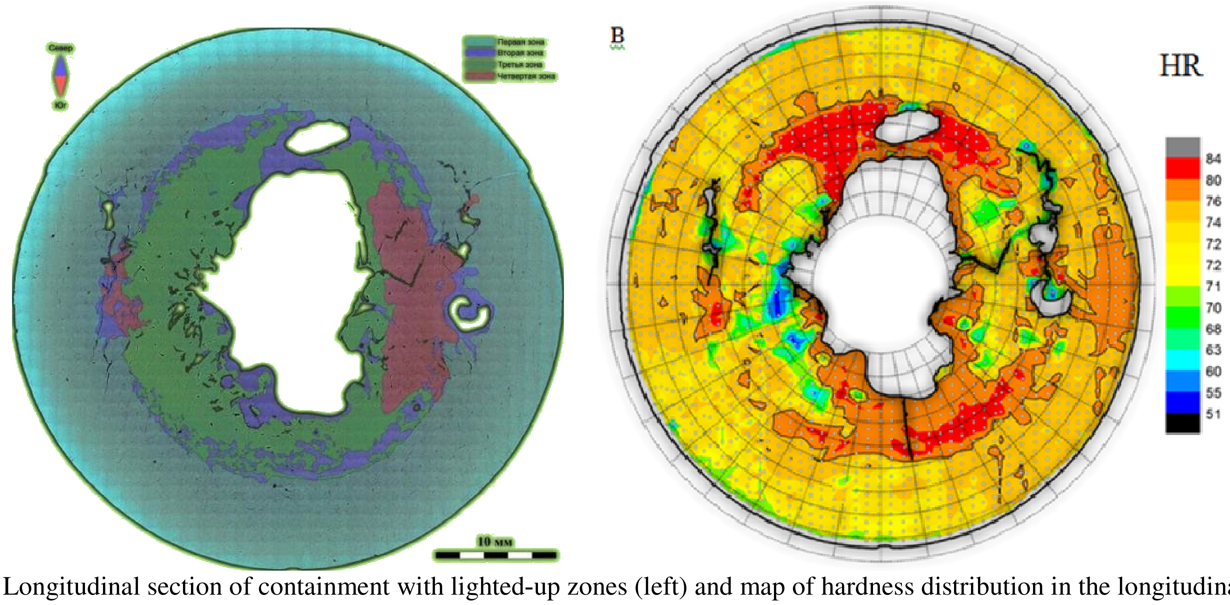
Study of physical properties of a material subjected to a high-rate intense loading is of great interest, since, along with a fast compression of the material up to high pressure values and its adiabatic heating-up, the processes of elastic-plastic deformation, fracture, polymorphic and phase transformations, chemical reactions, phenomena of electrical polarization, ionization, and other physical and chemical phenomena are extremely speedy as well. In this way, a unique possibility of investigation of fundamental properties of materials and nonequilibrium processes under extremal conditions becomes open up. High values of pressure and temperature are momentary achieved most simply and effectively via thorough spherical explosive loading.

The work presents the results of metallographic investigation of a thick-wall spherical containment, made from an alloy of uranium with molybdenum and zirconium, that underwent a shock-wave loading (SWL). The investigation was carried out using methods of optical microscopy and hardness measurements in the longitudinal section of the containment..

There are revealed four approximately concentrically located zones that are featured by different structural state, level of microhardness, degree of defectiveness, concentration, average size, and volume fraction of nonmetallic inclusions.



Longitudinal section of containment with lighted-up zones (left) and map of hardness distribution in the longitudinal section (right).

Processing and presentation of the experimental data which give information on the volumetric distribution of the physical parameters under study was performed with the help of color mapping.

Based on the analysis of the experimental data gained, several conclusions are made on the details of the physical processes taking place in the course of loading and leading to local changes in structural state and defectiveness, as well as on the related structure-sensitive parameters: hardness, microhardness, and distribution of metallurgical inclusions.

SLABBING AND SHEAR FRACTURE, HARDNESS, AND MICROHARDNESS OF CONTAINMENT MADE FROM U–1.5% Mo ALLOY AFTER EXPLOSIVE LOADING

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To develop and verify kinetic many-level strength models of a new generation that open up enhanced prognostic opportunities, systematic experimental data on the kinetics of nucleation, development, and healing of slabbing and shear micro-, meso-, and macrodefects are required. In particular, information is necessary to gain both upon explosive loading of samples and parts and upon subsequent examination with metallographic and fractographic methods.

The aim of this work is to present one of the approaches to attestation of a defective material, as well as a method of processing of the results of statistic analysis of completeness and character of slabbing and shear defects revealed in the longitudinal section of a thick-wall containment made of alloy U-1.5Mo after thorough quasisymmetric explosive loading.

Measurements of distribution of microhardness and macrohardness, as well as of geometrical characteristics of defects, were conducted on the surface of the longitudinal section of the containment undergone explosive loading. Information on the defectiveness is gained through the mathematical processing of large digital panoramas of the longitudinal section.

The suggested method of processing of quantitative data on the defectiveness in relation to definite criteria allowed one to sort all the defects revealed into meso-, micro-, and macrodefects, as well as to specify their position and orientation in the longitudinal section..

Along with the statistic processing, for a more convenient and productive combined analysis of heterogeneous spatially distributed data there was suggested a specially adapted method of color mapping of physical values.

When analyzing, there were studied maps of distribution of defects over orientation, concentration, and size and compared with the map of defect distribution over the longitudinal section. A correlation of the distributions obtained was found and conclusions on their peculiarities conditioned by the processes proceeding in the course of momentary high-intense explosive loading are made.

EXPERIENCE AND METHODOLOGY OF THE ENHANCEMENT OF THE LIFETIME CHARACTERISTICS OF THE BN600 REACTOR SUB-ASSEMBLIES

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The prototype Beloyarsk NPP BN600 reactor power unit has been steadily operating in the mode of the commercial electrical and thermal generation mainly due to the results of the work on the introduction of the advanced designs and materials of the fuel sub-assemblies, control rods and other reactor sub-assemblies. The evolution of the BN600 core which has undergone three modifications for 32 years of operation is continuously accompanied by the enhancement of the lifetime characteristics of the standard and experimental reactor sub-assemblies.

The additional R&D were required as early as at the first stage of bringing the core to full power in the 80s of the last century when the design characteristics of the core of the first type of loading (core 01) with the fuel burnup of 10 % of h. a. were not achieved due to the inadequate reliability of the design structures and materials. The utility was obliged to decrease both the peak burnup of the oxide uranium fuel down to 7.2 % of h. a. and damage dose of the materials down to 44 dpa with the fuel sub-assembly lifetime equal to 200 to 300 efpd.

As a result of the first core modification (core 01M) carried out in 1987 the burnup was increased up to 8.3 % of h. a., the peak damage dose up to 54 dpa and the residence time up to 330 efpd. The design fuel burnup of 10 % of h. a. was achieved only in 1993 due to the second modification of the core (core 01M1) with the fuel sub-assembly lifetime equal to 480 efpd with the peak damage dose of 75 dpa. The first two modifications were carried out as a result of the accomplishment of "The first comprehensive programme of the development of the radiation-resistant materials for the fast reactor cores" by a number of the industry enterprises (Pervouralsky Novotrubny Works, All-Russian Research Institute of Inorganic Materials, IPPE, Research Institute of Nuclear Reactors, Sverdlovsk Branch of Research and Design Institute of Power Engineering, Beloyarsk NPP) on the basis of the comprehensive testing and study of a number of the prototype and commercial steels of three grades as followed by the selection of the most radiation-resistant ones among them. For the manufacture of the wrappers of the standard fuel sub-assemblies of core 01M2 the 12Cr13Mo2NbVB ferritic-martensitic steel (EP450-Sh) was chosen whereas for the manufacture of the fuel cladding the cold-worked 06Cr16Ni15Mo2Mn2TiVB austenitic steel (ChS68 c. w.) was selected.

The third modification of the core (core 01M2) was prepared in the first decade after the breakup of the Soviet Union and significant shortening of the scientific and technical support of the state. The BN600 reactor was changed over to core 01M2 without any change in the design of the sub-assemblies and materials of their components owing to the organizational and technical measures taken by the concerned organizations under the circumstances of the transfer of the manufacture of the wrapper and cladding tubes from the Pervouralsky Novotrubny Works to the Mashinostroitelny Zavod in Electrostal. The third modification was accomplished in 2004 to 2006 after the reliable computational and experimental justification of the enhancement of the lifetime characteristics of the standard reactor sub-assemblies had been developed. The lifetime was extended on the basis both of the systematic step-by-step adoption of the engineering solutions by the utility to extend the length of particular cycles of the reactor in the period of 1995 to 2003 and testing of the standard fuel sub-assemblies about 1000 in number with 560 accumulated effective full power days or less. With core 01M2 the reactor has been successfully operating in the standard mode since 2006 with the fuel sub-assembly lifetime of 560 efpd up to the peak design fuel burnup values of 11.1 % of h. a. and damage doses of 82 dpa. For recent six years of the operation of the third modification core no fuel pin failures of the standard fuel sub-assemblies occurred.

The report presents the methodology of the post-irradiation examination of the fuel sub-assembly serviceability as developed on the basis of the experience accumulated during technological investigations of the main (nonirradiated) condition of the structural materials and post-irradiation investigations of the condition of the irradiated components of the reactor sub-assemblies accumulated extra effective full power days.

Now using this methodology the achievement both of the immediate goal, i. e. the extension of the lifetime of the bulk of the standard core fuel sub-assemblies up to 592 efpd with the fuel burnup of 11.7 % of h. a. at a damage dose of the cladding manufactured of the cold-worked ChS68-ID steel of the new generation as high as 87 dpa, and next stages, i. e. the increase both of the peak fuel burnup values up to about 14 to 16 or 19 % of h. a. and damage dose up to about 104 to 116 or 140 dpa with the replacement of the cladding material by the improved cold-worked EK164-ID steel, is studied.

SWELLING OF FUEL CLADDING MADE OF 304SS(SA) STEEL AS A FUNCTION OF THE IRRADIATION TEMPERATURE AND FAST NEUTRON FLUENCE

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The report presents the results of the analysis of the parameters of the dependences of the swelling of the fuel cladding manufactured of 304SS(SA) steel on dose and temperature. The data obtained during the old experiments designated PNL3, PNL4 and PNL5 in the irradiation temperature range from 380 to 500°C at a fluence of fast neutrons with E>0.1 MeV as high as $1.5\cdot10^{23}$ n/cm^2 or less were kindly provided by Dr. F.A. Garner. With neglecting the irradiation temperature effect on swelling in the above-mentioned temperature range the swelling rate actually amounts to the universal value in the range from 2 to 4 % / 10^{23} n/cm^2 as interpreted as 1 % / dpa.

However taking into account the typical distributions of the neutron fluence (damage dose) and coolant temperature as taken place along the height of the fast reactor fuel pins it seemed interesting to analyze the experimental data considering the actual temperatures of the irradiation of the PNL3, PNL4 and PNL5 specimens. The analysis was conducted in the framework of the simple presentations. The plots of the change in the volume of the specimens cut out from the fuel pin cladding sections with actually the same irradiation temperature versus dose were made. On their basis the incubation dose and swelling rate versus irradiation temperature were determined.

The relationships were compared with the similar ones obtained in [1] for the 18Cr-10Ni-Ti steel irradiated in the BOR60 [2] and BN600 reactors at damage dose rates of $7\cdot10^{-7}$ dpa/s and $2\cdot10^{-7}$ dpa/s respectively.

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INTERACTIONS BETWEEN VOID SWELLING AND IRRADIATION CREEP IN THICK 304 STAINLESS STEEL REFLECTOR BLOCKS IN RESPONSE TO GRADIENTS IN NEUTRON FLUX-SPECTRA AND IRRADIATION TEMPERATURE

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Void swelling and irradiation creep are life-limiting phenomena for components of fast and light-water reactors, requiring predictive equations to forecast limits of operation. It is not generally recognized, however, that such equations were developed from limited numbers of specimens, generally of thickness 0.3-1mm. In such configuration there are no significant variations in temperature, stress or neutron flux-spectra across the thickness. In actual reactor components, however, thicknesses can be larger with gradients not only in environmental variables but in the resulting distribution of stresses and strains. There are currently no benchmark data fields that allow confident incorporation of such "thin" equations in design codes for "thick" and complex shapes, especially since swelling-creep interactions determine the local stress field and feed back into swelling and creep strains.

A series of five hexagonal cross-section reflector blocks (annealed 304SS, 50mm flat-to-flat, ~250mm length) were vertically stacked in a thin-wall hexagonal 304SS can in Row 8 of EBR-II in flowing sodium. During their residence they accumulated 0.5-33 dpa depending on axial position. Over the stack there were significant axial and radial gradients in both dose and temperature with gamma heating leading to significant internal temperature increases, producing a complex spatial distribution of swelling and creep strains.

Four of these blocks have been subjected to non-destructive examination, and two of these to extensive destructive examination thereafter. Measurements involved profilometry, ultrasonic exam, density change and electron microscopy. It was found that the complex internal distribution of microscopic strains arising from void swelling and carbide densification can be related to the macroscopic deformation of the blocks, producing slight bulging and twisting. The strains of the blocks could also be correlated with the strains of the hexagonal can that housed them.

ION-INDUCED VOID SWELLING OF FERRITIC-MARTENSITIC AND ODS-FERRITIC ALLOYS AT 100-600 DPA AND 400-550°C

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Austenitic steels have traditionally served as fuel cladding for fast reactors but their tendency to exhibit high void swelling at doses of ≤150 does not allow fuel burn-ups greater than ~12%. From the viewpoint of fuel economy ~30% burn-up would be optimum. However, that requires a cladding material that could reach higher doses without significant swelling. Two classes of material might serve to reach this goal. The first are ferritic-martensitic (FM) alloys and the second is oxide-dispersion-strengthened (ODS) ferritic alloys.

Unfortunately available test reactors cannot reach 200 dpa in 10-20 years, which is the minimum dose required to assess the swelling resistance of new alloys. Although charged particle simulation can reach such doses in much shorter time, there is insufficient understanding of the differences involved to allow confident prediction of neutron-induced swelling, but self-ion irradiation can forecast the relative swelling resistance of various alloys and can identify the eventual steady-state swelling rate.

An extensive series of ion irradiations using 1.8 MeV Cr^+ ions has been conducted at $1x10^{-2}$ dpa/sec on HT9, EP-450 and MA957 (ODS) alloys. After determining the optimum irradiation temperature at 100 -200 dpa, then irradiations are conducted to much higher doses, usually terminating the experiment if swelling exceeds 20%. The results indicate that the eventual steady-state swelling rate of FM alloys is ~0.2%/dpa, one fifth that of austenitic alloys. The duration of the transient regime is rather variable, however. Ferritic alloys generally enter the higher swelling rate regime at ~150 dpa, but tempered martensite alloys wait until 300-400 dpa. ODS alloys usually have a ferrite matrix and the swelling resistance of this class is critically dependent on how well distributed are the oxide dispersoids. In cases where the dispersion is highly variable the swelling in individual grains can vary from 0 to 50% at 400 dpa.

SECOND-ORDER RADIATION PHENOMENA IN AUSTENITIC AND HIGH NICKEL ALLOY INTERNAL COMPONENTS GROWING TO FIRST ORDER IMPORTANCE AT THE HIGHER DAMAGE LEVELS ASSOCIATED WITH PWR PLANT LIFE EXTENSION

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Austenitic stainless steels, especially AISI 304 and 316, form the core internals that frame and support the cores of pressurized water reactors. In some reactors alloys such as Inconel 600 or 718 were also used for selected in-core applications such as guide tubes and springs. The near-core portion of the baffle-former assembly receives relatively high neutron exposures (40-100 dpa) over a 40 year life-time. Extending the lifetime of these components to 60 or 80 years will lead to correspondingly higher damage exposures.

Within the 40 year licensing period a number of issues of first-order importance have been addressed, especially embrittlement, IASCC and irradiation creep. A number of second-order issues have been recognized but not considered to be life-limiting or deleterious. However, the non-linear nature of a number of second-order processes gives cause to worry that they might become first-order with extension of PWR life-times.

The first of these second-order process is the void swelling phenomenon which is clearly a non-linear and non-saturable process. The second of these second-order processes is the progressive promotion of the five naturally occurring isotopes of nickel to higher atomic weight via transmutation. One product of this transmutation sequence is the production of Ni-59, a non-naturally occurring isotope that continues to increase in concentration until a thermal neutron fluence of about 4×10^{22} n/cm^2 has been reached. The consequences of the Ni-59 production are a very high and continuously accelerating production of helium and hydrogen, concurrent with a generally unrecognized increasing rate of atomic displacement and increased nuclear heating, the latter two consequences arising from the highly exothermic nature of the Ni-59 (n, α) and (n, p) reactions. These processes become increasingly important for higher nickel alloys such as Inconel 600 and 718.

The third process is the now well-known tendency of hydrogen to be stored in helium-nucleated bubbles and voids, and for the increasing storage to promote formation of very high densities of bubbles not only in the matrix but also on grain boundaries. Cracks moving along grain boundaries or through the matrix will constantly be intersecting cavities filled with hydrogen with possible consequences on accelerated cracking.

The fourth process is the generally unrecognized but progressive radiation-induced movement of 300 series steels toward stress-induced martensitic instability, especially at very high damage levels.

These four processes will be shown in this paper to have already begun to reveal their growing presence. Based on the known parametric dependencies of these four processes it is expected that they will most likely interact in a very synergistic manner. These processes should be studied proactively before they become truly first-order in importance.

SWELLING, CREEP AND EMBRITTLEMENT OF D9 STAINLESS STEEL CLADDING AND DUCT IN FFTF DRIVER ASSEMBLIES AFTER HIGH NEUTRON EXPOSURE

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This report focuses on the swelling, creep and embrittlement behavior of 20% cold-worked D9 cladding and duct used in two mixed-oxide driver subassemblies designated D9-2 and D9-4. These assemblies were irradiated in the FFTF fast reactor to maximum exposures of 25.3 and 21.4×10^{22} n/cm^2 (E>0.1 MeV). The D9-2 subassembly operated at somewhat lower temperatures compared to those of D9-4, leading to different swelling behavior. Since the D9-4 duct operated at lower temperatures than the cladding, the swelling of the duct was relatively low, peaking at 6-7%. The fuel pin cladding reached swelling values of 21-28% in D9-4 and 37-38% in D9-2, with much of the pin having attained the terminal swelling rate of ~1%/dpa.

Void swelling was observed to vary with dpa rate, irradiation temperature and small heat-to-heat differences in composition, especially phosphorus. While no significant pin failures were observed during in-reactor operation, failure arising from severe void-induced embrittlement occurred in D9-2 fuel pins and duct during post-irradiation handling.

CORROSION OF IRRADIATED GRAPHITE AT ROOM TEMPERATURE IN A WET OXYGEN–CONTAINING AND OXEGENLESS ENVIRONMENT

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All the spent nuclear fuel from the reactors AMB-100 and AMB-200 of the First stage of the Beloyarsk NPP was removed from the reactors and is stored in two decay pools (BV-1 and BV-2). It is in the assemblies made of st. st. ”12Х18Н10Т” and carbon steel ”Ст.3”. The assemblies contain from 17 to 35 spent fuel element assemblies (SFEA). Approximately 36 % of all the SFEA are in assemblies designated “К-17у” made of carbon steel ”Ст.3”, that has a low corrosion resistance in water and is effected by both uniform corrosion and pitting. A life time of wet storage of case tubes of assemblies ”К-17у” was determined from the measurement data of water activity in the decay pools and is ~14.5 years. As a result of a long–term storage of 25 to 45 years (that exceeds the ‘wet” shelf time) in water of the decay pools the assemblies “К-17у” lost tightness of case tubes of all the assemblies ”К-17у” and the SFEA were found in contact with water of the BVs.

In order to eliminate that all the assemblies with SFEA were reloaded for “dry” storage into cases “PT5015.02” made of st.st. ”12Х18Н10Т”. The reloading does not include dewatering of the assemblies and discharge of water from the case tubes. A possible water quantity determined from a difference of mass of the assemblies with the SFEA before the loading and after the removal of water from the BVs can be not less than 350 l. In such conditions the corrosion processes will continue in cases “PT5015.02” with a participation of the component contained in the SFEA and assemblies “К-17у”. One of such component sis irradiated graphite of graphite bushings in the area of the radioactive column of SFEAs, the weight and surface areas of which can be about ~55 kg and ~6.3 m^2, respectively. Depending of the gas environment content the corrosion products of graphite bushings there can be CO, CO_2 and CH_4, containing radionuclide ^{14}C.

The Decision of the SC «Rosatom» № 1-2.5/6819 of 04.08.2010 states that the final stage of handling with the spent nuclear fuel of AMB reactor of the BNPP is a radiochemical reprocessing at the plant “PT-1” of «PA «Mayak». However, at present time there is no technical possibility to receive and reprocess spent nuclear fuel of AMB reactor of the BNPP, therefore it will be stored for undetermined time at the BNPP site. In order to substantiate and secure safety storage this fuel will stay in cases “PT5015.02” and then be transferred in transportation package design “ТУК-84/1” to на «PA «Mayak». For that the data on the kinetics of changes of the gas parameters (pressure, composition, temperature, humidity) are needed for a long time, that includes time for all the stages of transport–technology operations with the spent nuclear fuel of AMB reactor. The field tests were conducted for 247 days in sealed tight case “PT5015.02” in not dewatered assembly ”К-17у” #137 containing 16 SFEA after its stay in water of “BV-2” for 42.6 years. From the test results the corrosion rates of graphite bushings at RT were determined to be:

- $1.26\cdot10^{-2}$ g-mol/(m^2·day) and $1.44\cdot10^{-3}$ g-mol/(kg·day) in air environment with a formation of carbon dioxide gas,

- $1.04\cdot10^{-4}$ g-mol/(m^2·day) and $1.18\cdot10^{-5}$ g-mol/(kg·day) in oxygenless environment with a formation of methane.

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MICROSTRUCTURE AND MECHANICAL PROPERTIES OF BORON-ALUMINUM COMPOSITES WITH FUNCTION OF THE NEUTRON PROTECTION PRODUCED BY HOT ROLLING METHOD

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In the atomic engineering there exists a great demand for a special functional material for production of transport packaging containers (TPC) used for transportation of the irradiated fuel waste.

As such materials, there are widely employed aluminum-matrix composites reinforced with particles of boron carbides (Borals). Application of aluminum or its alloys as the base for a composite material results in an effective decrease of mass and helps heat removal, whereas filling the material with carbon particles provides radiation protection of products

In the work, the possibilities of production of non-detachable composite materials using a simple method of hot rolling have been investigated and conditions for compacting powder mixtures with micro and nanosize particles of boron carbide that provide the function of neutron shielding are determined. The influence of composition of the powder mixture, dispersity of boron carbide particles, and peculiarities of delamination of the layered composites made from aluminum and its alloys with a powder interlayer have been studied.

It is shown that the boron-aluminum composites produced by hot rolling possess enhanced mechanical characteristics in comparison with the metal bases AB and AMr3. The highest strength properties ($\sigma_{0,2}$ = 236 MP; σ_B = 273 MP) in combination with a satisfactory plasticity level are achieved in composites containing nanosize powder interlayers of boron carbides. The method of production of sheet boron-aluminum composite developed in this work was patented 08.06.2011, patent №2011123237.

Also, there were developed technological grounds for the production of monolith boron-aluminum composites by the method of hot rolling of a mixture of powders of boron and aluminum placed in a closed metallic case.

Promises for increasing the strength and fracture toughness of Borals can be realized via employment of external sheet cases made of aluminum alloys with an increased strength, dispersion of structure of layers by intense plastic deformation and additional introduction in the composition of powder mixtures of an interlayer with reinforcing disperse fibers.

EVOLUTION OF FINE STRUCTURE OF AUSTENITIC STEEL «CHS68» UNDER HIGH –DOSE NEUTRON IRRADIATION AND ITS RELATION TO RADIATION SWELLING

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An effect of neutron irradiation on austenitic steels used as fuel pin cladding in fast neutron reactors causes integrated structural changes such as a formation of dislocation loops and vacancy voids, a proceeding of segregation processes that lead to changes in the crystal matrix and a formation of secondary phases. All that makes a deleterious effect on changes in sizes and physico–mechanical properties of fuel elements.

A determination of characteristics of a fine structure of a steel in its original state and after an operation life permits to obtain information on the processes that take place under irradiation; the information is needed to predict physico–mechanical properties of fuel pin cladding. An original structure state influences an amount of deleterious changes (swelling, embrittlement and etc.,), occurring under irradiation. This paper describes the study of the evolution of a microstructure of austenite steel « ChS68» as a material of fuel pin cladding of BN -600 reactor by the methods of X-ray structure and electron- microscopic analyses. The evolution was studied as dependent on temperature and neutron irradiation dose. The study was aimed to reveal a relation of the evolution of the steel with its compliance to radiation swelling and an influence of the evolution on the physico- mechanical properties of the steel.

The results of the X –ray structure and electron- microscopic analyses of steel « ChS 68» after neutron irradiation within a temperature range of 370 to 580°C and doses to 80 d.p.a. are presented in this paper. For a range of 370 to 430 °C it is shown that a crystal lattice parameter and micro-stresses increase with irradiation dose and a degree of the micro–stresses varies significantly for different pin cladding. The changes in the lattice parameter and micro–stresses resulted from a formation of radiation defects and a change in a crystal matrix content. For higher temperatures 550…580 °C a decrease in the lattice parameter is observed, the decrease is mainly due to interstitial impurities leaving a solid solution for carbides that are forming. A back correlation of the lattice parameter in an unirradiated condition of the steel along with a compliance of the material to radiation swelling was noticed.

FERRITE FORMATION IN AUSTENITIC ALLOYS IRRADIATED IN BOR-60 AND HFIR NUCLEAR REACTORS

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Austenitic stainless steels are important structural materials common to various fusion and fission reactor systems. Usually these steels are nonmagnetic, but high-energy particle irradiation (e.g., neutrons and ions) can lead to the formation of magnetic phases, principally ferrite. Radiation-induced formation of magnetic phases may impact the material’s performance, and this could be especially important for fusion reactor systems which use high-strength magnetic fields. Also, the corrosion behavior of material with radiation-induced magnetic phase might be different from that of the base steel.

In the present work, the formation and accumulation of magnetic phases has been studied for a set of industrial austenitic steels and model austenitic alloys. These included AISI 304 and 316 steels and high-purity model alloys based on AISI 304 and AISI 316 compositions. The investigated alloys were irradiated in the Russian BOR-60 fast reactor at 5–47 dpa at 593K and in HFIR reactor at 0.7 dpa at 363-563K.

To measure the amount of magnetic phase in both nonirradiated and irradiated samples, a Fisher FMP-30 ferroprobe unit was employed. The device was calibrated using a regular set of etalon samples with delta-ferrite. The microstructure of the radiation-induced magnetic phase was characterized using scanning and transmission electron microscopy, and also electron backscatter diffraction. It was found that the magnetic phase was present in all irradiated alloys. The amount of magnetic phases increases with increasing damage dose in the range of 0–10 dpa, approximately following a linear relationship. Further increase of damage dose did not change the amount of magnetic phase significantly.

The results were analyzed using thermodynamic parameters associated with the ternary Fe-Cr-Ni phase diagram. A mathematical model was developed that relates the amount of magnetic phase with alloy parameters (element composition, grain size, cold work level). It was established that silicon and manganese additions strongly increase the rate of ferrite accumulation, but molybdenum and carbon additions tend to resist ferrite accumulation.

MARTENSITIC INSTABILITY DURING PLASTIC DEFORMATION OF HIGH IRRADIATED AUSTENITIC ALLOYS

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Austenitic stainless steels are prone to martensite formation during deformation, with increasing tendency as the nickel-equivalent decreases and temperature decreases. However, the question of how irradiation impacts the steel's stability is not well-defined. Some recent papers show that neutron irradiation tends to accelerate martensite instability, and it could be an issue during long term operation of nuclear power plants.

In the present work, martensitic transformation during plastic deformation has been studied for a set of commercial purity austenitic steels and model austenitic alloys. These included AISI 304 and 316 steels and high-purity model alloys based on AISI 304 and AISI 316 compositions. The investigated alloys were irradiated in the Russian BOR-60 fast reactor at 5–47 dpa at 593K.

To evaluate phase and structure transformations (twinning, α- and ε- martensite) electron backscattering diffraction (EBSD-OIM) has been employed. Also, magnitometry has been used to measure the amount of martensite in small deformed regions of miniature specimens. Finite element analysis (commercial COMSOL v.4.3. FEA software) has been employed to evaluate stress and strain distribution in the deformed samples.

For nonirradiated and irradiated alloys critical stresses and critical strains required to produce martensite are studied as a function of damage dose and material starting condition. , Kinetic of martensite accumulation are investigated for nonirradiated and irradiated alloys; special attention has been paid to possibility of martensite formation below yield stress limit (“stress” or “elastic” martensite).

Morphology of martensite as function of irradiation, stress and strain are analyzed and discussed. Using OIM data, nucleation sites for α- and ε- martensite formation were analyzed in details.

THE ROLE OF SCALE FACTOR DURING TENSILE TEST OF IRRADIATED METALS AND ALLOYS

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Miniature specimens are widely used to investigate the tensile behavior of irradiated metals and alloys, nanostructured materials, and different composites. At the same time, it is well known that dimensions and geometry of the sample can influence test results, and geometry and scale factor are one of the reasons lead to data scatter (a potential problem in analytical studies).

The main objective of the present study was to compare mechanical properties obtained using four different widely used tensile specimens which were machined from the same heats of materials. A comparison of the tensile properties determined with miniature specimens types was made by testing cold-worked and solution-annealed wrought 316L and modified cast austenitic stainless steels, and F82H and A522B ferritic steels. Samples of SS-1, SS-2, SS-3, and SS-J3 types, which are widely used in radiation material science, were tensile tested at room temperature at strain rate 0.00109 s^{-1} with use of optic extensometry method. The results (engineering mechanical properties and 'true stress – true strain' curves) were compared with standard ASTM sub-size type specimens.

An additional specimen type, SS-mini, was offered and evaluated. This specimen can be useful for special purpose experiments, for example, evaluation of welds.

Influence of geometry parameters (thickness to width and length to width ratios) and thickness to grain size ratio on mechanical test result was analysed in details for small specimen types listed above. Influence of sample geometry on tensile test results, peculiarities of neck formation and deformation localization development were discussed details using optic extensometry and full-field strain measurement data.

INFLUENCE OF THERMAL AGEING AND ION IRRADIATION ON NANOSTRUCTURE OF FERRITIC-MARTENSITIC STEEL RUSFER EK-181

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Heat resistant reduced activation steels are the most promising structural materials for new generation fusion and fission nuclear reactors. Elevated mechanical properties of this material at higher temperatures considered to be connected with formation of nanometer size structural features (different types of clusters and segregations) during heat treatment, that might serve as pinning centers for dislocations and sink for point defects. In Russia the foremost focus is set to 12% chromium ferritic-martenitic EK-181 steel with increased heat resistance [1-2].

Mechanical properties degradation of reactor materials is caused by ion irradiation and high temperature. Whereas disperse particles play a key role in mechanical properties alterations [3], information about behavior of microstructures these materials under influence of high tempreture and irradiation is necessary. The aim of present work is to study alterations in nanoscale state of steel RUSFER EK-181 by tomographic atom probe microscope after thermal ageing and ion irradiation. In this work iron ions were used, what allowed to simulate influence of cascade defect formation, that took place in reactor irradiation, on the fine structure of the material under investigation.

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THE CONCEPT OF THE INITIAL EXITED STATE AS THE CENTRAL LINK OF THE NEW PARADIGM FOR QUICKLY PROCEEDING MARTENSITIC TRANSFORMATIONS

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For martensitic transformations (MT) in alloys on the basis of the transitive metals possessing strongly pronounced signs of first-order transitions are characteristic considerable deviations from temperature of balance of phases. A typical example of such MT is $\gamma - \alpha$ MT in iron alloys.

Available experimental data specify on supersonic (in relation to longitudinal waves) growth speed of separate martensite crystals. In essence this fact long time was ignored, as couldn't be explained within the limits of existing theoretical representations. Really, for first-order transition , in the constrained conditions of a solid state, a presence or an occurrence (at a stage of heterogeneous nucleation) the quasiequilibrium nuclear representing localized area with different symmetry of a lattice, isolated from an initial phase (austenite) by some border. For such border the dislocation nature was traditionally supposed. Then growth of a crystal with necessity should be reduced to the analysis of a movings of a border. But it is possible to show [1] that moving of dislocations with supersonic speed demands the stress exceeding the theoretical ultimate strength, that is physically is not realized for spontaneous MT. The decision of the specified problem and the whole complex of problems connected with it became possible after understanding that the traditional picture of growth of crystals isn't unique.

Other scenario (leading to the adequate description of all observable features of MT) is based on the concept of the initial exited (oscillatory) state triggering a mode of supersonic growth of martensite crystals [1, 2]. Specificity of heterogeneous nucleation in elastic fields of rectilinear segments of separate dislocations is reflected by:

- the form of the exited state the extended rectangular parallelepiped (constructed on own vectors of a tensor of elastic deformations of defect);

- the type of threshold deformation (as a rule, deformation with a weak distortion plane);

- the characteristic spatial scales (the cross-section size of the exited state makes an order of a hundredth part of the size of volume which is free from defects).

The additional account of the mechanism of generation of elastic waves by nonequilibrium electrons and the inclusion in structure of the control wave process, along with the pairs of quasilongitudinal displacement waves (which are responsible for the formation of the habit plane), the shorter longitudinal waves allow to solve such fundamental problems as existence of the critical size of grain for MT occurrence (and also to obtain its important consequences) and the description of supersonic formation of fine twin structure within martensite crystals.

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ATOMIC SCALE INVESTIGATION OF PHASE DECOMPOSITION OF Fe-22%Cr SOLID SOLUTION DURING THERMAL AGING

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The comprehension of the processes mechanisms in condensed matter at the nano-and atomic-scale levels as well as study of the correlations between these changes and macroscopic properties is a key goal of modern science of materials. Considerable efforts are focused on binary iron based systems as basic for the structural materials industry, mainly Fe-Cr alloys. This binary alloy is notable for formation and behavior peculiarities of defect structure. The explanation for this behavior was given in the past few years, where the key role of magnetism in the interaction of atoms in the lattice was shown with ab initio calculations. This result requires a review of the theoretical concepts and calculations of the defect structure properties. To verify the developing models experimental data on these alloys nanoscale changes under the influence of various factors such as temperature, radiation, etc. is required.

The increase of the chromium content in the alloy results in better corrosion resistance. However the excess of Cr concentration over 10% leads to phase decomposition in the solid solution in α and α' phases (iron- and chromium-rich, accordingly). Formerly, the main techniques of experimental investigation of phases mentioned were: microhardness and magnetoresistance tests, Messbauer spectroscopy, small-angle neutron scattering, transmission electron and field-ion microscopy. However, all these techniques provide not the full data. Therefore, recently the atomic probe tomography has become widely spread. The instrument allows the three-dimensional reconstruction of up to hundreds of millions of atoms with a resolution of 3Å and the associated chemical information, thereby providing the most complete information about the alloy behavior in the phase decomposition.

The present work is devoted to nanoscale quantitative investigation of phase decomposition of Fe-22at.% Cr binary model alloy during thermal aging using atom probe tomography. It is shown that the behavior of supersaturated solid solution over time does not fit classical behavior - the theory of Lifshitz-Slezov. The stages of nucleation, growth and coalescence are considered, their parameters are quantitatively described.

APPLICATION OF SURFACE OXIDATION FOR MECHANOSYNTHESIS OF Fe-BASED OXIDE DISPERSION-HARDENED MATERIALS

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Creation of new high-strength steels and alloys, including reactor materials that possess high creep and long-term strength is a topical problem of material science. Conventional strengthening of steels is realized via precipitation of particles (carbides, nitrides, intermetalics) which hamper the motion of dislocations. Along with the above types of strengthening particles, of significant interest are disperse oxides.

Steels and alloys dispersion-hardened with oxides (DHO) of yttrium and titanium are highly resistant to such external factors as high temperatures and neutron irradiation. This is conditioned, on the one hand, by a high thermal stability of oxides and, on the other hand, enhanced resistance to vacancy swelling owing to a large number of sinks of point defects in the form of boundaries of nanooxides. Note that no ordinary refinement of initial high-strength yttrium oxides to 2-4 nm takes place upon a prolonged milling of powders in a ball mill.

Earlier we proposed a new approach to creation of new reactor DHO steels and alloys, whch consisted in the involvement in the process of mechanical alloying of low-stable iron oxides as oxygen carriers, which upon deformation dissolve in metallic matrixes essentially easier than yttrium oxides that are difficult to dissolve because of high energy of interatomic bonding. It was shown that the employment of iron oxides as an initial phase significantly accelerates the process of formation of solid solutions of oxygen in steels upon mechanoactivation, which provides the precipitation of disperse oxides of Y and Ti 2-4 nm in size in the course of subsequent high-temperature annealing, provided the steel was preliminarily alloyed with these elements.

Along with the reactor materials which are hardened with yttrium and titanium oxides, high-strength materials without these costly elements are in demand as well. We performed a series of works on the strengthening of pure iron with the iron oxides. As the starting material, a powder of pure iron was subjected to surface oxidation by heating in air, which results in the formation of an oxide film on the powder surface. A subsequent treatment of the powder in the ball mill led to a dissolution of the oxide film due to its fragmentation upon deformation and development of the low-temperature diffusion of oxygen atoms into the material bulk. This is accompanied by the formation of solid solutions of oxygen and subsequent precipitation of secondary oxide particles upon annealing.

The work was supported by the Russian Foundation for Basic Research (project № 10-03-001130) and the Presidium of RAS (project 12-П-2-1043).

MECHANICAL SYNTHESIS OF MODEL STEELS ALLOYED WITH INTERSTITIAL ELEMENTS (B, N) FOR PERSPECTIVE APPLICATION IN REACTOR INDUSTRY

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The results of investigation of model alloys of iron with interstitial elements that were produced by the methods of severe plastic deformation via shear under pressure and via mechanoactivation in ball mills are reported. Using Mossbauer spectroscopy, X ray analysis, measurements of magnetic susceptibility, and electron transmission microscopy, it has been established that the deformation-induced processes in the samples produced proceed with the formation of solid solutions saturated with nitrogen and boron in quantities that cannot be achieved with the conventional modes of treatment applicable in material science. Data gained in the course nanostructured phase transformations involving disperse borides and nitrides are of practical interest for designing materials resistant to external actions (in particular, to irradiation), which are in demand in reactor industry [1-2].

Analysis of the experiments conducted presents evidence to the formation of a oversaturated crystalline solid solution of the interstitial type in the FCC matrix of Fe-Ni alloys with a concentration of boron of 1…3 at.%. The oversaturated solid solution is unstable and coexists with metastable borides of the $(FeNi)_3B$ type.

Deformation of stainless steel nitrided by plasma sputtering is accompanied by a reverse phase transition $\alpha \rightarrow \gamma$, dissolution of nitrides, formation of solid solutions oversaturated with nitrogen and secondary nanonitrides.

The work was carried out according to the theme “Structure” and supported by Ural Branch of RAS (projects № 11-2-9-PRO and 12-U-2-1020) and Russian Foundation for Basic Research (projects № 12-03-00040-a and 12-03-00929-a).

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EFFECT OF STRESSES ON DEVELOPMENT OF VACANCY VOIDS, SWELLING AND CREEP STRAIN IN IRRADIATED BY NEUTRONS Fe-18Cr-10Ni-Ti AUSTENITIC STEEL

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This paper presents the results of a research of the influence of compressive and tensile stresses on swelling, microstructure and creep strain of Fe-0.08C-18Cr-10Ni-Ti steel. The gas-pressurized specimens of complicated geometry (standard and coaxial) were fabricated from austenitic steel Fe-0.08C-18Cr-10Ni-Ti. They were irradiated in the BOR-60 reactor at 350 – 420°C up to a damage dose of over 70 dpa.

We used the methods of researches the physical and mechanical properties of steels and changes in linear dimensions of gas pressurized samples, metallography, microhardness to obtain reliable results the influence of stress on swelling and deformation creep. Research of the microstructure of both irradiated and unirradiated gas-pressurized specimens was performed by means of transmission electron microscope JEM-2000FXII [1].

We made comparisons between the influence of compressive, tensile and "zero" stress on the swelling, parameters of vacancy voids and creep Fe-0.08C-18Cr-10Ni-Ti steel. The results can be used to test models of the influence of different types of stress on irradiation swelling and deformation creep.

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PHASE γ→α'-TRANSFORMATION DURING LOCALIZATION OF DEFORMATION OF 12Cr18Ni10Ti STEEL IRRADIATED WITH NEUTRONS

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In modern reactor materials science great attention is given for studying of martensitic transformation during deformation of irradiated austenitic stainless steels. Studying of localization of deformation influence on γ→α'-transition is especially important.

Cylindrical stainless steel samples were austenizated (1050°C, 30 minutes) and irradiated in WWR-K nuclear research reactor core at <80°C. Fluencies were up to $1.3 \cdot 10^{20}$ n/cm^2. Mechanical tensile tests were conducted with strain rate 0.5 mm/min at room temperature. During plastic deformation amount of martensitic α'-phase, induced in the sample and sample's geometry changes were registered.

As a result of experiments graphs "«true» stress – local «true» deformations" and martensitic α'-phase deformation dependence were constructed. "True" characteristics of strength (σ), plasticity (ε) also kinetics of martensitic transformation parameters were defined.

The concept of intensity of martensitic transformation as «$dM_f/d\sigma$» function is offered. Changing of martensitic γ→α'-transition intensity values during plastic deformation is analyzed. During the analysis maximums on «$dM_f/d\sigma$-σ» curve located in limits 800-1200 MPa are found.

Using existing results conclusions of several stages existence during plastic deformation localization are made.

ATOM PROBE TOMOGRAPHY OF RADIATION INDUCED PRECIPITATES IN FERRITIC-MARTENSITIC STEEL EUROFER97 AFTER NEUTRON IRRADIATION IN BOR-60 UP TO 32 DPA

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In current paper 9%-Cr reduced activation ferritic martensitic steel Eurofer97 irradiated in BOR-60 reactor up to 32 dpa (at 332°C) has been studied by means of atom probe tomography. Data analysis revealed the high number density (10^{24} m^{-3}) of nanoscale clusters enriched in Cr, Mn and Si atoms. Size of observed clusters lies in a range of 3-5 nm. Analysis of the distribution of chemical elements showed the chromium depletion of the material matrix up to 6 at.%.

TOMOGRAPHIC ATOME PROBE INVESTIGATION OF CHEMISTRY ALTERATION IN OXIDE DISPERSION STEEL ODS EUROFER UNDER HEAVY ION IRRADIATION

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The main purpose of this work was to investigate the processes of evolution of oxide particles in ODS Eurofer steel (9%-CrWVTa+0.5%Y2O3) under heavy ions irradiation to simulate neutron damage. Experiments on the Fe-ion irradiation of the samples of ODS Eurofer perspective steel for fission and fusion reactors to different damaging doses (≤ 32 dpa) have been carried out. The analysis of distribution of different chemical elements in the volumes tested has revealed that under ion irradiation a change in the composition of nanosized clusters (2-4 nm), which are present in the initial material takes place [1]. Comparison of the data obtained with the results of reactor irradiation of the ODS Eurofer steel up 32 dpa [2] has been carried out. These data testify a correspondence between nanoscale changes in the steels oxide dispersion strengthened in imitation experiments and under the conditions of reactor irradiation.

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NANOSIZED STRUCTURE OF STEEL CHS-139 AND EK-181 SAMPLES IRRADIATED WITH FAST NEUTRONS

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Economical expedience of advancement of nuclear power industry calls forth the designing of such reactors that allow one to extend the campaign of fuel assemblies and enhance the fuel burnup to 15-20%. In this connection, the development and creation of new structural materials that preserve their technological characteristics upon irradiation with a dose of up to 150-200dpa is in a strong demand.

Promising materials for the fuel-element claddings are low-activated 12%Cr ferritic-martensitic steels EK-181 and CHS-139, which possess enhanced heat resistance. The martensite phase in them is stabilized with nano-size clusters, enriched in different elements, via special treatments. These steels are characterized by a high resistance to radiation swelling and high-temperature radiation embrittlement; yet they show up a tendency toward low-temperature embrittlement. A topical task nowadays is to search for new ways of eliminating this shortcoming.

The work is devoted to studying the nanosized structure of samples made from steels EK-181 and CHS-139 irradiated in an atomic reactor IBB-2M, at a temperature of irradiation of 340K, with the fast neutron fluences (E > 0,1 MeV) – $1x10^{18}$, $1x10^{19}$, and $5x10^{19}$ n/cm^2. The samples were investigated both in the as-supplied state (industrial heat treatment) and after special treatments by schemes: quenching from 1100^{o}C + tempering at 720^{o}C, and quenching + tempering + thermocycling at different temperatures. The influence of the heat treatment and irradiation with fast neutrons on the size of precipitates has been analyzed. It is established that the most typical is the presence in the samples of nanoparticles 1-2 nnm in size, as well as of the second mode described by a power size distribution with the averages value of 6-12 nm.

The work was performed according to the Plan of RAS “Impulse” (project № 01.2.006 13394), with a partial support of the Ministry of Sciences (State Contract №16.518.11.7032), the Program of Basic Research of the Presidium of RAS “Quantum mesoscopic and disordered structure (project № 12-P-2-1019 Ural Branch RAS), and the Program of Basic Research of the Department of Physics of RAS “Neutron investigation of structure and fundamental properties of substances”(project № 12-T-2-1006 Ural Branch, RAS).

INVESTIGATION OF DEUTERIUM BEHAVIOR IN FLUORID MOLTEN SALT

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Investigation of deuterium interaction with fluorid molten salt was done. Temperature dependences of deuterium permeation, diffusion and solubility factors for the molten salts Flinak and 77LiF -6ThF_4 -17BeF_2 are received.

EFFECT OF DISPLACEMENT RATE ON CHARACTERISTICS OF POROSITY FORMED IN STEEL «EK164» UNDER HIGH DOSE NEUTRON IRRADIATION

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At present time the austenitic steel «EK164-ID» c.w. (hereinafter «EK164») is considered as advanced steel capable to reach a high fuel burn – up, «EK164» is more resistant to radiation swelling as compared to the «ChS68-ID» c.w.(hereinafter «ChS68») currently used as a standard material of fuel claddings in the BN -600 reactor. At damage doses of 75…78 d.p.a. «EK164» swelling is by a factor of 1.5 less [1] than that of «ChS68». The voids formed in it are smaller than in « ChS68», but their concentration is higher. Swelling is not of a linear dependence on dose, and to predict it one needs to know a dynamics of voids growing versus neutron irradiation characteristics. The objective of this work was to reveal a dependence of characteristics of radiation porosity formed in steel «EK164» under high dose neutron irradiation on a displacement rate.

In this paper the research results on the «EK164» steel fuel claddings taken from fuel elements after their operation life in two fuel assemblies positioned in zones of low and high enrichment of the BN -600 reactor are presented. In the zones the conditions of the neutron irradiation effect on the claddings are differentiated by a displacement rate. The specimens were chosen so that the displacement rate was different in the same temperature ranges and for the same exposure time. Size distribution histograms were plotted from the electronic–microscope images obtained. They were also used to calculate a concentration of voids and swelling. The latter was determined by the hydrostatic weighing method as well. The comparison of the radiation porosity characteristics of the specimens permitted to ascertain that the size of voids increases with the displacement rate, and their concentration tends to decrease at the same irradiation temperature. As it was noticed in earlier research works on irradiated austenitic steels the similar manner of the changing is caused by an increase of irradiation temperature [2].

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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.

CORROSION AND STRUCTURE VVER-1000 FA COMPONENTS FROM E635 ALLOY AT BURNUPS UP TO 72 MW·DAY/KGU

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The use of irradiation resistant E635 alloy as a structural material of fuel rod cladding and skeleton elements of the VVER-1000 fuel assemblies advanced (FAA) has ensured the stability of the FA geometrical dimensions, minimized their bending and distortion, increased fuel cladding shape changing resistance at burn-up to 72 MW·day/kgU at a 6-year operation. Post-irradiation investigations of the VVER-1000 FAA components (fuel rod claddings, guide thimbles, central tubes, and rigid angles at frames) of E635 alloy show that in terms of their major operational characteristics, their resources for the 6-year cycle have not been exhausted yet. The geometrical parameters, corrosion, hydrogen absorption, tensile properties and structural-phase state of the components did not reach the values that would inhibit their further performance.

The oxide film thickness and the hydrogen content of E635 alloy are correlated over the core length, grow with burn-up and are determined by thermo-irradiation influence (temperature and neutron fluence). The oxide film thickness increases up to 80 µm at height coordinates of ~ 3100 mm, on the outer surface of the guide thimbles and rigid angles its thickness less than 42 µm. Hydrogen content in the cladding is less than 0.03%; in rigid angles around the bend it reaches 0.06%.

TEM study of dislocation structure, chemical and phase composition of E635 alloy components revealed structural characteristics influenced by temperature and neutron irradiation. The Laves phase precipitates and the matrix composition change due to SPPs depletion of iron in the irradiated fuel cladding, guide thimbles, central tube and rigid angles as a result of temperature parameters changes and neutron fluence, that determines their mechanical properties and shape changes resistance.

EFFECT OF IRRADIATION WITH FAST NEUTRONS ON STRUCTURAL STATE OF FERRITIC-MARTENSITIC STEELS EK-181 AND CHS-139 AFTER DIFFERENT HEAT TREATMENTS (NEUTRON DIFFRACTION STUDY)

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Physico-chemical origin of low-temperature radiation embrittlement (LTRE) as a typical phenomenon for metals with BCC crystal lattices have scarcely been studied so far (in comparison with high-temperature strength), though an important part taken in the phenomenon of LTRE by both initial structure-phase states of steels, which are controlled via initial compositions and TMT modes, and changes in these states upon neutron irradiation has been shown [1].

High-chromium ferritic-martensitic steels fabricated in the JSC "VNIINM" for perspective nuclear fission and fusion power reactors are exemplified by 12%Cr-steel EK-181 (low-activated) and CHS-139 [2-4]. Studies of structure-phase states of these steels and their changes upon the low-temperature neutron irradiation after different thermomechanical treatments (TMechT) are in a strong demand for further improvement of functional properties of the steel developed.

In the work presented the results of neutron-diffraction studies of the influence of low-temperature neutron irradiation on the microstructure and phase composition of steels EK-181 and CHS-139 after different modes of TMechT are reported. Neutron diffraction method allows one to gain important information on the real structural state of massive steel samples (microstructure, phase composition, presence of fine precipitates, microstresses in the bulk, etc.) and its changes upon different TMechT and neutron irradiation.

The work was performed in accordance with the Plan of RAS "Impulse" (project № 01.2.006 13394) with the partial support of the Programs of Basic Research of the Presidium of RAS (project № 12-2-032-BN Ural Branch, RAS) and State Contract (project № 14.518.11.7020).

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INFLUENCE OF HEAT TREATMENT ON STRUCTURAL STATE OF FERRITIC-MARTENSITIC STEELS EK-181 AND CHS-139 (NEUTRON DIFFRACTION STUDY)

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High-chromium ferritic-martensitic steels, including their low-activated modifications (with a fast decrease of activity) are promising structural materials for the development of nuclear fission and fusion power reactors [1-4]. Steels of this class are characterized by high functional physico-mechanical properties, which yet are to be significantly improved to employ the materials in power reactors of new generation. The improvements are required for both high-temperature (heat-resistant) and low-temperature (LTRE – low-temperature radiation embrittlement at temperatures of neutron irradiation up to 400 ^{0}C) properties of steels of this class (BCC–crystal lattice). Difficulties in the fabrication of steels of this class with enhanced radiation functional properties are caused by the fact that the means of improving heat resistance and weakening of the tendency to LTRE are alternative. Such an alternative brings developers of perspective steels to optimize methods of their fabrication (in the first place, to vary compositions and modes of thermomechanical treatments (TMechT)), with the aim to gain structure-phase states and properties of these steels meeting the requirements for both heat resistance and LTRE.

In the work, the results of neutron-diffraction study of steels EK-181 and CHS-139 after different heat treatments are presented. It is shown that, depending on the conditions of HT, in the samples there are formed solid solutions with the precipitation of carbide phases, which results in the formation of a stressed structural state.

The work was performed in accordance with the plan of RAS “Impulse” (project № 01.2.006 13394) with the partial support of the Programs of Fundamental Studies of the Presidium of RAS (project № 12-2-032-BN Ural Branch, RAS) and State Contract (project № 14.518.11.7020).

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HIGH-DOSE NEUTRON IRRADIATION SOFTENINING AND EMBRITTLEMENT OF STEEL «ЭК164»

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The steel «ЭК164» is considered as a candidate material for fuel coatings of fast neutron reactors. The experimental data available show that «ЭК164» radiation swelling is higher than that of the steel «ЧС68» used as a standard coating material of fuel in BN-600 reactor. It was found earlier from a research of irradiated fuel coatings made of steel «ЧС68», that an embrittlement and loss in strength of the coatings after their operation life are, to a greater extent, due to high swelling [1]. Therefore one can expect that the «ЭК164» steel coatings will be impacted by irradiation softening and embrittlement much less than the «ЧС68» claddings. The research on the influence of irradiation conditions of the «ЭК164» coatings on the softening and embrittlement of the steel «ЭК164» has been conducted.

The mechanical properties of «ЭК164» coatings after their operation life in the BN-600 reactor to different damage doses (up to 77 dpa.) have been determined and the results are presented in this paper. For mechanical tests the specimens of the coatings from different fuel assemblies were chosen so that their exposure temperatures were close, and the damage doses being of some difference. This permits to accumulate data to build the plots of the «ЭК164» steel mechanical properties against the doses at different irradiation temperatures.

The mechanical properties have been determined from the results of the tests of two types: the uniaxial tension of annular specimens made out of the fuel coatings and the internal pressure by moldable filler applied to tubular specimens[2].The tests on the annular specimens give a conservative value of the mechanical properties, it does not allow to estimate adequately a residual performance capability of the coatings but to obtain comparative data with quite a representative statistics on the strength and ductility characteristics of the specimens under irradiation conditions. The tubular-specimen test results describe, to a greater extent, the mechanical properties of the fuel coatings under true loading conditions, but they are of poor statistic, because these specimens have to have a larger size.

It has been found from the tests that a tensile elongation of annular specimens at a tensile temperature of 20 °C and swelling of more than 3 % equals to zero or takes on values close to it, the ultimate strength being approximately 600 MPa and more. At higher test temperatures of 500…600 °C a tensile elongation of annular specimens irradiated at temperatures higher than 480 °C becomes zero irrespective of a swelling value, and the ultimate strength being 50…200 MPa, that testifies to a high temperature embrittlement.

On tubular samples it is shown in reduction in a uniform relative lengthening at a test temperature of 600 °C, thus the general relative lengthening (more than 4 %) and strength (more than 600 MPa) keeps rather high values, testifying to a sufficient residual performance capability of the fuel coatings made of steel EK164for the life time prescribed.

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VERTICAL LITHIUM LIMITER FOR EXPERIMENTS ON T-11M TOKAMAK

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Unique properties of lithium are a basis of possibility of its use as the element contacting to tokamak's plasma. Before property of lithium were studied for use as the effective heat-transfer agent of nuclear power installations [1]. Lithium has the maximum value of a superficial tension: 406 mN/m [2]. It in a combination to low density defines unique capillary properties of lithium.

The basic principle of work of a lithium limiter on the basis of capillary porous system (CPS) is that over a surface of a limiter the plasma layer of lithium and its natural impurity, absorbing energy of a coming stream of plasma is formed.

Within the research program on tokamak T11-M the limiter realizing the concept of the lithium emitter-collector was designed. The concept of the lithium emitter-collector assumes existence of the lithium emitter located in hot area of contact of hot plasma with a limiter, and the lithium collector located mainly in colder area, but at the same time in area where the emitted lithium gathers. The emitter and a collector should be connected by system of transportation of lithium for maintenance of circulation of lithium in such system (fig. 1).

For implementation of the concept of the emitter collector the lithium reception element is made the greatest possible length. The lithium reception element contacts to plasma in a local zone from which in plasma lithium arrives. The ends of a reception element are lithium collectors as being "cold" and remote from a point of contact to plasma catch lithium. CPS plays a role of transport system of lithium in which lithium moves at the expense of capillary forces from lithium collectors (the element ends) to the lithium emitter (a zone of contact to plasma) in such execution.

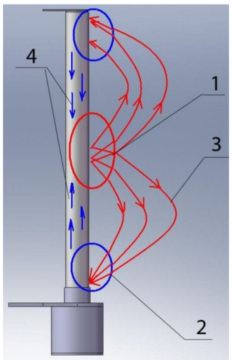

Fig. 1. Lithium streams in the lithium reception element: 1– hot zone of the limiter (the lithium emitter), 2 – cold zone of the limiter (the lithium collector), 3 – lithium streams in plasma, 4 – lithium streams in CPS

The created model of a stationary lithium limiter of vertical execution is tested on tokamak T-11M. For the end of 2011 more than 500 shots are carried out.

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DEFORMATION CHARACTERISTICS OF FUEL CLADDING MADE OF EK164-ID COLD-WORKED AUSTENITIC STEEL AND IRRADIATED IN BN600 REACTOR UP TO PEAK DAMAGE DOSE OF 95 DPA AND PEAK BURNUP OF 13.2 % OF H.A.

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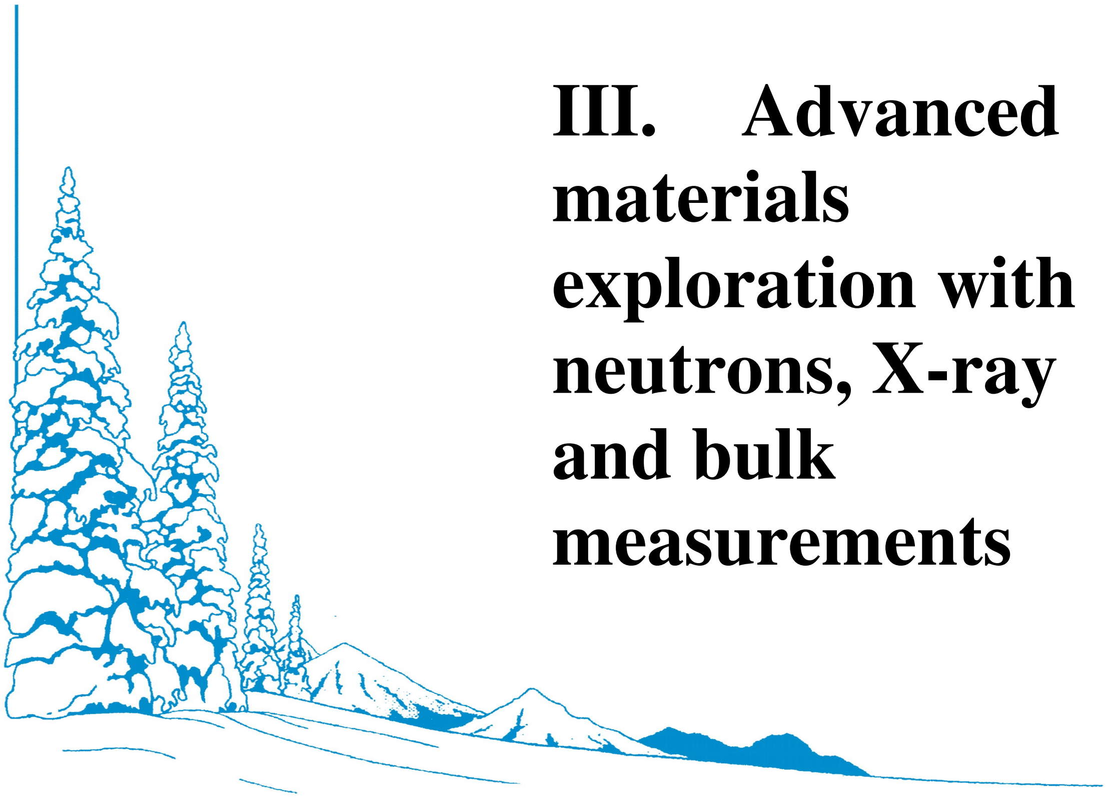
The work was carried out by the results of the study of the characteristics of the deformation of the fuel pin cladding manufactured of the austenitic steel of the new generation designated EK164-ID c. w. and irradiated as a part of four experimental sub-assemblies of the BN600 reactor. The technique and facility for obtaining the fuel pin cladding material swelling parameters from the high-accuracy measurement of their geometric dimensions are presented. The obtained results are shown in comparison with the data of the profilometry of the fuel pins of which the cladding is manufactured of the industrial grade steels used earlier as standard materials.



III. Advanced materials exploration with neutrons, X-ray and bulk measurements

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.

MAGNETIC EXCITATIONS IN $EuCu_2(Si_xGe_{1-x})_2$: BETWEEN VALENCE INSTABILITY AND MAGNETISM

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$EuCu_2Si_xGe_{2-x}$ series represents to date the only known case [1], among the variety of Eu- and Sm-based valence-unstable systems, where the state in the phase diagram is tuned from the valence-fluctuating one to heavy-fermion and then to magnetic-ordered state, with possibility for existing of a quantum critical point near x≈0.3. Here we present the inelastic neutron scattering study of spin dynamics in $EuCu_2Si_xGe_{2-x}$ (x=1, 0.8, 0.5, 1.2), performed in a wide temperature range (5-200K) related to the balk valence state of Eu defined by L_3-edge spectroscopy. Neutron scattering provide the detailed information about the spectral structure of dynamical magnetic response.

At x=1 the magnetic excitation spectrum [2,3] was found to be represented by the double-peak structure just below the energy range of the Eu^{3+} spin-orbit (SO) excitation $^7F_0 \rightarrow {}^7F_1$, so that at least the high-energy spectral component can be assigned to the renormalized SO transition. Change of the Eu valence towards 2+ with increase of the temperature and increase of Ge concentration [4] results in further renormalization (lowering the energy) and gradual suppression of both inelastic peaks in the spectrum, along with developing sizeable quasielastic signal. The origin of the spectral structure and its evolution is discussed in terms of excitonic model for the mixed-valence state. Possible phase diagram of $EuCu_2Si_xGe_{2-x}$ is considered in connection with structure and its temperature evolution of magnetic response spectrum.

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INFLUENCE OF THERMOMECHANICAL TREATMENTS ON THE STRUCTURE AND PROPERTIES OF U-Nb ALLOY

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Structural heredity is a phenomenon of recovery of size, shape, and orientation of initial grains of a high-temperature phase in a metal or alloy undergone a direct (upon cooling) and reverse (upon heating) phase transformations.

In the alloy U-Nb, which after quenching consists of plates of the metastable phase α'', the effect of heredity results in some cases in the formation of a coarse-facet brittle fracture and decrease of dynamic plasticity.

To suppress the structure heredity in the alloy U-Nb, it is necessary to establish a structural correlation between the high-temperature and low temperature phases. This can be achieved by either cold deformation or eutectoid decomposition. Based on these principles, 4 routines of thermomechanical treatments have been developed:

1. Quenching into water from 1000ºC + deformation ~50% + quenching into water from 700ºC.

2. Quenching into water from 1000ºC + deformation ~50% + annealing at 600ºC + quenching into water from 700ºC.

3. Quenching into water from 1000ºC + annealing at 600ºC + quenching into water from 700ºC.

4. Quenching into water from 1000ºC + slow cooling from 700ºC to 600ºC + quenching into water from 700ºC.

After heat treatments the samples were subjected to tests for impact toughness and metallographic and fractographic examinations.

The results of metallographic studies on an X ray diffractometer and optical microscope testify to the existence in all samples of one-phase α''-structure. Yet, the grain size significantly differs in the samples treated by different regimes. For instance, for the 2nd egime the average grain size makes up ~15 µm, whereas for the 4th regime, 100µm and more. At the same time, the microhardness of all samples is lower than for material in the as-supplied state and equals 130 – 150 kg/mm^2.

The results of tests on a pendulum pile-driver did not show up any significant increase of the impact toughness for the fine-grained state in the comparison with the coarse-grained one.

Fractographic examination of the surface fracture revealed a ductile character for all samples both at room temperature and liquid nitrogen temperature. The fracture proceeded by the mechanism of formation and coalescence of micropores. The centers of formation of pores were mostly brittle oxicarbonitride inclusions, which are abundantly present in the matrix of the alloy.

The metallographic studies conducted show the necessity for improvement of the regimes of thermomechanical treatments for an assured production of a homogeneous fine-grained structure in the alloy U-Nb. Moreover, a positive effect can also be exerted by a more careful refinement of the alloy from impurities.

4f SHELL COLLAPSE IN CeNi: METASTABLE AND HIGH-PRESSURE PHASES

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Strongly correlated electronic systems are in focus of interest of both theorists and experimentalists [1]. This class of objects includes heavy fermion and intermediate valence systems. Intermediate valence systems demonstrate puzzling phase transitions with a collapse of the 4f-electron shell. The physical picture of this phenomenon is still missing. Such phase transitions have been observed in cerium and plutonium (collapse by 15% and 26%, respectively).

Intermetallic system CeNi demonstrates many anomalies in electronic and lattice properties (see [2] and references therein). One of the most striking effects in CeNi is a unit cell volume collapse under relatively low pressure [3].

The true space group of the high-pressure phase of CeNi is unknown. This fact is puzzling since in last years many groups from Russian and foreign research institutes tried to solve the problem. In [4,5] the fit of the neutron diffraction patterns collected at high pressure provided the following solution: tetragonal symmetry with lattice parameters a = 3.748 Å and c = 5.796 Å. This solution is in contradiction with the result of the current work obtained on metastable CeNi.

The main goal of the current work was to investigate the unit cell volume collapse in the intermediate valence system CeNi which is a cerium-based plutonium homologue. Experiments have been performed at high pressure for the parent CeNi phase and at ambient pressure for the metastable CeNi phase. The outcome of the X-Ray and neutron diffraction measurements is presented.

For the first time the metastable volume-collapsed CeNi phase was synthesized at high pressure (9 GPa) and high temperature. This CeNi phase demonstrates very high degree of the cerium 4f electrons delocalization.

The measurements of the structural properties were performed at high pressure with diamond and sapphire pressure cells. The metastable CeNi phase was investigated at ambient pressure on the position sensitive diffractometer.

With work was supported by the Russian Foundation for Basic Research (RFFI project 11-02-01171-a).

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MAGNETIC RESONANT MODE IN CeB_6

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Resonant magnetic excitations are widely recognized as hallmarks of unconventional superconductivity in copper oxides, iron pnictides, and heavy-fermion compounds. Numerous model calculations have related these modes to the microscopic properties of the pair wave function, but the mechanisms underlying their formation are still debated. Recently, we reported the discovery of a similar resonant mode in the non-superconducting, antiferromagnetically ordered heavy-fermion metal CeB_6 by inelastic neutron scattering [1]. Unlike conventional magnons, the mode is nearly non-dispersive, and its intensity is sharply concentrated around a wave vector separate from those characterizing the antiferromagnetic order (Fig. 1). The magnetic intensity distribution rather suggests that the mode is associated with a coexisting antiferro-quadrupolar order parameter, which has long remained "hidden" to the neutron-scattering probes. The mode energy increases continuously below the onset temperature for antiferromagnetism, in parallel to the opening of a nearly isotropic spin gap throughout the Brillouin zone. These attributes bear strong similarity to those of the resonant modes observed in unconventional superconductors below their critical temperatures. Such an unexpected commonality between the two disparate ground states indicates the dominance of itinerant spin dynamics in the ordered low-temperature phases of CeB_6 and throws new light on the interplay between antiferromagnetism, superconductivity, and "hidden" order parameters in correlated-electron materials. A recently developed theory [2] has offered a description of the spin-exciton mode in the framework of a fourfold degenerate Anderson lattice model, which treats both order parameters in CeB_6 as particle-hole condensates of itinerant heavy quasiparticles. Future experiments addressing the magnetic-field dependence of the resonant excitation, as well as its dispersion and complete three-dimensional structure in the reciprocal space could clarify its origins and offer a direct way to verify the newly proposed theory. We expect these experiments to provide a long-awaited clue to the puzzle of the "hidden order" phase in CeB_6, as well as to the mechanisms underlying the formation of similar resonant excitations in a broad class of correlated metals, including unconventional superconductors.

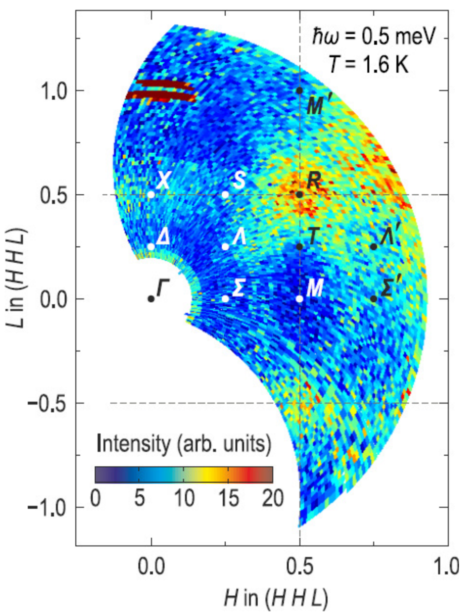

Fig. 1. (a) Inelastic neutron scattering signal at 0.5 meV energy transfer along the (*hhl*) plane in the reciprocal space. The measurement was done in the low-temperature anti-ferromagnetic phase of CeB_6 (T = 1.6 K) in zero magnetic field. The labels represent different high-symmetry points, and the dashed lines mark Brillouin zone boundaries. The measurement was done at the ILL using the IN14 spectrometer equipped with the *FlatCone* multianalyzer.

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STUDIES OF NEUTRON ELASTIC AND INELASTIC DIFFUSE SCATTERING IN SINGLE CRYSTALS

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The presence of defects in the regular periodic order of a crystal lattice is reflected by a modification of the intensity, position and shape of the δ-function like Bragg peaks of the original structure and sometimes accompanied by an additional signal appearing at other positions in the reciprocal space. While the effects concerning directly the Bragg peaks are frequently investigated, the supplementary signal, apart of superstructure reflections revealing the appearance of additional order, is subject of less attention. The main reason probably being interpretation difficulties arising from ambiguities in relation between experimental data and predictions of existing theoretical models [1]. It is also important to realize that in the X-ray case, generally more accessible and more favorable in terms of Q-resolution and intensity, at any temperature the measured diffuse scattering intensity contains in addition to defect scattering also the integral over the whole spectrum of lattice vibrations, themselves eventually affected by the presence of lattice defects.

In this sense the case of neutron scattering is more favourable due to the readily available energy analysis, which permits to separate the static and dynamic components of the response with a reasonable efficiency. Recent developments of the neutron three-axis spectrometers (TAS), boosting their performance both by massive beam focusing and by implementation of arrays of analyzer/detector channels have provided access to very efficient data collection schemes. Maps of diffuse scattering over several Brillouin zones can be collected in less than an hour from crystals of a modest size ($\approx 10^{-1}$ cm^3). Moreover, the flat-cone geometry [2] can be employed to map response in nonequatorial planes, permitting to carry out systematic surveys over three-dimensional intervals in reciprocal space.

In this lecture, we will mainly concentrate on fundamentals of diffuse scattering phenomenology and on experimental possibilities offered by the ILL *FlatCone* [3] multianalyzer, illustrated by examples in diverse fields ranging from relaxor ferroelectrics [4] to quantum magnetism.

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EXAMINATION OF INCLUSIONS IN URANIUM – 6.3 wt. % NIOBIUM ALLOY

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Main nonmetallic impurity in uranium are compounds with carbon (carbides), oxygen (oxides), and nitrogen (nitrides)[1]. Carbides, oxides, and nitrides possess isomorphous crystal lattices and in the course of melting can form inclusions of a cuboid shape, which include carbide, oxide, and nitride – U(CNO) and may be named as uranium oxicarbonitrides.

Methods of scanning electron microscopy and energy-dispersive X ray microanalysis were applied to compare inclusions in the alloy U-6.3 wt.% Nb from different batches supplied.

Image of the most peculiar types of inclusions for the given alloy have been obtained; morphology and elemental composition have been determined.

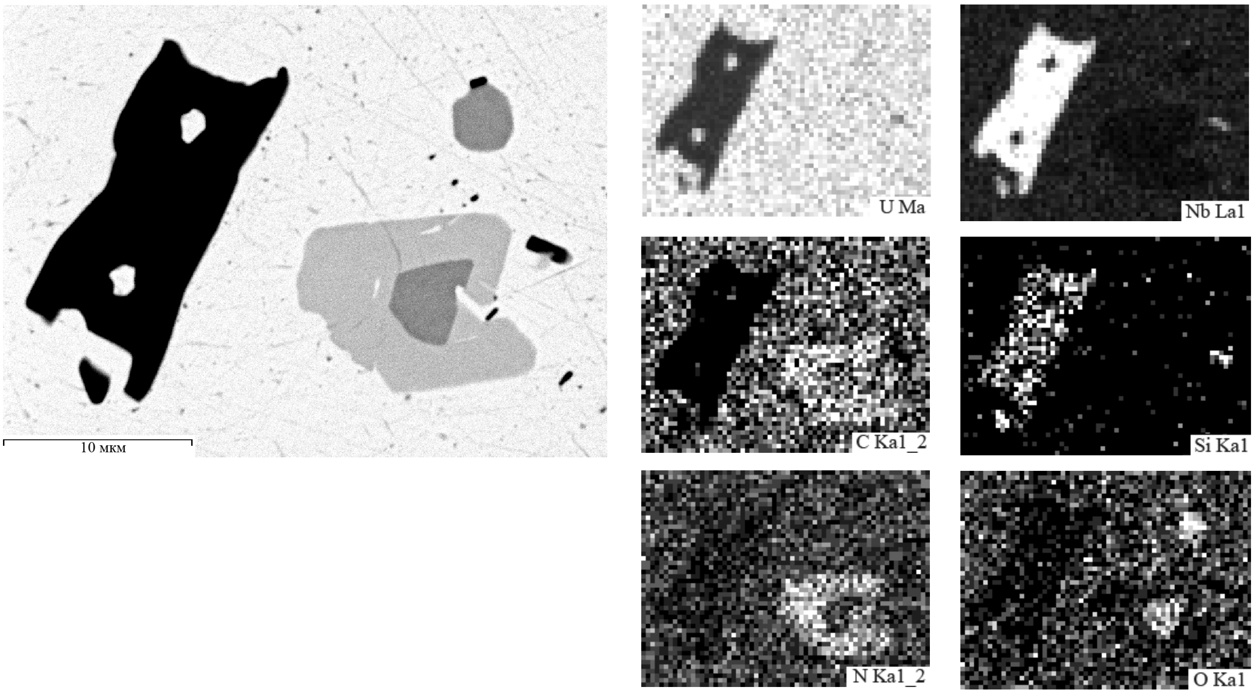

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Figure 1. Images of inclusions in the alloy U-6.3 wt.% Nb taken in the scanning electron microscope a) on the secondary electrons; b) maps of distributions of chemical elements (in the right lower corner of each map there is shown a symbol of characteristic X ray radiation based on which the map is drawn.

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MAGNETIC EXCITATION SPECTRUM OF α- AND δ- PLUTONIUM

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Transition between localized and delocalized (itinerant) behaviour embodies a forefront of physics of strongly correlated systems. The localized-itinerant 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 around Ce. In lanthanides, high pressure gives an increased overlap leading to a delocalization and, in some cases, to structural phase transformations accompanied by a volume discontinuity. The most famous example is cerium, which exhibits the isostructural $\gamma \to \alpha$ volume-collapse phase transition upon either cooling or application of external pressure. There has yet to be a quantitative and definitive determination of this phenomenon [1]. Also, the problems of plutonium ground-state and the number of 5*f* electrons in Pu are still debated.

Now more and more arguments appear that plutonium can be understood as a system with intermediate (mixed) valence {2-6]. Investigation experience of 4*f*-elements based strongly-correlated electronic systems shows that many complicated problems have been solved and anomalous physical properties have been explained of valence-unstable materials in which electrons, like in plutonium, balance at the border between localized and delocalized behavior, using inelastic neutron scattering technique.

In [3,4] we suggested an empirical multiple intermediate-valence model of plutonium, which describes quantitatively such static properties of α- and δ-Pu as temperature dependence of magnetic susceptibility within the temperature range 0< T < 450 K, low temperature specific heat, and equilibrium volume. In the present work in terms of the MIV model we calculate magnetic spectral response $S(\vec{Q}=0,E)$ for α- and δ-plutonium, which can directly be measured by inelastic neutron scattering technique. We show that measurements of dynamical magnetic response of Pu by inelastic neutron scattering technique will allow us to establish (almost un ambiguously) the type (character) of plutonium ground state, to determine characteristic energies of the system, and to estimate occupation of Pu 5f shell taking into account its intermediate-valence nature.

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SPIN DYNAMICS IN GEOMETRICALLY FRUSTRATED MULTIFERROIC $Ni_3V_2O_8$

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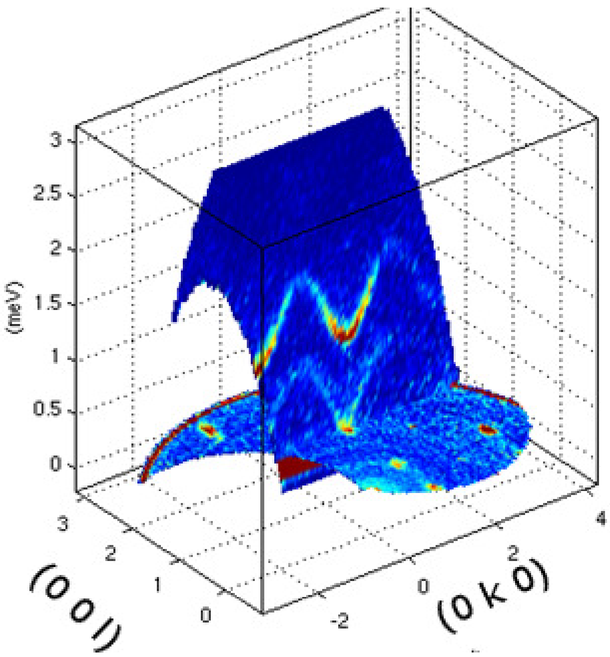

Fig. 1. Typical magnetic excitation spectrum of $Ni_3V_2O_8$ measured at T=1.4 K on Cold Neutron Chopper Spectrometer [2], Oak Ridge National Laboratory.

The coupling of magnetic and ferroelectric order has recently been drawing a lot of interest in condensed matter science given the fundamental interest and potential applications [1]. Ni3V2O8 is a S=1 magnet with Ni2+ ions arranged in a weakly coupled buckled Kagomé-staircase planes. Its complex magnetic phase diagram exhibits four different zero field incommensurate and commensurate magnetic phases below 10 K, with only one developing ferroelectric order. We present here a detailed study of low temperature magnetic dynamics in this geometrically frustrated spin system. Using single crystal inelastic neutron scattering technique we map the magnetic excitation spectra across all the magnetic phase transitions. We found that the spin-waves, well formed in the base temperature nonferroelectric phase at T < 3 K, are considerably damped when the system enters the low-temperature incommensurate phase with ferroelectric order (3.9 < T < 6.3 K). Finally, we discuss models that describe the coupling between magnetic and ferroelectric properties in the incommensurate magnets.

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HOMOGENEOUS MICRO-SCALE PHASE OF THE SUPERCONDUCTIVITY AND ANTIFERROMAGNETISM COEXISTENCE IN $CeRhIn_5$

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Nowadays it has been established that in the heavy-fermion intermetallide $CeRhIn_5$ Cooper instability is induced in the vicinity of the critical pressure at which the destruction of long-range antiferromagnetic order occurs [1]. As a result the phase of superconductivity and antiferromagnetism coexistence is formed without segregation on the separate antiferromagnetic and superconducting regions up to the microscopic scale [2]. An interest to $CeRhIn_5$ is dictated by the fact that the application of an external magnetic field shifts the boundary of the antiferromagnetic phase to the high pressure region [3]. This means that antiferromagnetism is induced by an external magnetic field in some region.

In this paper in the framework of the extended periodic Anderson model a phase diagram of $CeRhIn_5$ has been constructed, which contains antiferromagnetic ordering, the superconducting state, and the region of superconductivity and antiferromagnetism coexistence. It has been shown that both antiferromagnetic and superconducting orderings are induced by the exchange interaction between the localized 4f-electrons.

Taking into account that increasing pressure which is applied to the intermetallide leads to a growth of the energy of the localized f-states, it has been shown that the destruction of the antiferromagnetic ordering is implemented with increasing pressure. This is due to the fact that, the population of localized states decreases when a localized level moves up the energy band. For the chosen system parameters superconducting and antiferromagnetic orderings are in competition with each other. It has been confirmed by the fact that the maximum of the superconducting order parameter is attained when magnetization falls to zero. As a result of the mentioned above competition the amplitude of the superconducting order parameter in the phase of superconductivity and antiferromagnetism coexistence is much less compared to that which would have been without a presence of antiferromagnetic ordering.

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SPIN-DEPENDENT ELECTRON TRANSPORT IN THE FERROMAGNETIC METAL/INSULATOR/SEMICONDUCTOR HYBRID NANOSTRUCTURES

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Hybrid nanostructures consisting of semiconductor and ferromagnetic elements combine a huge potential of traditional semiconductor electronics and the ability of magnetic materials to control the electron transport via the spin state of electrons [1]. We present the results of investigations of the magnetotransport properties of the Fe/SiO_2/p-Si hybrid structure.

The features of the dc transport properties of this structure are caused by the metal-insulator-semiconductor (MIS) transition with the Schottky barrier that forms at the SiO_2/p-Si interface [2]. The structure exhibits the magnetoresistive effect; the observed magnetoresistance (MR) is positive or negative, depending on temperature and bias. The positive MR is related to the processes occurring when the current flows in the semiconductor volume (p-Si); the negative MR is caused by a thin inverse layer that forms near the SiO_2/p-Si interface.

The features in the behavior of the real and imaginary impedance parts result from recharging of the local surface states at the SiO_2/p-Si interface. For these states, two recharging processes with different relaxation times are implemented. The first process is trapping-emission of charge carriers with the participation of the surface states and the valence band. The second one is electron tunneling between the Fe electrode and the surface states through the SiO_2 potential barrier. The surface states are responsible also for the frequency-dependent giant magnetoimpedance of the structure. There are two mechanisms of the effect of an applied magnetic field: 1) the energy levels of the surface states shift relative to the valence band, which leads to the change in the characteristic recharging time; 2) the magnetic field controls the spin-dependent tunneling of charge carriers through the potential barrier.

The search for effective ways of controlling the magnetotrasport properties of hybrid structures disclosed the giant (up to 10^4%) magnetoresisitve effect induced by optical radiation in Fe/SiO_2/p-Si. The observed effect is also related to the presence of the «magnetic» surface states, which simultaneously participate in the optical transitions and the spin-dependent tunneling.

The results obtained open a new direction in silicon spintronics: the use of the spin-dependent tunneling and spin transport as a whole in hybrid structures with the participation of the «magnetic» surface centers.

This study was supported by the program no. 20 of the Presidium of the Russian Academy of Sciences, project no. 20.8, program of the Division of physical sciences of the Russian Academy of Sciences, project no. II.4.3, and the Siberian Branch of the Russian Academy of Science, complex integration projects nos. 43, 85, and 102.

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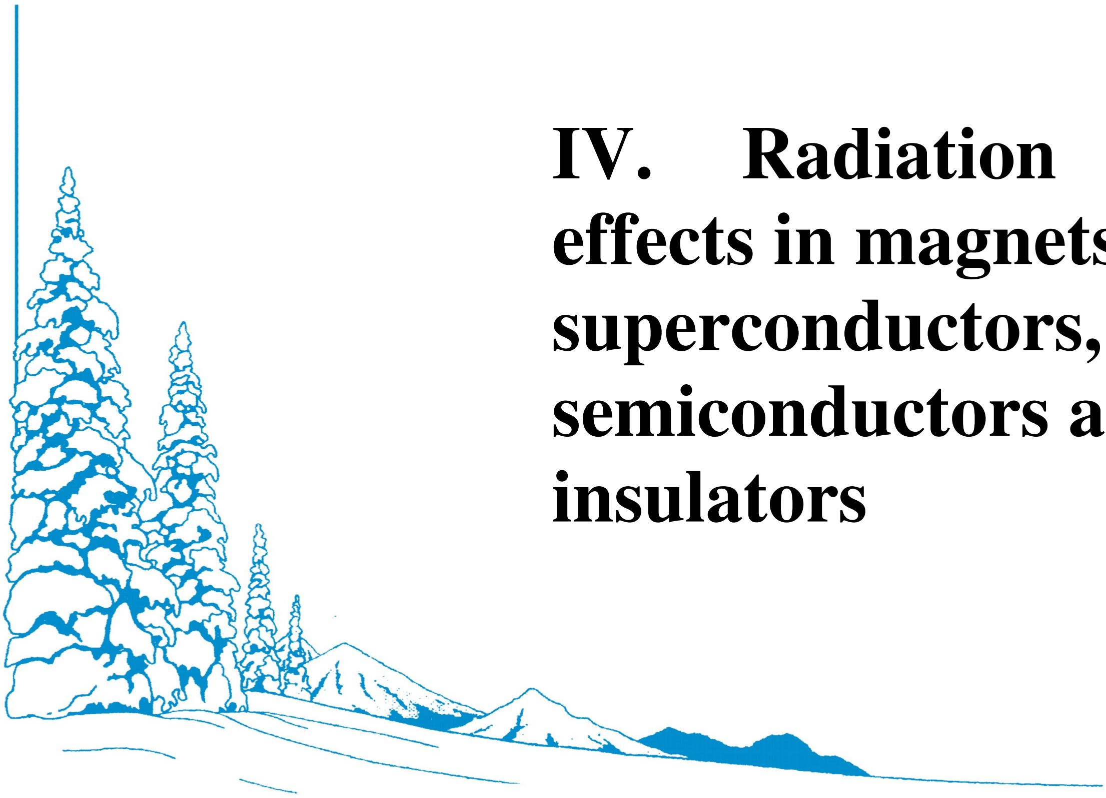
IV. Radiation effects in magnets, superconductors, semiconductors and insulators



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.

ON THE NATURE OF LOW-TEMPERATURE COLOR CENTERS IN OPTIC FIBERS IN OH IMPURITIES

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By measuring the spectra of optical absorption (OA) and thermo-luminescence curves (TLC) the formation of color centers (CC) and luminescence is studied in γ-irradiated «Polemico» quartz-quartz optic fiber waveguides (OFW) with impurities of OH ~1000 pmm. The CC's are studied at 77K in γ-irradiated OFW. Thermal relaxation of CC in γ-irradiated OFW at 77K are studied in the ranges of 77-315K. The TLC's are studied in the ranges from 9 to 315K. In OA of the γ-irradiated OFW at 77K one can see bands of additional absorption with peaks at 210, 260, 330 and 550 nm.

The thermo-relaxation of these absorption bands (AB) demonstrates that they have different temperature in the region of destruction. The AB at 210 nm disappears at 72, 100 and 310K. Destruction of AB at 330 nm occurs at temperature 95K, whereas AB 260 nm at temperatures 100, 180 and 220K. In TLC's of γ-irradiated OFW at 9K there are peaks at 17, 53, 72, 106 and 220K with activation energies of 0.03, 0.11, 0.14, 0.21 и 0.46 eV. Comparison of TLC position and destruction region of AB in γ-irradiated OFW at 77K demonstrated that position of AB destruction at peaks at 210 nm coincides with the TL peaks at 72 and 100K, AB at 330 nm with TL peak 95K, whereas AB at 260 nm with TL peaks at 100, 180 and 220K. The AB with peaks at 210 nm disappears at 310K destructs without luminescence.

Based on these studies we draw a conclusion that the OFW's with OH impurity of ~1000 pmm irradiated at 9K have at least 3 types of E′-centers (210 nm). Position of the first type E′ -center destruction corresponds to the TL peak at 72K, and the second E′-center TL peak corresponds to 100K peak. The third E′-center at 310K destructs without luminescence.

INFLUENCE OF ELECTRON IRRADIATION ON MAGNETIC PROPERTIES OF SINGLE CRYSTAL $La_{0.67}Ca_{0.33}MnO_3$

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Perovskite manganites $La_{1-x}A_xMnO_3$ are referred to the class of magnetic semiconductors that are featured by strong coupling between lattice, charge, and magnetic degrees of freedom. Upon substitution of part of ions La^{3+} by two-valence ions A=Ca, Ba, Sr or upon deviation from the stoichiometry there appear new ions Mn^{4+}. Ferromagnetic interactions (FM) Mn^{3+}-Mn^{4+} lead to changes in the magnetic order from antiferromagnetic (AFM) to FM. In the vicinity of Curie temperature T_C there is observed the effect of colossal magnetoresistance (CMR). The maximal effect is found in compositions of the system $La_{1-x}Ca_xMnO_3$ with x close to 0.3, which at low temperatures are FM metals, while above T_C they exhibit a semiconducting character of conductivity. To explain the CMR effect in a nonconductive paramagnetic phase, nanoscalled charge-ordered polarons are considered. Dagotto [1] introduced a new temperature scale according to which in the range $T^*>T_C$ there can exist correlated and noncorrelated magnetic polarons, whereas in the range of high temperatures $T_{pol}>T>T^*$, only noncorrelated polarons with an enhanced magnetic moment. Data on the magnetic susceptibility at T>400K are scarce; therefore, there is still an open question about temperatures at which a homogeneous paramagnetic state transforms into a inhomogeneous polaron state.

Peculiarities of manufacturing manganites can cause changes in the chemical composition and physical properties. Electron irradiation creates point defect without changes in composition. The work deals with studying the influence of local distortions and interfaces on the magnitude of T_C and polaron states in $La_{0.67}Ca_{0.33}MnO_3$. Measurements of magnetic susceptibility χ_{dc} of the initial single- and polycrystals and those irradiated with electrons with a maximal dose F = $9 \cdot 10^{18}$ e/cm^2 were carried out in the temperature range 80K<T<650K. Table 1 shows magnetic characteristics of the irradiated poly- and single crystals of $La_{0.67}Ca_{0.33}MnO_3$. Competition of local FM superexchange interactions upon displacement of ions from their positions and structural disorder results in a nonmonotonous dose dependence of T_C. Interfaces in the polycrystal serve as channels of relaxation of radiation defects. That is why, with increasing the dose of irradiation its T_C changes weaker than that of the single crystal. In the paramagnetic region in the vicinity of T_C there can exist correlated and noncorrelated polarons, as well as isolated Mn ions. In the temperature range $1.2T_C<T<2T_C$, only noncorrelated Varm's polarons with increased magnetic moment can form because of localization of e_g-electrons near Mn^{4+}.

The increase of the number of point defects favors the preservation of the region of inhomogeneous paramagnetic state up to higher temperatures T>650K.

Sample		F=0	F=5 ×10^{18} e/cm^2	F=9 ×10^{18} e/cm^2
Single crystal	T_C,K	244	226	241
	θ,K	292	327	316
	μ_{eff},μ_B	4.56 T>425 K	4.69 T>500 K	4.66 T>460 K
	T*	290	290	320
	T_{pol}	446	630	>630
Polycrystal	T_C,K	252	252	247
	θ,K	321	321	335
	μ_{eff},μ_B	4.60 T>500 K	4.70 T>480 K	4.68 T>480 K
	T*	290	290	290
	T_{pol}	470	>630	>630

The work was supported by the Program of the Presidium of RAS.

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RADIATION EFFECTS IN THE SEMICONDUCTOR COMPOUNDS III-N(BN, AlN, GaN, InN)

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In recent years the problem of radiation-induced effects in nitride compounds III-N(BN, AlN, GaN, InN) attracts high attention because of these semiconductors are more resistant to the influence of the hard radiation in the comparison with the others semiconductors from III-V group. Besides, the native lattice defects determine the properties of the grown material often, for example, n^+-type conductivity in indium nitride. But our knowledge about the structural defect in III-N compounds is still far from being complete. In the presented work the results of the radiation-induced effects investigation in the compound semiconductors III-N group after neutron, proton and electron irradiation are presented.

The local charge neutrality level energy position respectively to the top of the valence band (eV) in the compound semiconductors BN(3.9), AlN(3.5), GaN(2.7) and InN(1.7), which determines the electron properties of these semiconductors – n^{++}-type conductivity in InN and high resistivity v – type conductivity in BN, AlN, GaN after the saturation of these materials with radiation-induced defects has been calculated [1, 2].

The influence of the isotropic and anisotropic (in the basal plane and along the ***c***-axis direction) elastic stresses of expansion/compression on the lattice structural parameters and on the electron spectra of AlN, GaN, InN compounds are investigated. The expansion of the lattice constant ***c*** and at the same time the practical invariable value of lattice parameter ***a*** in GaN films on the sapphire upon the reactor irradiation and the numerical estimations of the proper elastic stresses in the irradiated material are fulfilled [3 - 5].

The changes of the electron properties of GaN films on the sapphire upon the high dose of neutron and electron irradiations have been investigated. The spectrum of the radiation-induced deep traps which determines the high specific resistivity in the irradiated material is presented. In the temperature range 20 – 1000^{0}C the isochronal annealing of the irradiated gallium nitride has been fulfilled. It was revealed that the main restoring of the electron properties and the lattice structural parameters in the irradiated GaN films takes place in the temperature interval up to 600^{0}C [6-10].

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INFLUENCE OF NEUTRON AND GAMMA IRRADIATION ON GaN HEMT-TRANSISTORS

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Stationary gamma and pulsed gamma-neutron radiation influence on output characteristics of HEMT-transistor based on GaN (CGH40010 manufactured by the company Cree (USA)) was studied.

Increase of drain-gate characteristic slope was detected after transistor irradiation with dose $\approx 3 \cdot 10^6$ Roentgen on isotope source Co^{60}. The increase value was ≈8%. Characteristic approaches to initial one under further irradiation.

Transistor drain-gate characteristics were measured under gamma-neutron irradiation directly at the impulse moment. The impulse parameters were: exposure dose $\approx 25 \cdot 10^3$ Rentgen, neutron fluence $\approx 1 \cdot 10^{14}$ cm^{-2}, impulse duration ≈100 μs.

The nuclear reactor radiation influence leads to parallel characteristic shift to the high voltages range. Maximum shift is observed under low (nitrogen) temperatures and amounts ≈0.5 V. Effect relaxation the time under the sample cooling increases and amounts to tens milliseconds.

RESEARCH OF RADIATION DEFECTS EVOLUTION IN STRUCTURES ON THE BASE OF GaAs

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The remote method for researching of damages evolution in structures based on GaAs after impulse irradiation was tested. The method is based on the functional dependence between the depth of trap levels and relaxation processes of nonequilibrium charge carriers.

The Schottky field transistors were taken for researching as samples [1]. Nonequilibrium charge carriers were induced by the GaN LED radiation. Experiments were made on pulsed nuclear reactor FBR-L [2].

We showed that shallow traps, which formed by neutrons, disappear during ~10 ms after reactor impulse. Deep traps with activation energy ~0,4 eV was formed during ~200 ms after reactor impulse.

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ELECTRICAL PROPERTIES OF POLY- AND SINGLE CRYSTALS OF $Nd_{0.7}Sr_{0.3}MnO_3$ PRIOR AND AFTER HIGH-PRESSURE TREATMENT

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Effect of colossal magnetoresistance in manganites with the perovskite structure $R_{1-x}D_xMnO_3$ (R - rare earth element, D - alkaline earth element) has been attracting attention of many researchers in view of a potential application. Active studies are mainly focused on the effect of magnetic field on the resistance, whereas the influence of electric field on the resistance (electroresistive effect) has not been fully investigated so far [1].

It has been shown that lattice defects and microstructure features can lead to changes in the electroresistive-effect magnitude. The lattice defects and microstructure features can be created and modified by high-pressure treatment (HPT). In particular, it was shown [2] that the electroresistive effect in the polycrystalline $Nd_{0.7}Sr_{0.3}MnO_3$ is highly dependent on the characteristics of microstructure which can be produced and governed by a unique method of HPT. This is evidenced by a very strong dependence of the resistivity of the sample on the value of the electric current passed.

In this work we studied the electrical resistivity of single- and polycrystalline $Nd_{0.7}Sr_{0.3}MnO_3$, prior and after the HPT at a quasihydrostatic pressure of 9 GPa and annealings at temperatures up to 1200K for 5-10 min with the subsequent quenching at 300K and 80K. A significant change in the form of the temperature dependence of the resistivity for the samples subjected to the HPT was found. Thus, for the polycrystals the resistivity increased by two orders, and the temperature of the metal – insulator transition (TMI) decreased by almost 100 K. The TMI temperature for the single crystal Nd0.7Sr0.3MnO3 after HPT also reduced but not so significantly - only by 20K, and the value of the resistivity increased less than two times. In addition, there were detected nonlinear current-voltage characteristics, the most stronger, in polycrystals after HPT.

This work was partly supported the fundamental research program UB RAS, project № 12-Y-2-1036 and the scientific school SS № 6172.2012.2.

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STRUCTURE, MAGNETIC, AND ELECTRONIC CHARACTERISTICS OF SEMIMETALLIC FERROMAGNETIC HEUSLER ALLOYS Co_2CrAl, Co_2CrGa, $Co_2Cr_{1-x}Fe_xAl$ AND Fe_2NbSn

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Synthesis of Heusler alloys and study of their properties, especially of those in half-metallic ferromagnetic state [1], are of special interest. One of the main features of these materials is the energy gap at the Fermi level in one of the spin subbands and semimetallic nature of the density of states in the other. This can lead to the 100% spin polarization of the charge carriers and these materials can be very promising for use in spintronic devices [2-4].

The half-metallic ferromagnetic state was predicted for the Heusler alloys such as Co_2CrAl, Co_2CrGa, $Co_2Fe_{0.6}Co_{0.4}Al$ and Fe_2NbSn. Since the properties of bulk (cast) alloys subjected to various treatments and "dimensional" (thin film) alloys can be very different, we have prepared the above mentioned Heusler alloys and investigated their structure, magnetic, and electronic properties. The samples were both in the bulk (cast) state and subjected to intense deformation by torsion - "dimensional" (film).

We studied the structure, magnetic, optical, electrical and galvanomagnetic properties of these alloys in the temperature range from 4.2 to 300K and in magnetic fields up to 10 T. It is shown that the cast alloys have an L21 structure, which is preserved after severe torsional deformation. Films of the alloys $Co_2Fe_{0.6}Co_{0.4}Al$ and Fe_2NbSn, obtained by magnetron sputtering and annealing, also have a crystalline structure. The experimental results are discussed in terms of the existing concepts of half-metallic ferromagnets and suggest that all these alloys show up a semimetallic ferromagnetic state.

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INFLUENCE OF THERMORADIATION ACTION ON THE STRUCTURE AND MORPHOLOGY OF THE IMPURITY – DEFFECTIVE COMPOSITIONS IN DOPED SILICON

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Modification of the monocrystallic silicon properties, based on the using dope process of the semiconductor matrixes by impurities, formed deep donor and acceptor levels in the forbidden region of silicon is one of the wide used applications of the technological methods in the modern solid – state electronics. Successful using of doped silicon is determined by the choice of the doped impurity, optimization of their concentrations and methods of doping. However during doping process in the sample volume simultaneously with formation of the deep level centers are formed micro defects, accumulations of impurity atoms in the form precipitates, defect complexes, arising at the thermo radiation action and etc., what strongly can act on their properties.

In this relation in the present work a structure and morphology of the impurity – defective compositions in the silicon doped by copper and palladium impurity before and after thermo radiation influence are studied by the electrical and structural methods.

For our research of the monocrystallic silicon of the n- and p-types conductivity with specific resistance of 5÷100 Ohm·sm were used. A dope of the silicon by the investigated impurities implemented by the thermo diffusion method in the temperature region 1000 ÷ 1280^{o}C during 0,5 ÷5 hours with further slow (with velocity co ~5 degree /min) and fast (with velocity of the ~250 degree/min) cooling. For taking into account thermal treatment and no control impurities, in parallel at the identical conditions was made anneal of the control samples, do not contains Cu and Ni. Irradiation was made by reactor neutrons up to the fluency $3 \cdot 10^{18}$ см$^{-2}$. A study of the types, structure and morphology of defective states was made on the modernized infrared microscope MIK-1. On the base of the carried investigations it was shown, that in the control samples was observed a tendency of the increase of the density and sizes of the dislocation pits with rise of the cooling rate and on the passing light can be observed micro defects, having an oval and roundish shape with laminated distribution, at that the sizes of the defect core is less than ~10 µm.

In the doped by cooper samples at the slow cooling dislocation sizes decrease, but in the sharply cooling samples in the result of the dislocation slip becomes their fusion with formation of the many petaline rosette and tubes. In the case of Si<B,Pd> at the sharp cooling can be observe dislocation motion to their fusion to the forming dislocation core.

In the sharply cooling samples of Si<B,Cu > after irradiation of neutron fluencies of $3 \cdot 10^{18}$ см$^{-2}$ with further anneal at 800^{o}C during 30 min occur a dislocation coupling and formation of the three petalines, arranged to each other on 120^o dislocation rosettes.

On the base of the obtained results suggested a mechanism of the low dimensional compositions formation with impurities and radiation defects participations and quazi chemical reactions, running in the doped silicon at the thermo radiation treatment.

This work was performed in the frame of Ф2-ФА-Ф121 grant at the Committee of coordination and development of science and technology at the Ministry Cabinet of the Republic of Uzbekistan.

IRRADIATION INFLUENCE ON THE MICRO SOLIDITY OF THE DOPED SILICON

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At the producing of silicon devices a hard requirements is needed for mechanical strength of using silicon, because many technological processes is related with contact interaction.

In the given work a process of the formation impurity – defect complexes in silicon, doped by copper, nickel and palladium impurities and influence of the thermo radiation treatment on the solidity parameters of the doped silicon are studied.

For the investigation were used monocrystallic silicon samples of n- and p- type of conductivity, grow by the Chokhralsky method with specific resistance 1÷100 Ohm·sm and dislocation density ~10^4см$^{-2}$. Doping of the silicon plates by the under research impurities were produced by the thermo diffusion methods in the temperature region 1000 ÷1280^{o}C during 5 ÷10 hours with further cooling with different rates.

Irradiation was produced by reactor neutrons VVR – SM up to $3{\cdot}10^{19}$ см$^{-2}$ fluencies. The study of the type and structure of defective states was made on the modernized infra red microscope MIK – 1. Test of the micro solidity under the Vickers on the (111) plane was measured on the PMT-3 device. Loud on the indenter was 1 H, and loading time 10 s.

On the base of the carried out researches was discovered that in all samples can be observed tendency to the rise of the dislocation pits density with rising of the cooling rate. At that their densities and sizes in the doped samples much greater then in control samples. Observed differences, probably, are due to the Cu and Pd impurities condensations on dislocations.

Investigations of the solidity parameters of silicon doped by the Cu, Ni and Pd impurities established a character of the impurity content influence on the silicon solidity. It was shown that Cu, Ni and Pd impurities lead to the loss of strength (due to the different covalent radiuses) of monocrystallic silicon. It was discovered, that oxygen precipitation suppress strengthening process due to the interaction of the diffusion atoms of Cu, Ni and Pd with oxygen and their capture by growing precipitates. It was established, that contribution into the strengthening of the doped silicon brings also dislocations, generated by the fields of the elastic tensions created by these impurities.

From the carried out investigations of the neutron irradiation influence on the silicon micro solidity changes, doped by Cu, Ni and Pd was discovered, that with rise of these impurities micro solidity of the irradiated monocrystallic silicon decrease, therefore doping of the silicon by these impurities suppress effect of the radiation strengthening of silicon.

This work was performed in the frame of Ф2-ФА-Ф121 grant at the Committee of coordination and development of science and technology at the Ministry Cabinet of the Republic of Uzbekistan

LOW-TEMPERATURE RESISTANCE AND MAGNETORESISTANCE HYSTERESIS IN POLYCRYSTALLINE $(La_{0.5}Eu_{0.5})_{0.7}Pb_{0.3}MnO_3$

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The behavior of temperature dependences of electrical resistance and magnetoresistance of polycrystalline substituted lanthanum manganite $(La_{0.5}Eu_{0.5})_{0.7}Pb_{0.3}MnO_3$ at low temperatures was thoroughly studied. A broad hysteresis was found in the field dependences of electrical resistance in the low-temperature region. Above 40 K, no hysteresis feature was observed. The temperature T = 40 K coincides with the temperature of minimum electrical resistance and temperature T_N of the antiferromagnet-paramagnet phase transition of the material of the intergrain boundaries. In this work we propose the model which explains the observed features of the R(T) and R(H) curves at temperatures below T_N by the formation of a network of ferromagnet-antiferromagnet-ferromagnet tunnel contacts [1]

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INFLUENCE OF POSITIVE AND NEGATIVE PRESSURE ON MAGNETIC AND LATTICE PROPPPERTIES OF FERROMAGNET $La(Fe_{0.86}Si_{0.14})_{13}$

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In ferromagnets $La(Fe_xSi_{1-x})_{13}$ there is observed a giant magnetocaloric effect (MCE) and significant magnetostriction in relatively weak fields. In the work presented the results of measurements of temperature dependence of the lattice parameter are given for the ferromagnet $La(Fe_{0.86}Si_{0.14})_{13}$ at different pressures and temperatures. Also, the temperature dependence of the lattice parameter of this sample was measured after neutron irradiation with a fluence of $3 \cdot 10^{19}$ n/cm^2. The experiments were performed on two neutron diffractometers and a synchrotron. The temperature measurements without a pressure were carried out in the town Zarechnyi (diffractometr D7a); those under pressure, in the Kurchatov's Institute (diffractometer DISK). The dependence of the lattice parameter on pressure at room temperature was obtained using a synchrotron (Median station).

The measurements of the temperature dependence of the lattice parameter of the ferromagnet $La(Fe_{0.86}Si_{0.14})_{13}$ at pressures 0 and 11 Kbar revealed that in the absence of pressure in the temperature dependence of the lattice parameter there is observed a sharp fall in the range from 160 to 210 K, whereas at a pressure of 11 Кбар, the decrease takes place in the range from 110 K to 180 K. This testifies to changes of T_c under pressure from the 210 K to ~150 K. Also, we established that upon neutron irradiation of the sample, both T_c and the lattice parameter grow, whereas the spontaneous volume magnetostriction decreases. After irradiation the Curie temperature equals 240 K. The results of experiments were analyzed with the use of equations of states with magnetic and elastic subsystems of a ferromagnet, which were derived in [1]. The lattice expansion caused by the presence of defects formed in the sample under the neutron irradiation is simulated by application of a negative pressure.

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ELECTRONIC PROPERTIES OF n-GaN IRRADAITED WITH HIGH-ENERGY ELECTRONS

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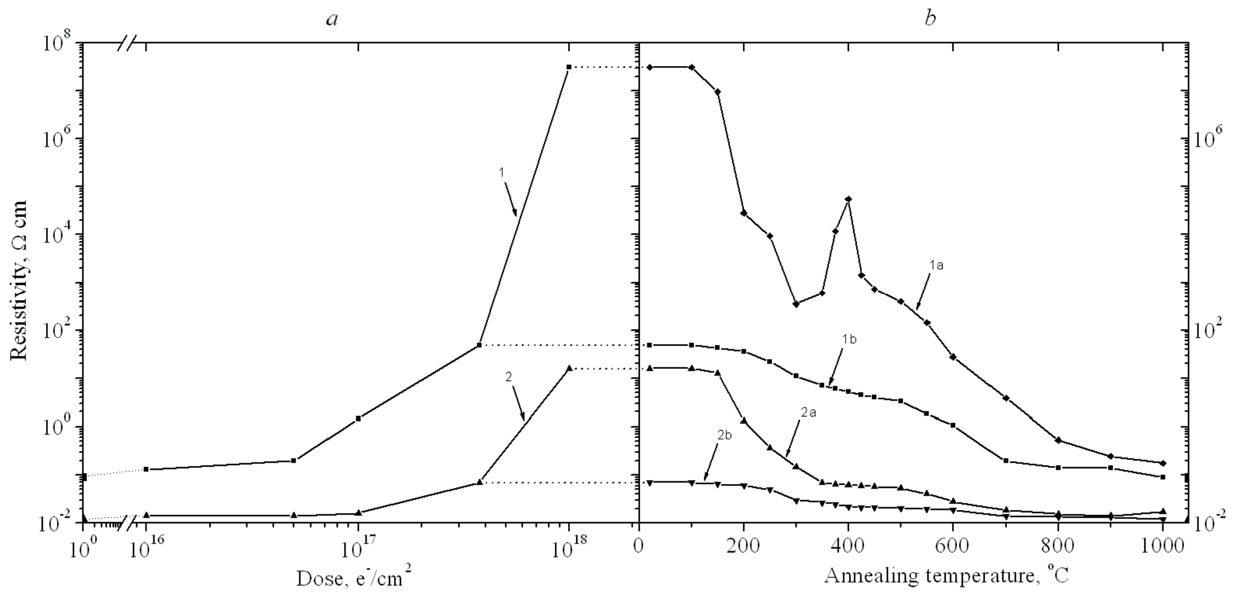
The influence of irradiation with electrons (E = 7 MeV, D = 10^{16} –10^{18} cm^{-2}) and subsequent heat treatments in the temperature range 100–1000°C on the electro-physical properties of epitaxial layers of n-GaN (d=4μm) alloyed with silicon (n=2·10^{17}, 2·10^{18}cm^{-3}), which were grown on the substrate of Al_2O_3 by the MOCVD method, is discussed. It has been discovered that upon electron irradiation, the resistivity of n-GaN increases, which is conditioned by shifting the Fermi level to a limiting position in the vicinity of Ec–0.91 эВ. The spectrum of deep traps in the initial state of n-GaN and that after irradiation was investigated. It is shown that the recovery of initial properties of the irradiated material takes place in the temperature range 100–1000°C, the main stage being near 400°C. For the samples with n=2·10^{17} cm^{-3}, in this range there was detected the stage of reversal annealing.



Dependence of resistivity of the epitaxial film GaN on the dose of electron irradiation (a) and temperature of annealing (b) for samples with different initial concentration of charge carriers n, [cm^{-3}]: 1 – 2·10^{17}, 2 – 2·10^{18};

The work was supported by the Ministry of Science and Education, FCP “Researches and Developments on the Priority Directions for Advances in Scientific and Technological Complex of Russia for 2007-2013“.

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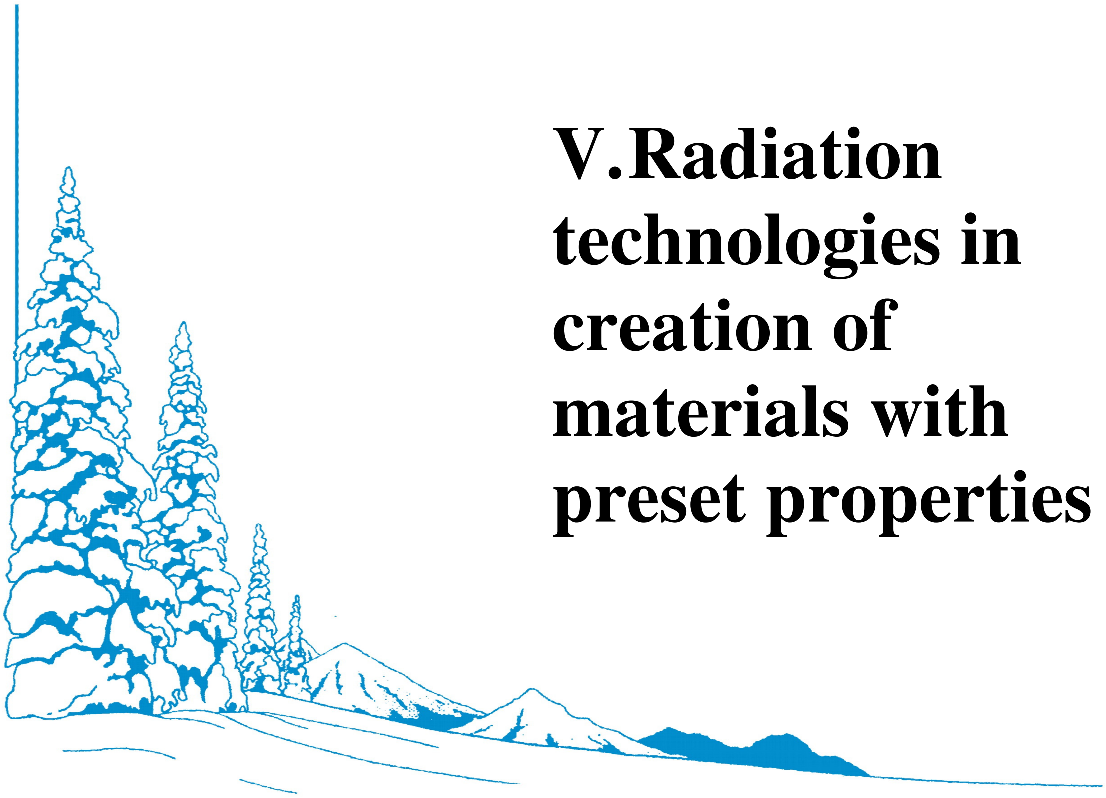

V. Radiation technologies in creation of materials with preset properties

The Seminar Program includes a section, which is intended to introduce the attendees to the latest developments in the sphere of radiation material science concerning the methods for production of new functional materials, including nanostructural materials. Presentations will be made on the formation of nanostructures by the method of radiation modification, specifically, the ion implantation and the shock-wave effect.

EFFECT OF IRRADIATION WITH MANGANESE IONS OF DIFFERENT ENERGIES ON CHANGES IN COMPOSITION OF SURFACE LAYER, SURFACE MORPHOLOGY AND MECHANICAL PROPERTIES OF CARBON STEEL

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In the beginning of last century it was shown that the state of surface, namely, presence of scratches, cuts, signs of treatment, etc, as well as topology and composition of surface, control many properties of solids, from their exterior to strength characteristics. Modification of the surface layers results in changes of properties of metallic materials. Up to date, a great many of methods for the surface treatment have been developed, thermomechanical, chemical, etc., of which one is ion-beam irradiation, being actively applied during the last decade. Purposefully choosing impurity atoms and modes of irradiation, one can provide with the method of ion implantation a variety of useful properties of surface layers: increase in the ultimate strength, yield strength, impact toughness, crack resistance, corrosion resistance, etc. [1,2]. In comparison with conventional ways of chemical-heat treatment, ion implantation allows one to shorten the duration of treatment by a factor of tens and decrease essentially its temperature, as well as to selectively treat separate portions of a part.

Earlier, we performed a series of researches into the influence of irradiation with manganese ions with doses from the range $2 \cdot 10^{16} - 10^{17}$ ion/cm^2 [3] and current densities,10 – 50 μA/cm^2 [4] on the formation of composition of surface layers, surface morphology, and changes in the mechanical properties of carbon steel St3.

This work deals with the influence of irradiation with manganese ions 10 - 40 keV in energy with the doses $5 \cdot 10^{16}$ and current densities 10 μA/cm^2 on the surface morphology and structure and composition of surface layers of carbon steel St3. The changes of fatigue strength, wear resistance, and microhardness of the surface layers of carbon steel depending on the energy of manganese ions are found. Regularities of the formation of elemental and structure-phase state of the surface layers, as well as of the surface morphology, with changing the energy of irradiation are discussed.

The work was supported by the Program of the Presidium of RAS (project №12-П-2-1040) and the Russian Foundation for Basic Research (project №11-08-00559).

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ION SYNTHESIS OF SILICON NANOSTRUCTURES

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The contribution presented consist of three parts covering both new and earlier published results of works that contain conclusions on synthesis, properties, andphysical models of formation of nanostructures produced by implantation of ions into silicon substrates..

1. Properties of self-organized SiGe quantum points formed by ion implantation of Ge ions into silicon have been studied with the help of SEM, AFM, and Auge-spectroscopy. It is established that after annealing a spatially ordered distribution of Ge atoms is observed in the implanted layers of silicon. The annealing leads to the formation of nanosize regions in which the content of Ge is 10–12% higher than in the surrounding matrix of solid solution SiGe. Optical properties of the layers of SiGe quantum point were investigated by the methods of combined light scattering and low-temperature photoluminescence. An intense luminescence peak was observed in the wavelength range 1,54–1,58 μm at room temperature [1].

2. A new result is the observation of formation of nanostructures upon ion implantation of rhenium ion into silicon. The profile of spatial distribution of clusters correlates with that for implantation of Re ions (maximum of the distribution coincides with R_p). Electronic Auge-probe was used to study elemental composition of the nanoclusters formed in which enrichment in Re atoms was detected. Atomic concentrations of Si and Re inside the clusters and beyond their limits depend on the conditions of implantation. It is established that increase of the frequency of ion-beam pulses results in the increase of cluster concentration, the dose of implantation being kept equal. Other parameters of the clusters formed (phase composition, size, etc.) also depend on the conditions of implantation. In view of the results published earlier on the synthesis of nanostructures by ion beams, a model of the process of formation of nanoclusters is suggested [2].

3. The results of etching with a focused ion beam of single-crystalline silicon with the formation of a nanosize relief on the surface are presented. The appearance of periodic ring edges at the walls of craters of etching with the Ga ion beam is observed. An explanation of this phenomenon is based on the effect of radiation plasticity [3].

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CHANGES IN STRUCTURE AND PHASE COMPOSITION OF HOT-WORKED 1960 ALLOY (Al–Zn–Mg–Cu) IRRADIATED WITH ACCELERATED Ar^+ IONS

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The effect of Ar^+ ion irradiation with an energy of 40 keV on the structural and phase state of the hot-worked 1960 alloy of the system Al–Zn–Mg–Cu has been studied.

Samples were irradiated by continuous Ar^+ ion beams using an ILM-1 facility for ion beam implantation, equipped with a PULSAR-1M ion source based on a glow discharge with a cold hollow cathode. The irradiation dose was varied in the range of 10^{15}–10^{17} cm^{-2}; the ion current density was 400 μA/cm^2.

Electron microscopy of thin foils, prepared from a section parallel to the irradiated surface at a distance of ~150 μm from it, revealed that after hot deformation the 1960 alloy has a nonuniform subgrain structure with a subgrain diameters from 1 to 5 μm. Subgrains contained dense dislocation tangles and clusters of randomly distributed intermetallic compounds Al_7Cu_2Fe and Al_8Fe_2Si of crystallization origin in the form of laths and lamellas up to 1.5 μm in length.

Low-dose Ar^+ ion irradiation ($2.5 \cdot 10^{15}$–10^{16} cm^{-2}) of the alloy provide us to eliminate nonuniformity of the subgrain structure: the fracture of subgrains with a diameter of 3–5 μm increased and their shapes became more equiaxial. The amount of excess phases at subgrain boundaries and the density of dislocations decreased. Simultaneously, the number and size of intermetallic compounds Al_7Cu_2Fe and Al_8Fe_2Si was reduced, which precipitated during crystallization and retained after deformation in the alloy. The average length of these particles in an irradiated sample did not exceed 300 nm.

In addition, the supersaturated solid solution decomposed under ion irradiation in the hot-worked alloy with the formation of fine particles belonged to metastable $\theta''(\theta')$ ($CuAl_2$) and η' ($MgZn_2$) phases and to stable η ($MgZn_2$) one with a diameter less than 15-20 nm and also with the formation of T-phase $Al_{49}(Zn,Mg)_{32}$ lath-shaped particles with a length from 150 to 300 nm.

An increase in the radiation dose to $1.9 \cdot 10^{17}$ cm^{-2} led also to dissolution of intermetallics Al_7Cu_2Fe and Al_8Fe_2Si of crystallization nature and to solid solution decomposition followed by the formation of $\theta''(\theta')$, η', η phases. Moreover, there was found coarse precipitated particles of stable ternary phases T ($Al_{49}(Zn,Mg)_{32}$) and S (Al_2CuMg) in the form of lamellas and lathes.

Thus, it was found an improved structure of the hot-worked 1960 alloy after low-dose irradiation with accelerated Ar^+ ions, i.e., a more perfect and uniform subgrain structure compared to the initial one, and detected dissolution of the coarse intermetallic compounds Al_7Cu_2Fe and Al_8Fe_2Si formed during crystallization as well as layers of excess phases at grain boundaries. This all resulted in an increase in ductility of the alloy from 9% to 14%.

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MANIFESTATIONS RANGE EFFECT OF ION IMPLANTATION IN STUDIES OF THE ALLOY FOIL $Cu_{50}Ni_{50}$

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Rolled $Cu_{50}Ni_{50}$ are irradiated with Ar^+ ions under various ion energies, ion current densities and doses of irradiation. Modification of defect structure in abnormally deep layers of target is found. Non-monotonous distribution of defects with depth is revealed.

The investigation of the microhardness and elemental composition of non-irradiated hand rolled alloy foils $Cu_{50}Ni_{50}$ with deposited on the irradiated side of the aluminum layer, subjected to implantation of Ar^+ ions with different energies, doses and current density.

The study ended with a non-irradiated side showed that as a result of ion implantation is a redistribution of material components (changing ratio of the concentration of atoms of copper and nickel), despite the fact that the thickness of the foils is several orders higher than the calculated depth of the changes in the composition and structure of the material as a result of ion implantation.

Microhardness unirradiated sides also highlighted the influence of ion irradiation on abnormally high (according to the theory Lindhardt-Shaft-Schiott) distance from the irradiated surface.

Studies have shown that with the non-irradiated side of the foil microhardness depends essentially on the irradiation parameters and the load on the indenter, from which it can be concluded that the micro-hardness of the material uniform depth. In addition, the microhardness of the irradiation parameters are diverse, depending on the load on the indenter. This may indicate a dependence of the characteristics are formed by ion implantation of inhomogeneous structures of irradiation parameters: microhardness, and hence the structure of the various layers of materials under irradiation varies nonmonotonically.

In our opinion, this is due to the initial non-equilibrium state of the samples after rolling. Ion implantation is self-propagating structural changes upon irradiation of the target incident ions create local thermal spikes. The excess energy causes the generation of elastic waves, and the energy carried away by the waves, is sufficient to transform the source of the defect structure of the material, including the initiation of chain reactions (associated with unlocking dislocation annihilation of various types of defects). As a result of the non-irradiated foil the redistribution of material components due to coupling of the atoms with a certain kind of met in the flow of ion implantation defects.

Thus, the ion-beam processing of metallic systems with a suitable choice of parameters can be used for different products aimed to create ultra-thin surface layers of a given composition and structure.

This work was supported by RFBR (10-02-96039_ural) and the Presidium of the Russian Academy of Sciences 12-F-2-1013.

MODIFICATION OF MACROSCOPIC VOLUMES OF CONDENCED MEDIA UPON THEIR SURFACE IRRADIATION WITH ACCELERATED IONS

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It is known that metastable condensed media can transit into an equilibrium or nearly equilibrium state under external effects.

According to [1], the tendency of metastable media to structural phase transitions from a state 1 to a state 2 with a lower free energy induced by the post-cascade shock waves substantially depends on the fulfillment of the following relations:

$$(\alpha\tau)^{1/2} \ll R_o < (E/(4/3\pi n\Delta f))^{1/3}, \quad (1)$$

$$\Delta F > 2\beta\Omega\Gamma\Delta f, \quad (2)$$

where R_o is the effective radius of the cascade of atomic displacements; $l = (\alpha\tau)^{1/2}$ is the characteristic length of the heat; $\tau \sim 10^{-12}$s is the thermalization time; E is the energy of the accelerated ions; n is the atomic density of the medium; Δf is the energy of a transition potential barrier; v is the shock wave velocity; Ω is the wave shape factor (for a Gaussian profile of the solitary wave $\Omega = 1.06 \approx 1$); Γ is the wave width (according to [2], $\Gamma \sim 1$ nm); $\beta = \delta/v$ for a plane wave, and $\beta = \delta/v + 1/R$ for a spherical wave; and δ is the decay factor.

In [1, 3], the size of atomic cascades and energy density ε released in cascades (for heavy ions implanted into metals at E = 10–50 keV) were estimated using hydrodynamics, Monte-Carlo and molecular dynamics approaches and the variation ranges of all above mentioned parameters were analyzed. These data and those of direct experiments on the measurement of energy ε released in the atomic cascades (0.5–0.6 eV per atom of cascade, which agrees with the calculated data; at Δf being no more than 0.2–0.3 eV) [4], allow us to make the following conclusions. Virtually in all metastable media (even in media with minimal stored energy ΔF, which is only hundredths or even thousandths of eV per atom), solitary waves with sufficiently high amplitude ($\varepsilon \sim \Delta f$) can propagate without decay. Such waves are able to rearrange these media, This refers to the process of migration of individual atoms, unlocking of dislocations, cooperative atomic rearrangements in solids, etc.

The energy density in the self-propagating (undamped) solitary wave in the steady state: $\varepsilon^* = \Delta F/(2\beta\Omega\Gamma)$ [1], is such that the scattering speed of this energy in the medium is exactly equal to the rate of energy release at the expense of the transformation at the wave front.

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IRRADIATED-AMORPHOUS STATE OF RAPIDLY QUENCHED ALLOYS $R_2Fe_{14}B$ (R=Nd, Er)

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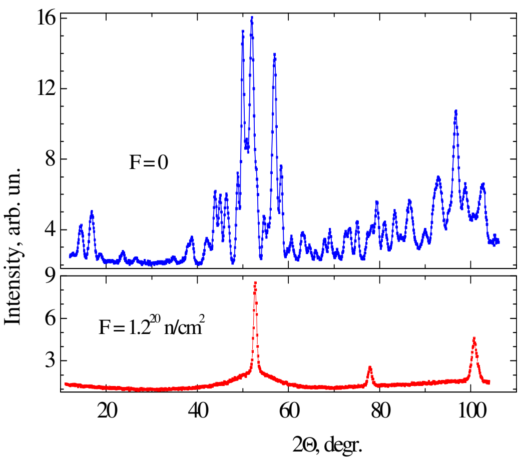
Based on $Nd_2Fe_{14}B$ phase permanent magnets possess record value of maximal energy product. At the same time, simple estimations show that a specific magnetization of such magnets is lower than that of iron and their coercive force is much less than an anisotropy field. One of way to increase a magnetization and a coercive force of these magnets is creating of composite magnets, formed by exchange-coupled magnetically hard (crystalline) and magnetically soft (amorphous) phases. Therefore, an attainment of amorphous state of the $Nd_2Fe_{14}B$ phase is of interest of both fundamental investigations and practice. Rapidly quenched Nd-Fe-B alloys are used in modern magnet production. A procedure of getting of rapidly quenched alloy consists in a cooling of a liquid melt on a surface of a fast-rotating wheel ($V_{tan} \approx$ 40 m/sec.).

In this research an amorphous state of rapidly quenched $Nd_2Fe_{14}B$ and $Er_2Fe_{14}B$ alloys were gotten at the first time and their basic magnetic properties have been studied.

An amorphous state has been attained by irradiation of the fluence of fast neutrons of $1.2 \cdot 10^{20}$ n/cm^2. Neutron diffraction experiment was carried out on diffractometers D-2 and D-3 (reactor IWW-2M, Zarechny, Russia); neutron lengths λ = 1.8 and 2.4 Å have been used.

Fig. 1 presents neutron powder diffraction patterns of initial (up) and irradiated-amorphous (bottom) states of rapidly quenched $Nd_2Fe_{14}B$ alloy. One can see that reflections, originating from nuclear and magnetic coherent neutron scattering on initial $Nd_2Fe_{14}B$ phase, disappeared. Instead of theirs only reflections with large half-width take place on bottom diffraction pattern, so there exists neither nuclear nor magnetic long-range orderings. On bottom diffraction pattern three reflections, which have narrow half-widths, are related with coherent neutron scattering on α-Fe phase.



We studied basic magnetic properties of the $Nd_2Fe_{14}B$ and $Er_2Fe_{14}B$ phases in the amorphous state and found that saturation magnetization and Curie temperature of the $Nd_2Fe_{14}B$ phase didn't change visibly in compare with that in crystalline state. However, a coercive force decreased in amorphous state almost to zero; a phenomenon of a magnetic nonsaturable disappears over region of low fields. Then, if particles of the amorphous phase are exchange-coupled with a crystalline phase, they are oriented fully along a direction of an exchange field. This will be accompanied by an increasing of the magnetization.

In case of the amorphous $Er_2Fe_{14}B$ alloy is observed a noticeable decreasing (at about of 200 K) of Curie temperature that causes corresponding magnetization lowering (almost two times) at room temperature.

This work was partly supported by the project of RFBR 12-02-12065-OFI_M.

FORMATION OF COMPOSITION OF SURFACE LAYERS IN CARBON STEEL DEPENDING ON DOSE OF PULSE IRRADIATION WITH CHROMIUM IONS

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Service characteristics of metals and alloys, including endurance, wear resistance, corrosion and erosion resistance, and some other properties, are controlled by the structure-phase state of surface layers. Consequently, the surface characteristics of metals and alloys can be significantly improved by means of surface modification. It looks promising to employ the implantation method [1] as a way of treating surfaces. This method makes it possible to cut time and temperature of action onto a material by a factor of tens, as well as to automate the process of treatment. Besides, surface strengthening of low-alloyed carbon steels is one of the current trends in the machine building industry. Yet, with a lot of researches conducted in this direction, many fundamental and technical problems related to the service treatments of metals and alloys still remain unsolved because of a variety of factors affecting changes in structure and properties upon ion-beam treatment. At the same time, depending on the mode of action, both positive and negative effects on the material properties can be observed. In this connection, the aim of the work was to study the influence of the does of pulse irradiation with chromium ions on the changes in mechanical properties of carbon steel St3.

The pulse irradiation with chromium ions was carried out at the following parameters: the energy equal to 30 keV; current density at pulse, 0,8 mA/cm^2; frequency of pulse sequence, 25 Hz; pulse duration, 0,4 ms. The dose of irradiation was varied from 10^{16} to $5 \cdot 10^{17}$ ion/cm^2. The endurance and hardness of surface layers have been found to change depending on the dose of pulse irradiation. Regularities of formation of elemental and structure-phase state of surface layers, as well as morphology changes of the surface with increasing the irradiation dose are discussed.

The work was supported by the Programs of the Presidium of RAS (project №12-P-2-1040 и №12-P-2-1013) and by the Russian Foundation for Basic Research (project №11-08-00559).

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INFLUENCE OF PULSED LASER RADIATION ON MICROHARDNESS AND COMPOSTION OF SURFACE LAYERS OF $Cu_{50}Ni_{50}$ FOILS

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The purpose of this work consists in studying the influence of defocused laser radiation on the processes of mass transfer in the surface layers of nonequilibrium foils $Cu_{50}Ni_{50}$ with one side sputtered with Al, depending on the number of laser pulses.

To solve the problem we employed methods of X ray phonoelectron spectroscopy (XPES), atomic force microscopy (AFM), and measurements of microhardness. Laser impact on the samples was preformed by an fiber-optic ytterbium laser LDesigner.

The experiments carried out allowed one to establish that after irradiation of foils, chemical composition of the surface layers of the foils changes (Fig.1), as well as the surface microhardness (Fig.2). The AFM data evidence no changes in the relief of the foil surface either at a macro- or microscale in the zone of irradiation. Calculation of temperature in the irradiated region shows up that the thermal influence in the zone of irradiation was not sufficient for the origination of the thermodiffusion mechanism of mass transfer of the system elements. Consequently, one can assume that in the given case the change of the surface composition of the foils is conditioned by the wave mechanism of elemental transfer due to a shock laser action. A decrease of microhardness of the irradiated foil side can be caused by an increase in internal stresses and plastic deformation of the irradiated system.

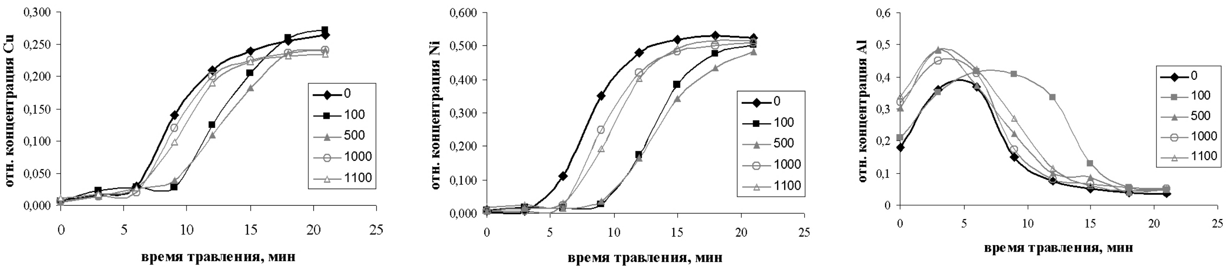

Fig.1. Distribution of elemental concentrations in ratios over the depth from the irradiated side of the $(Cu_{50}Ni_{50})$+Al system depending on the number of laser pulses.

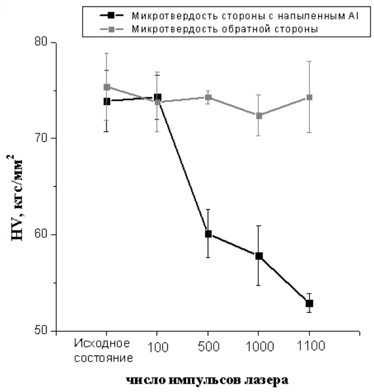

Fig.2. Microhardness of foils $(Cu_{50}Ni_{50})$+Al

The work was supported by the Russian Foundation for Basic Research (project 10-02-96039_ural).

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.

HYDROGEN-VACUUM TREATMENT OF PALLADIUM POWDERS USING IN THE PRODUCTION CATHODES FOR MAGNETRONS

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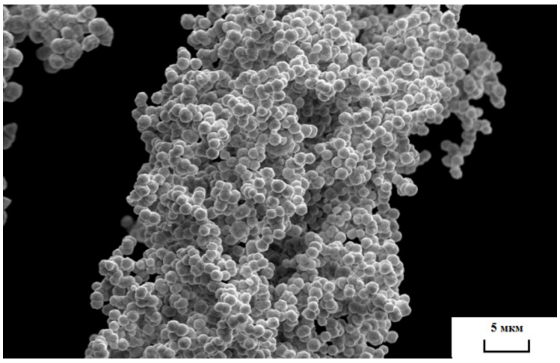
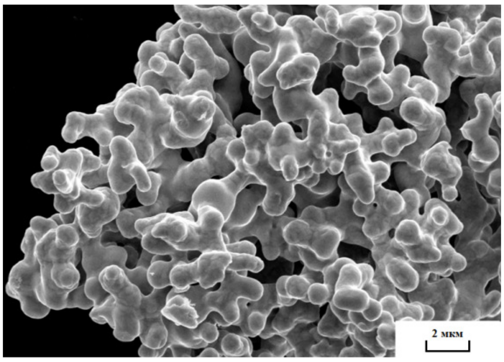
Practically instantaneous availability (no more than 0.5 seconds) of nonincandescent magnetrons is its characteristic feature. Such availability is provided by a special design of the cathode unit that does not require its heating.

Cathode assembly in nonincandescent magnetrons consists of alternating washers and field-electron secondary emission cathodes. In these magnetrons during feeding the anode width modulated voltage a field emission current from the field-emission cathodes (AEC) initiates the generation of microwave oscillations. And secondary-emission cathodes (SEC) support operation of devices during the exploitation period. The washers ~ as 4 microns of thickness from tantalum foil used as AEC predominantly. SEC consists of palladium and palladium intermetallic compound Pd_5Ba powders must have stable emission characteristics and to be resistant to the ion and electron bombardment.

In the paper it has been investigated in detail the operation of the initial palladium powder preparation, its structure and elemental composition, the distribution of fractions of powder size and opportunity to improve the homogeneity of the size distribution of the powder particles. After subsequent operations of the cathode preparation these factors provide an uniform distribution of the emission component on the surface of the cathode.



Micrograph of the original palladium powder surface



Micrograph of palladium powder subjected to hydrogen-vacuum treatment

To improve the uniformity of the particle size distribution of palladium, emission-uniform distribution of the active component and emission characteristics of cathodes in this work it has been carried out the investigation to stabilize the size of the palladium powder particle by its annealing in hydrogen and subsequent tempering in a vacuum.

Conclusions

1. The method of hydrogen-vacuum treatment of palladium powder for the manufacture of palladium-barium cathodes of nonincandescent magnetrons has been proposed.

2. It has been shown that application of the method improves the efficiency of the cathodes. Using of the cathodes in nonincandescent magnetrons of both 2-cm and 8-millimeter wavelengths allowed to increase by 1.5 times the yield rate instruments.

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HOW CAN TEM WITH *IN SITU* ION IRRADIATION OF THIN FOILS PREDICT NEUTRON IRRADIATION DAMAGE IN BULK?

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We have performed a series of experiments using TEM of *in situ* ion irradiation of thin Mo foils designed to closely couple to computer model simulations. Measured defect densities, sizes and 3D distribution with foil depth, as functions of ion dose, dose rate, and temperature [1] were used to advise and validate a cluster dynamic reaction rate computer model [2] for exactly the same set of conditions. The same model kinetic parameters were employed to simulate neutron irradiation damage in bulk Mo and compared with similar TEM data from neutron irradiated Mo from the same material source. The results demonstrate a promising direction in understanding and predicting neutron damage in bulk with *in situ* ion irradiation of thin films closely coupled with computer modeling.

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RPV LOW TEMPERATURE ANNEALING INTENSIFICATION BY ADDITIONAL IRRADIATION

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As a main barrier against radioactivity outlet reactor pressure vessel (RPV) is a key component in terms of NPP safety. Therefore present-day demands in RPV reliability enhance have to be met by all possible actions for RPV in-service embrittlement mitigation. Annealing treatment is known to be the effective measure to restore the RPV metal properties deteriorated by neutron irradiation.

There are two approaches to annealing. The first one is so-called «dry» high temperature (~475°C) annealing. It allows obtaining practically complete recovery, but requires the removal of the reactor core and internals. External heat source (furnace) is required to carry out RPV heat treatment.

The alternative approach is to anneal RPV at a maximum coolant temperature which can be obtained using the reactor core or primary circuit pumps while operating within the RPV design limits. This low temperature «wet» annealing, although it cannot be expected to produce complete recovery, is more attractive from the practical point of view especially in cases when the removal of the internals is impossible.

The first RPV «wet» annealing was done using nuclear heat (US Army SM-1A reactor). The second one was done by means of primary pumps heat (Belgian BR-3 reactor).

As a rule there is no recovery effect up to annealing and irradiation temperature difference of 70°C. It is known, however, that along with radiation embrittlement neutron irradiation may mitigate the radiation damage in metals. Therefore we have tried to test the possibility to use the effect of radiation-induced ductilization in «wet» annealing technology by means of nuclear heat utilization as heat and neutron irradiation sources at once.

In support of the above-mentioned conception the 3-year duration reactor experiment on 15Cr3NiMoV type steel with preliminary irradiation at operating PWR at 270°C and following extra irradiation (87 h at 330°C) at IR-8 test reactor was fulfilled.

In fact, embrittlement was partly suppressed up to value equivalent to 1,5 fold neutron fluence decrease. The degree of recovery in case of radiation enhanced annealing is equal to 27% whereas furnace annealing results in zero effect under existing conditions. Mechanism of the radiation-induced damage mitigation is proposed.

NEUTRON STUDIES IN MATERIAL SCIENCE

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Neutron scattering studies of materials including irradiated ones regarding to the development of analytic complex at the reactor PIK with high flux neutrons are discussed. It is analyzed the state of researches of amorphous and crystalline materials: reactor constructional steels and alloys under irradiation and mechanical loading, welded joints of power plant's reactor vessel, membranes conducting protons for hydrogen power, inorganic fibers for thermal isolation, elastomers including nanoparticles. The experimental goals of non destructive neutron methods are considered (analysis of structure in the bulk, selective contrast, sensitivity to isotopic composition and light elements (hydrogen), mobility of atoms and structural defects (vacancies, interstitial atoms, dislocations). The expected characteristics are presented for the material science instrumental complex including reactor PIK.

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EXPERIMENTAL FACILITY FOR MÖSSBAUER EFFECT OBSERVATION UNDER ION IRRADIATION

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There are experimental data that material characteristics change under ion bombardment not only in the area of ion deceleration, but at a depth well above the projected range of the particles [1, 2]. These processes were called "long-range effects." A lack of sufficient explanation for them is partly due to the fact that all studies on ion effects were so far conducted only "post factum" [1, 2], including Mössbauer studies [3]. It was assumed in [2] that the observed phenomenon might be related to the formation and propagation of post-cascade shock waves in material and excitations, which propagate in the electron subsystem and are able to influence the distribution of outer shell electrons in atoms.

A special equipment for gamma resonance (Mössbauer effect) under irradiation of ^{57}Fe-containing targets ("in situ") with Ar^+ ions (or other gas ions M >10 amu) was built in the laboratory of beam exposure of the Institute of Electrophysics of UB RAS to detect radiation-supported electron and phonon excitations in matter. Comparison of the Mössbauer spectra of the samples taken before, under, and after the irradiation allows indicating the changes in atomic and electronic structures of crystals.

To implement the experiment we used an equipment that included a facility for ion-beam modification of condensed matter [4], with a plasma ion source PULSAR-1M [5], which generates continuous ion beams with an energy up to 40 keV and an ion current density up to 500 μA/cm^2, and a precision Mössbauer one built on the basis of a standard SM2201 spectrometer. A doppler modulator, a detector, and the sample were placed in a vacuum implanter chamber of so that the gamma-axis of spectrometer intersects with the axis of the beam in the center of the sample – the foil with a thickness of 10 μm.

The use of specially enriched material for a scintillation crystal-converter and a new circuit solution made it possible to eliminate a detector overloading due to the presence of deceleration radiation (0-40 keV), arising during the ion source operation, on the background of the resonant γ-radiation with an energy of 14.4 keV and to increase the Mössbauer spectrum reading speed.

This work was supported by the Presidium of the Ural Branch of Russian Academy of Sciences (program OFN no. 5 "Physics of new materials and structures").

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ABOUT PULSED PRESSURE UNDER ELECTRICAL BREAKDOWN IN FUSED SILICA

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Paper [1] for the first time presented the results in Russian periodical literature on investigation of potential behavior macroscopically anisotropic carbon-carbon (C-C) composites under absorption of pulsed electron radiation energy. Small value of Gruneisen coefficient of such composites requires using high-sensitivity piezogages (for example, piezoceramics TsTS-19 [1]) and acoustic delay of registered pulse of thermo-mechanic stress, which permits to increase measurement resistance to electrical noises appearing under accelerator launching. As practice showed, the selection of materials for using as a delay can not be arbitrary. Absorption of bremsstruhlung energy [2] in delay materials having Gruneisen coefficient at the level of 1…2 (aluminum or titanium alloys) leads to formation of "parasitic" pressure pulse, whose amplitude can be comparable with amplitude of thermo-mechanical stress in the sample under study.

Application of delay materials having small Gruneisen coefficient (for example, fused silica of KV grade [3]) permits to decrease the amplitude of "parasitic" pressure in it by one- two orders. However under irradiation of CC composite samples 4KMS with the thickness that is less than accelerator electron path, application of silica led to appearing a signal from piezogage of "parasitic" pulse of another origin. For this composite, polarity of such pulse (Fig. 1, the first positive pulse) differs from polarity of a signal related to thermo-mechanical stress, whereas their amplitudes are comparable. While studying complicated profiles of thermo-mechanical stresses, their interpretation can be a problem.

Appearance of "parasitic" pulse of such type is conditioned by pressure developed in fused silica under electrical breakdown, caused by electrons that passed through the composite sample. The difference of this pulse from the pulse of thermo-mechanical pulse is a short front (~ 40…80 ns). Much longer front of thermo-mechanical pulse in silica is determined by a profile of electron energy absorption in it. Fig. 2 shows oscillogram of a signal obtained from a gage using fused silica plates as acoustic delay and irradiated sample.

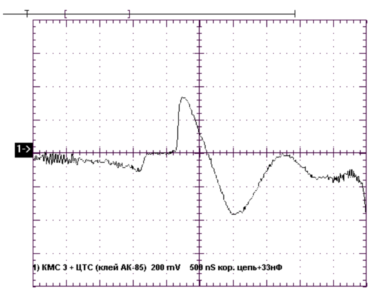

Fig. 1 Oscillogram of a signal from the gage for C-C composite sample 10 mm thick. Time base - 500 ns per a division.

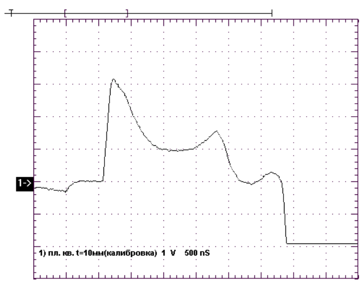

Fig. 2 Pressure profile formed in fused silica sample under electron energy absorption. Time base - 500 ns per a division.

At first, positive polarity pulse is registered, front duration is about 80 ns. Its time profile shows that at the cost of breakdown, pressure pulse was formed at the rear sample side relatively to electron beam falling. The second positive peak on oscillogram is related to the formation of thermo-mechanical stress pulse. Complicated resulting signal profile is conditioned by time overlapping of these two pulses having different duration. Their maxima are scattered in time at the cost of different spatial formation of pressure profiles. For this accelerator launching, amplitude of pressure pulse, formed under breakdown, was ~ 1,3 MPa. Despite the fact that with this method of breakdown realization, profile of its pressure pulse is difficult to distinguish, it is possible to asses its duration as ~ 0,2 μs.

Analysis of irradiated fused silica samples confirmed that after irradiation, it is possible to observe a picture of branching, which is formed under electrical breakdown in dielectrics (Fig 3). For correct reproduction of thermo-mechanical stress profile in C-C composite, using acoustic delay out of fused silica, it is desirable to have sample thickness larger than electron path in it.

Fig. 3 Photo of a picture formed in fused silica sample after a series of irradiation by electron beam.

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