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October 10-15
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FUNDAMENTAL PROBLEMS AND MODERN TECHNOLOGIES OF MATERIAL SCIENCE (FPMTMS)

Altai State
Technical University
Barnaul, Russia

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FUNDAMENTAL PROBLEMS AND MODERN TECHNOLOGIES OF MATERIAL SCIENCE (FPMTMS)

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The main problems of this Conference were as follows: Structure-energetical transformations in condensed materials, taking place at difference influences: temperature, high pressure, high energetical influence, annealing e.t.c.; problems of formation of amorphous phases and nanostructures; role of defects struture - energetical transformations in materials; influence of microgravitation on cristallization and phase transition in materials; the development of making technique of metastable phases; properties of metastable phases; problems of making of new materials with prognosticating set of physical properties.

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THE RESEARCH OF THE STABILITY OF POLYSYNTHETIC TWINS IN THIN FILM WITH FOLIATED SUPERSTRUCRURES OF AB STOICHIOMETRIC COMPOSITION

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In the present work the stability of the twins structure in the metal ultrathin film and alloy surface with foliated superstructures of AB stoichiometric composition is considered. The investigation is performed using in the limits of the model of stochastic diffusional atomic ordering. Ordered metal thin film with hard square lattice, where twin antiphase boundaries (from 1 to 8) are formed in the direction <11>, is studied. The sensitivity of pine-like domain structure with regular alternation of axis C to the temperature is investigated. The ratio of ordering energy in the first two coordination spheres, when twin boundaries keep in the definite temperature interval, is determined empirically. Parameter of long-rang order is determined in the layers, situated on both sides from the boundary and inside domains one. It was obtained, that temperature of phase transition Tc changes in the dependence on density of twin boundaries. With the growth of density of twin boundaries, transition temperature increases. The density of the twin antiphase boundaries, when the structure of the domains appears to be stable till high temperature, is determined.

STABILITY OF TWINS STRUCTURE IN ULTRATHIN FILM WITH FOLIATED AB SUPERSTRUCRURES

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In the present work the stability of twin structure in the metal ultrathin film and alloy surface with foliated superstructures of AB stoichiometric composition is considered. The investigations are made using the stochastic methods.

Twin antiphase boundaries (from 1 to 8) are formed in the direction <11> in the initial material. The atomic reconstruction of the material is realized under the diffusion of atoms at the vacant points of the crystal lattice. The sensitivity of pine-like domain structure to the temperature is investigated. The ratio of ordering energy in the first two coordination spheres, when twin boundaries are kept in the definite temperature interval, is determined empirically.

It was obtained, that the temperature of order-disorder phase transition changes in the dependence on density of twin boundaries. With the growth of density of twin boundaries, transition temperature increased. The density of the twin antiphase boundaries, when the structure of the domains appeared to be stable till high temperature, is determined.

EVOLUTION OF THE THIN FILM STRUCTURE WITH ANTIPHASE BOUNDARIES IN THE ORDERED PROCESS

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The evolution process of the thin film structure in the transformation order – disorder was investigated in the limits of computer experiment. It was used the model of diffusion in the two-dimensional binary thin film (AB) with hard square lattice. The following parameters are varied: temperature of annealing, concentration of vacancies, initial meso- and micro- structure of thin film. The initial structures of the modeled thin film contained antiphase boundaries were considered.

It was studied mechanisms of domains coalescence and relaxation of antiphase boundaries, dividing them. The influence of boundaries length on the process of the antiphase boundary struc-

ture evolution at different annealing temperatures was examined. Also it was studied the effect of boundaries "washing" and their transformation in interphase boundaries. It is established that phase transition order-disorder passes wide two phases sphere and heterophase fluctuations of ordered phase proceeds to it. Four main mechanisms, leading the thin films to disordered state, were obtained.

STRUCTURE-ENERGETICAL CHARACTERISTICS OF CRYSTAL LATTICE NEAR COMPLEX PLANAR DEFECTS IN SHAPE MEMORY ALLOYS

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Nowadays application sphere of ordered alloys is wide because they have uniqul phisico-mechanical, electro-magnetical and thermal properties, depending on structural features of ordered state of material. In the result of their comparison with pure metals major part of defects can be formed in ordered alloys. Investigation of their energies and atomic features is considered to be important. Ordered systems $D0_3$ (alloy Fe_3Al), $L1_2$ (alloy Ni_3Al), $D0_{24}$ (alloy Ni_3Ti) and $D0_{19}$ (alloy Ti_3Ni) were investigated in this paper. Energetic and structural features of planar defects were found in basic and prismatic orientations of main sliding systems for antiphase boundaries and in pyramidal – for twins the method of computer simulation. Also it was obtained interaction of antiphase boundaries with point charges.

It can be noted, that sedimentation of substitution defects and vacancies at antiphase boundaries leads to deformation of crystalline structure, having many layers. Their zones, saturated with point defects, interchange with unsaturated zones. It was established that such crystalline reconstruction (at the given conditions) can appear in result of thermoactivated processes. Energies of complex defects (point defect and antiphase boundary) decrease in comparison with energy formation of single antiphase boundary.

CONSTRUCTION OF INTERATOMIC POTENTIALS IN ANISOTROPIC CRYSTAL STRUCTURES

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It is known, that the stability of anisotropic crystal structures with hexagonal and tetragonal lattices of the knots can not be reached by the use of isotropic central pair potentials of interatomic interaction. In this connection the most acceptable in the use of anisotropic non-central potentials, which take into account the symmetry of the crystal lattice. For the description of interatomic interactions in hexagonal crystals, we made an attempt to construct a similar potential on the basis of sufficient approved Morse function. The parameters of interatomic potential were determined from the conditions of the stability of crystal HCP lattices. Numerical values of the parameters were determined for the metals: Cd, Co, Hf, Ti, Mg, Zr, Zn. At the description of the properties of ordered alloys and intermetallids with the superstructures $D0_{19}$ and $D0_{24}$, the same type of interatomic potential was used. The values of potentials parameters, describing the interactions of atoms of the same type, were the same as in pure metals. The set of the known properties of the definite alloy was used for the determination of the parameters of interatomic potentials, describing the interactions of the atoms of different types. In particular, the values of the lattice parameters, ordering energies and formation energies of antiphase boundaries were taken into account at the determination of the potential parameters in the alloy Ti_3Al.

CONDENCED PHASES STRUCTURE AND THEIR COMMON CRITICAL POINT

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Among processes of production of many materials the leading role belongs to metallurgical technologies of deriving of metallic blanks and products from melts. It is known that an unsoundness of a solid material essentially depends on quality of a melt and an evolution of defects. Therefore researches of physical properties of substances in a liquid state and their changes in crystallization processes are uniformly important with traditional material-science by researches of solid materials during thermal, mechanical, chemical and beam influences.

The list of researched physical properties of substances and materials is very wide but the special importance is represented a density and it defects in macro- and microvolumes, and also atomic volumes v_a in individual substances and in alloys. For example, a long time is known the rule Hume-Rothery: the metallic alloys are received stables, if the residual of atomic volumes of components does not exceed 15%. It means in particular that dimensions of atoms themselves are rather stable within the limits of temperature technological modes including a melt state, crystallization and solid substance (material). The emerging and research of metallic clusters and also deriving nanocrystalline and cluster materials was made the problems of nanostructure determination especially actual.

In this work some results of research about correlations of rigid and liquid condition of elementary substances are given on the basis of cluster model of a structure of substance in condensed states. The temperature interval of these condition makes from $T = 0$ K up to the T_C - temperatures of the critical point " liquid / vapour (gas) ". This interval includes also the point melting-crystallization T_L, near to which are rather well known a macrophysical property of many substances, including macrodensity ρ, interatomic distances R_1 and coordination numbers Z_1 in nanostructure. Before was shown ([1] etc. earlier), how the structure of crystal characterized by numbers R_{1S} and Z_{1S}, will be transformed to a structure of liquid with the meanings R_{1L}, Z_{1L}. Essentially that after melting $R_{1L} < R_{1S}$ but $Z_{1S} = Z_{1L}$ at many substances. In other hand the comparative study of literary data about meanings R_1 of majority of elementary substances in liquid and solid states was realized. ([2] etc.) This research has shown that R_1 in the time of heating of metal crystals in an interval (0, TL) is increased less than by 2 % if structural transformations are not present in concrete substance. As show many experimental data values R_1 and Z_1 of liquids do not practically depend on temperature in an interval (T_L, T_C) or decrease a little.

These results well correspond to the theory of a cluster structure of liquids developed by us. In this theory we assume, that a natural elementary cell of crystal and liquid both are stable minicluster consisting of central atom and Z_1 atoms of the first coordination sphere on a distance R_1. The identity of elementary cells in an interval (0, T_C) allows calculating a critical density ρ and also the temperature T_C and pressure P_C value. At the same it used of a model of spherical atom by a diameter $d_a = R_1$ and van der Waals equation of state. On this basis the accounts of main properties the critical point "liquid / gas" of many substances having various structures of a crystalline condition are conducted: the PC (Z_1=6), BCC (Z_1=8), HCC (Z_1=12). They have a little bit distinguished theoretical parameters of a minicluster model owing to a difference in Z_1 and denseness of atoms packing in a crystal.

The results of all estimates have shown good concurrence known experimental (only Hg, Cs, Rb, K) and other data ρ_C, T_C and new settlement values at many metals. Thus the obtained evaluations once again testify to genetic coincidence of solid and liquid state of substance. It is exhibited first of all in uniformity and invariance of main nanosructural characteristics of condensed states: $Z_{1L} = Z_{1S}$ and $R_{1L} \cong R_{1S}$, rigidity of spherical volume of atoms v_a and stability of a number of other values. All this specifies also a duality of atomic structure of liquids and different character of packing of atoms in micro- and in macrovolumes. In microvolumes (in miniclusters) the atoms of a liquid are situated as in the crystal. In macrovolumes the liquid consists obviously of chains of miniclusters, joint by rigid connections between separate atoms of the first coordination spheres of

connected miniclusters. By increasing of temperature the volume of atoms and miniclusters remains constant but intercluster volume increases. The space disposition of chains can rapidly change as a result of mechanical or thermal effect. This ensures mutability of a structure, high fluidity of liquids and many other special properties exhibit also in the critical point "liquid/gas". In the close vicinity of critical point the miniclusters begin to break up that causes of fast growth of a thermal capacity. With $T = T_C$ all mass of substance turns to gas for which $Z_1 = 1$. Process of gas cooling close of critical point from a condition $\rho = \rho_C$, $T = T_C$, $P = P_C$ first of all reduces to formation of free clusters, then cluster aggregates, which are linked (are condensed) in small drops of a liquid. In a gravitational field these drops turn in macrovolume of liquid.

In carried out researches all circumscribed transformations are considered as thermal though it is obvious that in their basis the quantum processes in electronic subsystems of substances ensued feed or removal of energy lie.

1. Basin A.S.. Transition of a structure of a crystalline lattice in a structure of a liquid // Evolution of defective structures in condensed mediums. - Barnaul: Altai State Technical Univ., 1996. - P.29.
2. Basin A.S. A ratio of dimensions of atoms in nanostructure of solid and liquids // Evolution of defective structures *Kochanenko D.V.* in condensed mediums. - Barnaul: AltaiSTU, 1998. - P.18.

WEAR RESISTANCE SURFACE LAYERS ON METALS FORMED BY MULTICOMPONENT ELECTROEXPLOSIVE ALLOYING

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The impulse effect on metals of plasma jets generated at electrical explosion of conductors, results in melting away of thin surface layers and interaction of a melt with vapor-plasma and condensed products of explosion. The main features of electroexplosive alloying are determined by action on a surface by action on a surface by thermal impulse and gas-dynamical pressure, hydrodynamic processes in a melt, heterogeneous structure of jets. The comparative analysis of the available references shows the large potential opportunities of development in this direction. The wide choice of materials of exploding conductors causes wide opportunities of application of a method. For one pulse of treatment it is possible alloying of surface layers by the area up to 5...10 cm^2 and thickness up to 20...40 cm. The application of electrical explosion and phenomena, accompanying it in various technologies of treatment of materials, now has resulted in creation of the appropriate equipment distinguished by simplicity of a design, low cost, high reliability and ecological safety. In this paper are presents the results of metallographic investigations of treatment of titanium alloys and steels by aluminum and carbon and by aluminum and boron also. The electroexplosive alloying carried out for creating at once layers heat resistance or wear resistance. Measurement showed that properties of surface are increases on a several times.

FORMATION OF A GRADIENT STRUCTURE OF METAL AT TO DIFFERENTIAL QUENCHING OF RAIL STEEL

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Now already it is possible to ascertain, that the uniformity of metal materials used in the practical purposes, not always is desirable. The large interest is represented by materials with, so-called, gradient structure. In such material, structure and, hence, all properties are monotonous or unmonotonic function of coordinate, in which role distance from a surface up to a considered deeper layer acts more often. As the practice shows, the creation of gradient structures can be very perspective with the purpose of increase of operational resistance and durability of railway rails.

The traditional heat treatment does not allow to receive such complex of properties of rails, which to the full answered the requirements, showed to them. The most simple and effective way of artificial creation of a demanded gradient structure of a rail is the differential quenching, at which during short time, but very intensively are cooled from temperature of an austenization a surface and surface layer, with the subsequent rather slow general cooling of other volume of a material. Such quenching forms in a surface layer the gradient structure having raised hardness and durability, the most favorable heterogeneity of the head of a rail is created; a firm, strong top layer and rather soft central part.

In the given work is shown, that the differential quenching of rail steel forms in the head of a rail a surface layer (depth of 1-2 mm) raised hardness, with the expressed gradient structure. Within the limits Of this layer the characteristic unmonotonous dependences of the size of a grain and parameter of thin structure of a pearlite (thickness of plates of ferrite and cementite) from distance up to a surface of processing, because of the special thermal conditions are revealed which are created by a differential quenching in a surface layer of metal.

CLASSIFICATION OF POIINT DEFECTS AND THEIR COMPLEXES FOR TWO-DIMENSIONAL HEXAGONAL CRYSTAL LATTICE

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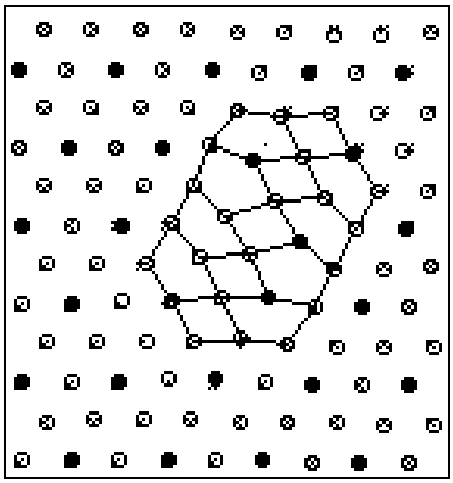
Classification of point defects such as vacancies and their complexes, point defects of substitution (PDS) and their complexes for two-dimensional crystal lattice was made in the given paper. Main energetical and structural characteristics for static and dynamic systems were calculated. All possible, configurations of point defects and their groups were shown. It was made the analysis of structural and energetic peculiarities in the area of point defects and their complexes.

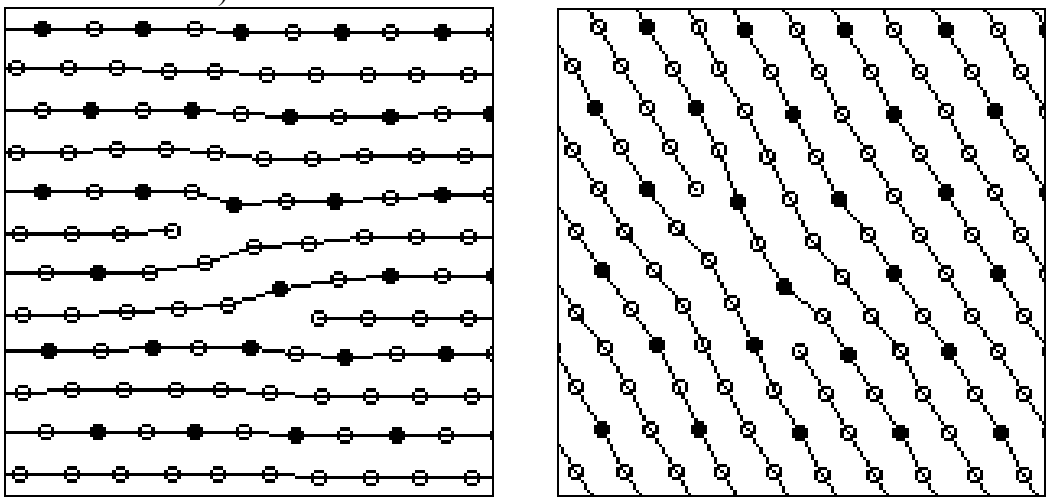
Possible combinations, structure and configurational energy of point defects and their complexes of different types, which can form in two-dimensional thin film of atomic planes (111) of $L1_2$ superstructure were studied in the model of hard spheres. It was studied energetical advantage of unification of single point defects (vacancies, PDS) into complexes: divacancies, threevacancies and their complexes, consisting of two and three PDS. The maximum value of bond energy of single vacancies at the unification of single vacancies into complexes was reached, when the distance between vacancies was equal to the radius of the first coordinational sphere. This value decreased with the increasing of the distance between vacancies. Annular substitution of the pairs of PDS at the first coordinational spheres along one of closely packed crystal-graphic directions was advantageous at the unification of single PDS into complexes. Geometrical figure, having PSD at their apexes took the shape of a disk. Local structure near the complexes of the nearest divacancies, re-

ceived by the method of molecular dynamics, was changed, taking into account the displacement of atoms in the result of relaxation. The elements of atomic packing, corresponding to the symmetry of non-crystal, the fifth and other orders appeared in the crystal structure. Such areas could be called as nanocrystal cluster or quazi-crystal cluster (pic.1). Atomic-structural reconstruction was studied as the formation of the dislocations in three-dimensional crystal (pic.2).



a)

Pic.1. Configuration, consisting of three vacancies, taking into account the relaxation: a) the areas of local distortion of lattice symmetry, where the displacement of atoms is more than 20%.



a) b)

Pic.2. Pictures of packing of atomic rows are observed:
a) dipole;
b) disk of vacancy.

MODEL OF DEFECTS EVOLUTION IN ION-IRRADIATED FCC-METALS

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Various aspects of the irradiation-induced evolution defect microstructures have been studied for a number of years both experimentally and theoretically. It has been a common practice to treat the problem of defect accumulation during irradiation within the framework of mean-field theory using chemical rate equations. However, under cascade damage conditions, none of the assumptions used in the conventional approach is valid because of a massive intracascade recombination and spontaneous clustering of vacancies and self-interstitial atoms (SIAs) already during the cooling-down phase of the cascades and subcascades. In an effort to overcome these discrepancies and to be able to incorporate the physical features of the damage production in multidisplacement cascades and subcascades have been proposed a new model called “production bias model” (PBM). The

model takes explicitly into account the consequences of intracascade recombination and spontaneous formation of clusters of vacancies and SIAs. The PBM also depends on the removal of SIAs clusters, which may occur via the one-dimensional glide of small SIA loops. It is necessary to note that the interaction of defects as a rule is shown at a nuclear level and to carry out a direct experimental research rather difficulty. An alternative way is the computer modelling by a method of Monte-Carlo with use of binary collisions approximation. The computer program is executed in frameworks PBM model with reference to an irradiation of fcc-metals by high-energy ions forming the cascade of damages, and simulates migration and interaction of defects, annealing of defects by means of their recombination and annihilation on sinks, ignoring interaction between separate atoms. It is based on a simple model defects diffusion and their interaction and physically is correct by relatively dilute concentration of defects. The similar computer simulation allows more completely to check up regularities influencing to migration and a reactions between defects, obtained by interactions of defects by molecular dynamics modelling.

MONTE-CARLOES SIMULATION THERMAL ANNEALING IN Cu

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The diffusion of defects in Cu after irradiation by high-energy ions can be investigated by Monte-Carlo methods in frameworks PBM model (production bias model). Clusters of both types (interstitials and vacancies) are thermally stable. Point defects and defect clusters centred on lattice sites, with radii related to their cluster size. Mobile defects move one lattice site at a time in randomly chosen directions. The order in with the defects are chosen to move is determined by random selection, depending on the number of mobile defects and assigned relative jump probabilities. Glissile clusters diffuses through the crystal lattice until it is trapped by any immobile defects. The mobility of the one-dimensionally diffusing glissile clusters is comparable with that of the single SIAs. Two defects interact when their separation falls within the assigned critical reaction distance for that interaction. The interaction product is placed at the target defect's lattice site. The annealing is continued until no mobile defects remain in the volume being annealed. When simulating the thermal annealing in a single cascade region, the cascade is placed at the centre of a volume that is somewhat larger than the cascade in all directions. For simplification of calculation were conducted for want of voids in simulated area. Such approach is reasonable by doze of irradiation below than 10-2 displacements per atom (dpa). The outcome received by repeated calculations at different sets of the defective configurations within the framework of given initial parameters. Under condition of low temperature ions irradiation, simulated a complete stage thermal annealing of the high-energy collisions cascade. On the basis of a computer program some features of evolution defective microstructure reshaped on a surface of metals after transit of the high-energy collisions cascade were investigated. The role of one-dimensional motion of interstitial clusters in a broad interval of different initial conditions was systematically studied. The analysis of influencing of mobility of vacancies on formation of all defective microstructure was conducted. The final distribution of defects on a cluster size was studied in case of short and full stages of a thermal annealing.

INTERRELATION OF REACTIVITY, STABILITY AND DEFECT STRUCTURE OF ENERGY MATERIALS

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This work is prolongation of cycle of works devoted to investigation of influence of defect structure heavy metal azides (tread-like crystals of leads azide and silver with average sizes

$10\times0,1\times0,03$ mm^3) on physicochemical processes, flowing past after energy effect. Experimentally set, that irrespective of a view of energy action (radiolysis, photolysis, electrofield decomposition) the sluggish decomposition heavy metal azides (HMA) flows past with formation of nitrogen (N_2), polymeric compound of nitrogen (N_6), metal, and is determined by defect structure of substance. Process of sluggish decomposition HMA is localized in reactionary regions (RR), which generated from edge dislocations in surface region of a crystal. The average sizes of RR make $10\times20\times5$ mkm^3 in AgN_3 and $20\times30\times5$ mkm^3 in PbN_6 (to detection of RR applied a method of pits). A role of dislocations in formation of products of decomposition estimated as follows. If by action on dislocation structure to deduce dislocations from a chip, at the subsequent energy action of decomposition is not observed within 20 clocks. During this time the chips are chemically inertial to the mentioned above energy actions. A requirement the shaping of a RR - presence of edge dislocations and presence in chips of impurities with concentration not less than 10^{-16} $см^{-3}$ is revealed experimentally. In a RR long-lived time after the termination of effect the processes of decomposition are prolonged, accompanied by generation of nonequilibrium electrons and holes, therefore in a RR the cluster of an intermediate product (N_6) the existence and which stability is confirmed by quantum-chemical calculations is shaped. The procedures of control of time of formation of a RR designed which allows targeted to set reactivity HTM, and also to drive time of formation of intermediate product.

THE ULTRASONIC SPECTROSCOPY OF POLYMERIC MATERIALS

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The ultrasonic researches allow to obtain a full and reliable information about physical properties of different systems, including polymeric materials. In samples the values of velocities of ultrasonic waves longitudinal and shear propagation, received by ultrasonic methods, are usually used for determination of elastic modulus. Our researches lead to conclusion about this, that on the basic of the ultrasonic measurements it is possibly to study the wide spectrum of polymer characteristics.

The unique correspondence between the elastic modulus and strength properties of the materials allowed to realize the estimation of their strength, the limit of forced elasticity and also cohesion energy.

The bond between the elastic modulus and thermophysical properties of the materials are stipulated the forces of intermolecular interaction, determined the character of oscillation processes in polymer chains. The obtained relations allowed to calculate their coefficients of thermal expansion, Debye temperatures, thermal capacities and thermal conductivities.

The modern model conceptions and special theories point the way of determination of the row of parameters of the interchain interaction, including the power indexes in potentials of attraction and repulsion and also Grunyez constants.

We showed that it could be received information about the structural peculiarities of the studied objects, using the ultrasonic measurements. On the basic of realized experiments the coefficients of polymer chains packing, values of unconfined space of some polymer chains and Rao constants, corresponded to them, are calculated. The values of average free path of the thermal phonons, founded from the acoustic measurements, show on sizes of ordered domains in the studied structures.

The comparison of parameters, obtained on the basic of ultrasonic data, with the results of direct measurements, establishes their satisfactory correlation. It gives the foundation to consider the acoustic methods are the more effective and reliable instrument for the spectroscopy of polymeric materials.

FORECASTING OF CYCLIC CRACKING RESISTANCE OF LOW-CARBON LOW-ALLOYED STEEL 0,09C2MN1S IN CONDITIONS OF THE UNIFORM STATE OF STRESS

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There are accelerated methods of an estimation of cracking resistance at static and cyclic loading. Under the real conditions the material is more often subjected to an completely cycling loadings. The methods of the accelerated definition of parameters of cracking resistance are effective enough and less time taking. Advantage of these methods is that at their use it is possible to calculate a theoretical curve of cracking resistance under characteristics of static strength, without testing.

In the given work cyclic cracking resistance of cylindrical samples with a circumferential notch was estimated on low – alloyed steel 0,09C2Mn1S (0,09%C, 2%Mn, 1%S). Samples in diameter 3mm and length of 300 mm preliminary were annealed at temperature 680°C during 30 minutes, then they were subjected to natural ageing.

Standard tensile tests were carried out on the "Instron" machine with record of the diagram in coordinates loading P – absolute elongation Δl. True stresses (S) and true deformations (ε) were determined by the method of plastic–destructive analysis and constructed stress – displacement relation in doubles logarithmic coordinates. Cyclic cracking resistance was estimated with the help of the kinetic diagram constructed as dependence of growth rate of a fatigue crack dl/dN on amplitude of stress intensity factor.

Limiting (critical) value of stress intensity factor (fracture toughness) was (determined) according to standard techniques. Stress range was estimated according to expression $\Delta K = 0.64\Delta\sigma\sqrt{\pi L}$, where $L=(D-d)/2$, D – external diameter of a sample, d – diameter of an isthmus in a plane of a circumferential notch. Quantity of loading cycles, necessary for appearance of cracks in the concentrator was estimated according to Manson-Koffin equations $\Delta\varepsilon_n N^{-0,6} = \varepsilon_k^{0.6}$, $\Delta\varepsilon_Y N^{1/m} = 3{,}5\sigma_{\text{Á}}.E$, where $\varepsilon_k=ln[1/(1-\varphi)]$ – initial plasticity of a material, E – the modulus of elasticity.

At known values of true stresses and deformations in this work calculation of quantity of cycles before formation of cracks was made depending on amplitude of plastic deformation.

Thus, in the work it is predicted cyclic cracking resistance of cylindrical sample from steel 0,09C2Mn1S with a circumferential notch in conditions of the uniform state of stress. At change of stress intensity factor ΔK=17 MPa/m^2 quantity of loading cycles before appearance of cracks was 200, strain amplitude was $\Delta\varepsilon$=1,5% and crack growth rate v=5,5·10^{-5} mm/cycle.

DUCTILE-BRITTLE TRANSITION IN ALLOYS ON THE BASIS OF FE-SI

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The rapid increase of ductile-brittle transition temperature $T_{d\text{-}b}$ in Fe-Si alloys is observed in process of growth of the silicon concentration. Transition of magnitude $T_{d\text{-}b}$ from range of the negative temperatures in range of the positive temperatures is happened when processes of atomic ordering begin to play a significant role. Value of $T_{d\text{-}b}$ in alloys on the basis of iron-silicon is structural-sensitive and depends on the grain size.

Influence of alloying elements on propensity to ductile fracture of the ordered alloys on the basis Fe-Si, was regularly observed, on the one hand, to reveal alloying elements which favorably influence to plasticity and establish their optimum concentration and, on the other hand, to understand the reasons of similar influence and finally to find out a nature of brittleness of alloys on the basis iron-silicon.

Analyzing the received data it is possible to pick out some alloying elements (Al, Ga, Nb, Cr and Ni), which reduce $T_{d\text{-}b}$ and expand an interval of plasticity of the iron-silicon alloys.

Practically all alloying elements lowering propensity to fragile destruction, to some extent influence parameters of atomic ordering of the investigated solid solutions. The only thing from the alloying elements, lowering $T_{d\text{-}b}$, but not varying parameters of atomic ordering, is Nb. It is possible to assume, that Nb influences electronic structure iron-silicon. With the purpose to be convinced of it studying electronic spectra of alloy Fe-11atom%Si alloyed 1atom% of Nb, with the help of a method of x-ray photoelectronic spectroscopy was undertaken. Appeared, that alloying Nb results to expansion a valence band and in shift of a maximum of a spectrum in area high energy of interatomic bond, and also to increase of an index of asymmetry 2p3/2 - a level of iron. It, apparently, is caused by increase of density of a charge at the Fe atoms, as accompanied by decrease of covalent component of bond.

We do not consider influence of the grain size to the plasticity, because all values $T_{d\text{-}b}$ were given in the standard grain size d_0, and the variation of the grain size for concrete structure is easy carry out, for example, at selection of a regime of preliminary thermomechanical treatment.

NANOSIZABLE STRUCTURES UNDER CONDITIONS OF ELECTROSTIMULATED DEFORMATION

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The synergetic scheme of the slaving of the plastic deformation by the large scale displacements in material is realized in [1]. The transition of the large scale displacements from the level of grain to the micro cracks level is remarkable phenomenon in the upper paradigm.

The universality and scaling leads to the formation of nanosizable structure of the carbide phase particles (Fe_3C) on the boundaries of material fragments [2]. Dislocations, forming boundary grains (dislocation walls – small angle boundaries) are characterized by scaling [2]. “Mobile” dislocations (“dilatation and shear on the one atom”) are formed by “electron wind”, and “fixed” dislocations are formed by drawing, and fatigue et cetera [1].

The scaling under (far) nonequilibrium conditions is discussed in [2]. Many experimental data on the electroplastic deformation are correlated with effective electron wind stresses $\sigma = (m\upsilon_F/e)\cdot j$ [1] with the good accuracy, where m – the electron mass, υ_F – the electron velocity on the Fermi surface, e – the electron charge, j – the electric current density.

So, the factor growth of own stresses of mobile dislocations (defermined by the electron wind) is the saurce of nanosizable structures in the material.

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ELECTRO-SLAG TECHNIQUE OF CAST DIE TOOL PRODUCTION

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The method of steel smelting is the essential for steel properties to be obtained as well as alloying and modifying processes. One of the main problems to be solved by metallurgists is the improving of steel quality that as a rule directly correlates with the purity of steel.

There are some metallurgical methods to obtain high quality steel: deoxidizing, alloying, refining and degassing and some methods of refine remelting – electron-beam remelting, electro-slag remelting, and so on. The electro-slag technique (electro-slag remelting ESR, electro-slag casting ESC) to manufacture a cast die tool is the most promising because of electro-slag refining process. This process is the most commonly used in industry and have advantages over others processes. In the course of ESR the electric current generates the heft in the synthetic slag bath. The heat maintains the slag bath in liquid state and melts the metal electrode to be remelted. Metal during remelting process is purified from impurities, gases, non-metallic inclusions because of interaction between drops of metal and active slag melt and progressive solidification of melt from the bottom to the top. That provides the forming of dense structure ingot. The ESR process is used for production of steel ingots of hard working tool, stainless, acid-proof, heat-resistant steels, low alloying steels for forgings and high-temperature strength steels. There is a tendency to increase both - ingot mass and a ESR unit capacity.

For the electro-slag crucible melting (ESCM) requirements to the shape and the surface of consumed electrode are minimal. Possible to melt electrode changeable in cross section and shape, assembled from different peaces of metal by welding. The electro-slag casting is suitable to get castings from any materials (steels, alloys, cast iron with globular graphite and so on). So, consumed electrode is composed from proper chemical composition blanks.

Electro-slag production process is clean enough. That allows locating bays of electro-slag centrifugal casting (ESCC) or electro-slag casting in metal moulds (ESCMM) directly in heat-treatment, welding or repairing workshops. The sufficient loading is the necessary condition to start the ESC bay in any enterprise. Different special-purpose equipment to produce wide range of blanks with the mass from kilogram to ton and more by ESCC and ESCMM methods was worked out in the welding institute named by E.O. Paton (Ucrane).

The foundation of ESC process is the melting of consumed electrode. Liquid metal moves from the edge of melted electrode to the mould through the liquid slag without contact with surrounding air. Solidification of casting occurs within the thing skin of a slag lining (skull). That results in negligible interaction with mould material and smooth surface of a casting that may be usually used without subsequent machining.

Refining process of metal to be remelt generally occurs during the contact with the slag of high activity. This contact takes place in thin layer of melted metal on the edge electrode to be melted, in drops of metal when move through the slag bath and in the boundary between slag and metal bathes.

The advantage of EDC over others casting processes is the possibility of selective refining from different impurities by adjusting a chemical composition of using slag.

INFLUENCE OF HIERARCHY OF STRUCTURAL DEFECTS AND INTENSE DEFORMED CONDITION ON PHOTOCHEMICAL DECOMPOSITION WHISKERS CRYSTALS B-AZID LEAD

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A perfection of a crystal structure of whiskers crystals b-azid lead and the developed methods of revealing dislocation have allowed to divide the influence of a concentration of linear defects (dislocations), dot defects and an intense-deformed condition into their photochemical decomposition by the light from an area of its own absorption.

In the report is shown, that the concentration growing dislocations is influenced on the photochemical decomposition. At a deformation by the bend in the field of elasticity occurs the movement of the dislocation, accompanying by the increase of an optical density WC b-PbN_6. The formation of nitrogen with the photochemical decomposition first of all begins on dislocations, caused by the background of a sample. From a comparison of curves of a dependence specific gas isolation from density dislocations is visible, that growing dislocations create in WC conditions for the more effective course of the process of photochemical decomposition, rather than again entered.

Within the limits of the used mechanism of elementary stages of photochemical decomposition b-PbN6 the increase of concentration of dot defects at the deformation results at initial stages to the primary formation of V_k-centers (holes seized on cation vacancies) and to the increase of the induction period of a beginning the gas isolation. At significant times of the photochemical decomposition, when the most part of cation vacancies will be filled by holes, there is a secondary capture of holes and an allocation of nitrogen.

The role of the intense-deformed condition, arising at photochemical decomposition or deformation, is reduced both to a separation of dot defects in fields of elastic strains and the formation of charging heterogeneities, and to the decomposition in the electrical field of charging heterogeneities or the field of a piezoelectric effect, found out in b-PbN_6. A dependence of influence of temperature on electrofield and the photochemical decomposition confirms the existence of area of phase transition b-PbN_6 at temperature 360-380 K to the centrosymmetrical condition. The maximum in the dependence of the specific gas isolation on the temperature falls on an area of segnetion phase.

STRUCTURE OF DIFFUSION FRONT ON SQUARE LATTICE

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The structure of diffusion front and dependence of parameters of this structure on time for a two-dimensional square lattice is investigated. The diffusion was simulated as a random walk on four nearest neighbours. Each particle at regular intervals jumps on one from four nearest node of a lattice, if this node is free. If it is occupied, the particle remains on a place. To exclude any correlations in transition of particles, the exhaustive search of particles on each step was made in a random sequence.

The diffusion front (shell) was constructed for each picture of diffusion. The concept of diffusion front (shell) can be introduced only in computer simulation and is closely connected to the percolation theory. The shell is self-similar fractal. Following parameters of shell structure was studied: fractal dimensionality, number of nodes, average coordinate along a direction of a diffusion.

The new concepts are introduced: a sceleton and boundary of the shell. For them the same parameters as for a shell were investigated. Many additional parameters of a shell also were investigated: number of nodes in closed loops of a sceleton, number of loops of a sceleton, number of dead

branches, number of ramifications of dead branches, averages of nodes in a loop of a sceleton and in one dead branch and so on.

All these magnitudes are power functions of time (number of steps). All indexes of power of these functions were calculated.

TRANSFORMATIONS IN DEFECT STRUCTURE AND PLASTIC DEFORMATION STAGES

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The paper is devoted to an analysis of dislocation ensemble organization on different work-hardening stages. The classification of dislocation substructures and dislocation-disclination ones observed at active deformation of metals and alloys is given on the base of experimental data received by the author with the colleagues. Transformations in dislocations subsystem which lead to substructure formation are considered. Order parameters determining these transformations are introduced. Signs of autonomous behavior of dislocation subsystem and development of transformations in dislocation ensemble which similar with kinetic order-disorder transformations are analyzed. Basic peculiarities of phase transformations of dislocation subsystem are determined. Two main sequences of transformations of dislocation structure (low-energy dislocation structure - LEDS and high energy dislocation structure- HEDS) observed at increase of dislocation density or deformation degree are introduced. Experimental data testified about self-organization processes in dislocation substructure are given : 1)parameters characterizing development of different substructure are connected by direct or inversely proportional dependencies; 2)there are bifurcation points on dependencies of local scalar dislocation density in a concrete dislocation substructure from average scalar dislocation density. A nature of change of the stages of work-hardening connected with substructure transformations is discussed. Data about a rate of accumulation of different defects on the different deformation stages which responsible for internal stress field and behavior of work-hardening coefficient are given : it is a scalar dislocation ensemble on stages II, dislocation charges on stage III and partial disclinations on stages IV.

NEW VIEW ON THE HALL- PETCH PROBLEM. STRENGTH OF ULTRA-DISPERSED MATERIALS

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The classical the Hall-Petch relation: $\sigma = \sigma_0 + kd^{-1/2}$ (σ_0 is a strength to sliding in a grain body, k is coefficient, determining a contribution of a grain size d) is known very long time.. It is possible to output this relation on a base of different models: (1) connecting a grain size with a stress in individual slip bands; (2) based on a dependence of a dislocation density from a grain size: (3) on a base of analysis of a role of a grain dislocation sources; (4) on a base of dividing all dislocations on statistically stored ones and geometrically necessary ones. With a development of a physics of ultra-dispersed materials it was determined that coefficient k is not a material constant. It is changed when an average size of grains is changed. Besides the coefficient k depends from a type of grain boundaries, a possibility of sliding on grain boundaries, a presence of disclinations in joints of grain boundaries, a material texture and other factors.

In the paper it is analyzed a behavior of the Hall parameter k at changing a grain size on several orders. A change of a deformation mechanism at a change of a grain size is considered and a role of local stresses on grain boundaries is analyzed.

PLASTICITY AND REACTIVITY OF WHISKERS SILVER AZIDE

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Silver azide is an initiating (primary) explosive. Physicochemical properties of silver azide are well studied and it is often used as a model material in solid state chemistry. However, a number of formerly unknown features of silver azide behavior was observed.

Thus, the sizes of diamagnetic silver azide crystals under a strain and in the magnetic and electric fields have been found to change. The relative lengthening of the samples is 10-3. It was established that the value and the sign of this effect was changed (i.e. the anisotropy was observed) depending on the orientation of a crystal in the magnetic and electric fields. The change of the dimensions results from the effect of the prolonged energetic force.

Moreover, we have studied first the slow decomposition of silver azide crystals under the mentioned influences. The availability of the momentary postprocesses after the energetic treatment has been found. The interdependence between the decomposition reaction and the effect of size change has been stated. The time required for the highest possible change of crystal sizes has been turned out to coincide with time when the maximal volume of the “trapped” gas evolution was observed.

It is assumed that the cationic sublattice affects on the change of the dimensions of silver azide crystals.

THE INTERACTION OF THE TiFe SURFACE STATES WITH SIMPLE ADSORBATES

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In the past two-decade the properties of metal surfaces have been the subject of an inreasing number of experimental and theoretical studies. The electronic properties of transition metal (TM) alloys are less investigated. It is known that adsorption of hydrogen or oxygen may modify the properties of TM interface growth. Surface oxygen can considerably improve surface order and enhance the magnetic properties. Hydrogen plays also a crucial role in the properties of various materials. However, the modification of surface electron properties by hydrogen or oxygen adsorption is not well understood. TiFe is known as hydrogen storage compound, one of the key material for the development of future clean hydrogen energy system but it is very difficult to activate. It is believed that the activation of a thin film of TiFe hydride is much easy. The main goal of the present work is to study the bonding mechanism between simple adsorbate and TiFe (001) and (110) surfaces states. A full potential linearized augmented plane wave method was applied for the calculations of the electronic structure for (001) and (110) *B*2-TiFe surfaces with hydrogen or oxygen in the different adsorbate sites. The surface was simulated by repeated slabs separated in z-direction

by a vacuum region. To determine the stable adsorption geometry we have allowed a minimization of the total energy with respect to the height of the adsorbed atom measured from the center of the top layer of the pure TiFe surface. Four different adsorption geometry (H adsorbed on-top of Fe or Ti atoms and H adsorbed on a bridge position between Fe or Ti atoms) were considered for (110) surface. In the case of (001) surface H (O) has been considered in the fourfold hollow position. The atomic positions were relaxed by minimizing the forces acting on the atoms. Our results suggest a possibility of the reconstruction of both (001) and (110) surfaces. The adsorption on the Ti-terminated (001) surface is found to be preferable. Comparing the total energies of the four H arrangements on the TiFe (110) surface we find that Fe-bridge adsorption is most favorable. The present results indicate also that hydrogen atom exhibits a larger affinity with Fe atoms rather than Ti atoms. The chemical bond between surface states of substrate and adsorbate is analyzed. As a result, it is shown that the hydrogen and oxygen adsorption characteristics are well understood in terms of the chemical bonds between atoms. The microscopic explanation of the local surface reactivity is suggested. The influence of hydrogen (oxygen) adsorption on magnetic properties of Fe-surface and subsurface atoms is also discussed. It is shown that the formation of surface oxide layer hinders the hydrogen adsorption.

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THE BAND STRUCTURE CALCULATIONS OF METAL-SEMICONDUCTOR INTERFACE

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The modern generation of highly polarized electron sources is based on photoemission from semiconductor nanostructures. Strained GaAs-based short-period superlattice structures are found to be the best for this purpose. To achieve considerable improvement of the both emitted charge and electron polarization an optimization the cathode heterostructure parameters is necessary. In the present paper a full-potential linearized augmented plane wave (FLAPW) method is used to investigate $(MeAs)_1(GaAs)_1$ (001) multilayer structures with Me=Al, In, Cs, Mn as well as clean and cesiated GaAs (001) and (110) surfaces. Such *ab-initio* calculation can elucidate the microscopic origin of change in the electronic properties in the interface area, in particular, the magnetic anisotropy of heterostructures consisting of ferromagnetic metal and semiconductor and to explain their so-called half-metallic behavior. In addition, we have studied the adsorption of alkali metals on the GaAs (001) and (110) surfaces that leads to a drastic decrease of the work function. This phenomenon is known to be quite different from that for the alkali metals adsorbed on the metal surfaces. For comparison the work function dependence on the coverage for cesiated Au (001) and Cu(001) surfaces is also evaluated and found to be in good agreement with experimental results. The atomic layer model for the Cs as well as for the metal and semiconductor substrates was used instead of the popular jellium model. The interaction of the surface states of GaAs and metal substrate with adsorbate and charge transfer is discussed. The layer resolved density of states, electron energy spectrum and single particle charge densities of some surface states are analyzed. The origin of the surface states within the fundamental band gap and the reconstructed surface properties with Ga-dimer in the surface layer of GaAs (001) (2x1) structure are discussed. The computer simulation allow one to

obtain the correct physical-chemical trends for realistic Me/Sc interfaces, to predict the properties of GaAs-based heterostructures and suggest their composition.

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CU-TIB$_2$ NANOCOMPOSITE AS MOTOR OIL ADDITIVE.

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There are some recent tendencies in development of additives to motor oils. One of these is the preparation of metalcladding additives able to growth copper metal layer at the wearing surface up to one micron of high. The perspective type of additive is characterized by great remedial activity of motor part surface. It is known, that attachment of remedial additive into lubrications results in formation between friction surfaces thick (up to 100 and more micron) layers, which are closing down wearing defects. A material of films is metal ceramic composite containing copper and hard inorganic substance, generally, alumina and silica.

The literature overview demonstrates, that one of the perspective challengers for the role of ceramic grains is the titanium diboride with his unique physical properties At target aggregate formation it is important to receive not simple fragments of ceramics in metal matrix of composite, but as more as possible shallow fragments, in a limit of nanometer sizes.

Aim of the present paper is the investigation of some friction pairs with introduced organometalceramic composition based on copper - titanium boride composition from the point of view of system friction coefficient.

Copper – titanium diboride composite material containing titanium diboride 1.3 – 3.5 nm particles in 50 – 100 nm copper grains was prepared via mechanochemical reaction of titanium and boron in copper matrix. Dispersion of composite particles in oil was made by mechanical treatment in high intensive planetary ball mill.

Friction pairs “steel-steel”, ”steel-bronze”, “steel-aluminum alloy” were studied in oil with additive. The measuring of moment of friction with the subsequent recalculation was conducted on the friction installation MI-1. Friction moment dependences upon temperature and load were observed. The main result of investigation one may formulate as next: for “steel-steel” pair the friction coefficient decreasing up to ten fold is observed.

The results are discussed in terms of correlation of shift module values of bulk and remedial materials. The relation of modules of steel and copper matrix composite is optimal among investigated materials.

MULTISCALE STRUCTURE of NANOCROCRYSTALLINE METALS

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The nanocrystalline (NC) metals with an average grain size of about 100 nm prepared by severe plastic torsion straining were objects of investigations in the given work.

Samples of Cu, Co, Fe, Ni, Pd, W and 18Cr-10Ni stainless steel were deformed by two deformation modes: torsion under quasihydraustatic pressure or equal channel angular pressing.

The micro-, atomic, hyperfine magnetic and electronic structure of metals was investigated by TEM, calorimetry, x-ray, EXAFS, Mössbauer spectroscopy as well as field ion microscopy, field

electron microscopy and field electron spectroscopy. According to the results of these investigations grain boundaries in NC metals have excess enthalpy. The first neighbor number and a value of local electron work function are decreased. NC metal contains atoms in two states. Atoms in the first state have parameters of hyperfine magnetic structure typical for usual coarse-grained iron while atoms in the second state have different parameters and low Debya temperature. It is important to note that their parameters are fixed. A thickness of a layer of these atoms near grain boundaries is about 10 nm. The local electron work function for grain boundary region in NC metal have decreased magnitudes.

A two-phase (grain phase and metastable grain boundary phase) model of NC material structure with is suggested for explanation of revealed features of structure and physical properties of NC metals.

THE MICRODEFECT ENSEMBLE EVOLUTION EFFECT ON CRACK BRANCHING.

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The microbranching of fast cracks leading to their dynamic instability is one of complex problem of fracture mechanics. The recent Russian and foreign experimental investigations of cracks have shown the main role of structure kinetics of material under failure and allowed us to consider the problem in the framework of the statistical theory of mesodefects. Using the results of this theory we obtained the non-linear constitutive equations for the tensor parameter of microcrack density and carried out the numerical simulation of the dynamic instability under crack propagation. The self-similar solutions of the kinetic equation showed the existence of a specific type of the developed stage of damage, which is characterised by the explosion-like kinetics of the microcrack growth on the spectrum of spatial scales. From the results of the self-similar solution analysis it appeared that the steady-state - branching transition occurs when the microcrack ensemble has no enough time for generation of the self-similar pattern and its evolution (it corresponds to nucleation and evolution of a daughter crack). In this case the statistical distribution of the material properties starts playing a considerable role in this process and the crack takes the other more effective way of dissipation of external energy.

The theoretical and numerical results were supported by the direct experimental study of crack dynamics in PMMA specimen using the high speed camera and experimental investigation of the crack surface. It was shown that in the branching regime the crack radiates an acoustic wave and its surface demonstrates the self-similar properties. We have processed the acoustic signal from the fast crack in terms of the correlation integral and established the existence of correlation indexes ($\nu \approx 0.4$) for this regime of crack propagation, which corresponds to the stochastic crack tip dynamics.

The main results of this work are:

- crack propagation and generation of daughter branches results from the blow-up kinetic of the microcrack ensemble localized on the spectrum of spatial scales;
- theoretical explanation of the reasons for crack branching and limits of the steady-state crack velocity;
- determination of the scaling properties of acoustic crack emission in terms of the correlation integral;
- computing of crack branching and acoustic emission from the crack tip.

STRUCTURE-ENERGETICAL TRANSFOR MATIONS IN THE STRONG DEFORMED ALLOYS 40XHЮ AND 36HXTЮ.

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Authors of the submitted work carry out research of influence of a high degree of cold rolling deformation on structural - phase transformations at the subsequent ageing industrial dispersionno-hardening alloys on basis Ni-Cr.

Research of thin structure was carried out on transmission electronic microscope JEM - 100CX (foil). For studying the common character of structure used an optical microscope " Neophot 21 " and diffractometer DRON –3 for studying phase structure of samples. Mechanical tests included one axis static tension with a measurement of breaking point σ_b, relative fluid limit σ_{02}, relative lengthening till gap δ (%). The fractography a cross break studied on electron-zoned microanalyzer SUPERPROBE 733 JEOL in a raster mode secondary electrons.

Result of the analysis of experimental data are the following conclusions:

1. The concrete modes of mehaniko-thermal processing including a high degree of deformation and the subsequent ageing are recommended, allowing to receive fine-grained structures with high properties of plasticity in alloys 36HXTЮ and 40XHЮ.
2. Formation of different types of structures is revealed at ageing strong deformed alloys: structures a microduplex in 40XHЮ and special microstructures from elementary cells of cellular precipitation (ECCP) in 36HXTЮ. The size and a volume fraction in an alloy of cells ECCP is determined by time of aging at the constant temperature of ageing.
3. It is established, that high degrees of in an alloy 36HXTЮ generally do not change morphology of structural - phase transformations, but instead of γ'- phases is cellular precipitation of η-phase. The new circuit of structural - phase transformations in an aging alloy 36HXTЮ is offered at 1023-1123K after flattering with $\varepsilon \geq 95\%$.

FORMATION OF FINE-GRAINED STRUCTURE IN ALLOYS 40XHЮ AND 36HXTЮ FOR INCREASE OF PLASTICITY.

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Using features of preliminary cold deformation at ageing alloys, it is possible to offer phase and structural transformations easily sold ways of reception of a ultra fine-grained microstructure in alloys 36HXTЮ, 40XHЮ, that will allow to realize in the given alloys transition in a superplastic condition.

Mehaniko-thermal processing of alloys 36HXTЮ and 40XHЮ (industrial dispersionno-hardening heat resisting alloys of standard structure) included training on a single-phase solid solution, flattering and ageing in vacuum is no worse 1 Pa. Research of thin structure was carried out on transmission electronic microscope JEM - 100CX (foil). For studying the common character of structure used an optical microscope "Neophot 21" and diffractometer DRON –3 for studying phase structure of samples. High-temperature tests of samples of an alloy 40XHЮ on a stretching carried out on installation 1246P-2/2500 in an interval of temperatures 1153-1323 K in vacuum no worse 10^{-2} Pa.

As a result of research conclusions are made:

1. Metallography and elektronno-microscopic researches it is established, that in an alloy 36HXTЮ to a condition of superplasticity there corresponds a special microstructure from elementary cells of cellular precipitation. The size and volume fraction in an alloy of these cells is de-

termined by time of aging at the constant temperature. A superplastic condition in an alloy 40ХНЮ the structure provides a microduplex.

2. One axis the stretching of samples of an alloy 40ХНЮ at high temperature has shown that preliminary processing, namely: training 1323 K (5 mines) + flattering with ε= 90% provides occurrence of a superplastic condition of an aging alloy in an interval of deformation's speeds 10^{-4} - 10^{-2} c^{-1} and in an interval of temperatures 1153 - 1323 K.

3. The concrete modes of mehaniko-thermal processing including a high degree of deformation and the subsequent ageing are recommended, allowing to receive fine-grained structures with high properties.

HARD ALLOY SURFACE LAYER MODIFICATION AFTER VARIOUS ION CURRENT DENSITY HIGH POWER ION BEAM TREATMENT

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Modifications of surface layer of hard alloy tool made from BK-8 (WC-92%, Co-8%) and T5K10 (WC-75%, TiC-5%, Co-10%) have been investigated to determine factors influencing the hardening covers adhesion increase.

To analyze the surface properties electron Auger spectroscopy and X-ray analyze method were used. Change of surface relief and microhardness was determined for different current density in these investigations. Observations show that surface roughness and microhardness have maximum value when current density reaches 70-100A/cm^2. Chemical and phase compositions changes have threshold level when current density reaches 200-250A/cm^2.

High power ion beam (HPIB) treatment leads to changing of physical-chemical properties of semiconductors and metals. Also, it has been observed by X-ray analyzes and metallographic investigation that surface layer significantly changed. Using of definition conditions of HPIB treatment results in significant enhancing of details working properties. It had been established that lifetime increases average in 2,5-3,5 times for cutting tools were treated by HPIB.

Expansion on source of HPIB lifetime and development of technology for hardening non-resharpened cutting tools results in practical application of this technology for hardening these tools for repairing of railroad engine wheels.

Using of HPIB is a perspective way of cleaning and surface activation before hardening covers coating such as TiN. Some of HPIB treatment conditions lead to significant increasing of cover adhesion strength and cover's durability and, as a result, to enhance operational functionality of hard alloy cutting tools. Earlier investigations shown that easy-melting impurities were vaporized from surface and free oxygen from grain boundaries was removed when surface layer was treated by HPIB. Thus, surface cleaning is occurred. Grain boundaries become less-defined and WC and Co inter-solution occurs. Consequence of that is healing of grain boundary defects with strongly constrained Co-W-C atoms.

Morphology change investigations of hard alloy surface layer in dependence on HPIB parameters are presented in report. Aim of the work is to determine of aggregate factors that leads to covers adhesion increasing.

THE PROBLEM OF K-STATES AND CONCENTRATION PHASE DISCONTINUITY

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The macroscopically nonuniform distribution of alloying elements in the continuous and monophase structure of steels and alloys in the low-temperature annealing range (K-state) was discovered experimentally more than half century ago. No more or less adequate explanation of this effect was given to it since the formation of stable segregations in a continuous phase could not be substantiated in terms of the then existing state of the art in the field of phase conversion thermodynamics. Hence, the K-states had to be recognized as extremely finely-dispersive precipitations of the second phase, the precipitations which result from the phase stratification corresponding to that phase diagram domain that stretches between the coherent and heterophase stratification curves [1]. The status quo has remained unchanged since then.

Meanwhile, based on the existing experimental data, the K-states can be concluded to arise exactly in a continuous phase which is stratification-free. This served an incentive in looking for new K-state problem solutions [2,3].

In the present paper we offer a correct thermodynamic substantiation of the existence of stable segregations in continuous phases of steels and alloys. The analysis of free energe of solid solutions indicates the presence of a domain of monophase states with thermodynamically stable nonuniform distribution of dopant concentrations (the domain of a K-state) directly above the destruction curve for a non-stoichiometric solid solution with a tendency to ordering (or formation of chemical compounds in the case with stoichiometric composition).

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COMPUTER MODEL OF DEVELOPING THE MACROSTRUCTURE OF GAS-THERMAL COATINGS

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The macrostructure of a gas-thermal coating is formed under continuous effect of some random factors (turbulence of the high-temperature gas flow, distribution of particles, different degree of heating, etc.). Earlier the author has developed the statistical approach to the description of the macrostructure of gas-thermal coatings. The Local density of a coating has been chosen as the characteristic of the macrostructure. The following assumptions have been made while constructing the statistical model:

local density of a coating is a random function of a distance to a substrate;

change of the local density by layers is a random Markovian process.

The aim of the paper considered is to reveal the main statistical regularities of developing the macrostructure of gas-thermal coatings on the basis of the elementary model of random packings on the plane.

The monodisperse flow of two-dimensional round particles falling on a smooth substrate is considered. It is assumed that during the contact between a particle and a substrate or another particle the solidification without deformation takes place. Thus a random packing of round particles is formed in the plane. To determine the local density in some region of a random packing we have calculated the total area of particles and their fragments entering into the packing. The program

formed in the MathCAD7 PRO has been used for the calculations. Characteristic realization of a random packing of particles on the plane is presented in the Figure where coordinates are in microns.

The following statistical regularities of the formation of random packings have been revealed: formation of regular tree-like structures is revealed which points to the existence of the stable correlation of local density between the layers of a random packing of particles; the same regularity is observed in gas-thermal coatings;

- average density of random packings near the substrate changes regularly: two maximum are observed at the distance of a characteristic size of particles; this regularity shows the influence of the state of substrate roughness on the distribution of average density of a gas-thermal coating; at removing from a substrate the average density is relaxing to the total density of a packing;
- variance of the local density varies nonmonotonously but it grows with the increase of the distance to a substrate; the same dependence is also observed in gas-thermal coatings.

EFFECT OF LASER TREATMENT ON WEAR RESISTANCE OF PLASMA COATINGS

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Plasma spraying of coatings is one of the promising methods of improving the wear resistance of machinery parts and mechanisms. In this case, to provide the necessary strength of adhesion to a base, plasma coatings are often subjected to fusion by different methods: in heat-treatment and induction furnaces, in a high-temperature gas current, by an electric arc, etc.

In the paper presented the effect of CO_2-laser fusion on wear resistance of plasma coatings has been studied.

A self-fluxing powder of the Ni-Cr-Si-B system with the dispersion 80-150 mcm has been used as a material for plasma spraying. Specimens for spraying have been steel cylinders with a 50-mm diameter.

Plasma coatings have been sprayed on under the following technological conditions: arc current – 210 A; arc voltag – 140 V; spraying distance – 120 mm; plasma producing gas – nitrogen.

Fusion of plasma coatings has been performed by a continuous CO_2 laser with the length of an emission wave 10,6 mcm under the following technological conditions: emissive power has been varied from 1 to 2 kw, rate of beam travel – from 30 to 80 mm/sec.

Coefficient of mixing, depending on the depth of layer melting-down and plasma coating thickness, has been taken as a characteristics of laser fusion.

Specimens with the fused coatings have been tested for wear resistance according to the "disk-disk" scheme under the conditions of boundary lubrication; degree of wear has been determined by the weight method.

The results of the tests show that there is a specific interval of the values of the coefficient of mixing within which wear of fused plasma coatings is minimum.

The data of the micro-X-ray spectrum and X-ray structure analyses of a treated surface show that the improvements of wear resistance is prompted by the formation of strengthening phases that takes place at the laser fusion conditions considered above.

FIELD EMISSION FROM NANOCRYSTALLINE METALS

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The enhanced interest to nanocrystalline (NC) materials is attributed to their unusual physical properties significantly different from those of usual coarse-grained counterparts. A large volume fraction of grain boundaries within NC metals and their special, non-equilibrium states play a significant role in formation of its specific properties. The specific behavior of physical properties from NC materials allows to wait the features of the electronic structure from these materials.

Specific features of an electron structure of the NC tungsten and NC nickel were studied by a method of field electron emission spectroscopy. The NC structure with average grain size about 100 nm was processed in samples by severe plastic deformation. The microstructure was studied by ion and transmission electron microscopy.

Depending on a probing area on the emitter surface (grain boundary, near grain boundary, far from grain boundary) the energy distribution of field-emitted electrons for NC samples either have additional maximum in the low energy region of distribution or have a break in high-energy edge or have one-peak form. On the basis of the our theoretical analysis it can be concluded that due to formation of NC structures (by means of severe plastic shear straining under quasi-hydrostatic pressure) paths of currents with low work function at grain boundaries occur in metal.

LIQUID-SOLID PHASE TRANSITION OF FESI ALLOY IN DROP TUBE.

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Amorphous liquid-solid phase transition of FeSi alloy was studied in the paper. By means of optical and a scanning electron microscope (SEM), morphology transition of primary phase and eutectic is found through observing the samples of different diameter. When the diameter of the sample is larger than 1.0mm, faces dominate in the sample, indicating the faceted growth mode.

Further with increasing the diameter of the sample, most morphology is spherical shape, and faceted shape is reduced. As the diameter of the sample is as small as 0.2mm, morphology of the primary phase is branch shape, indicating the morphology transition from faceted structure to dendrites. With the decreasing of the samples ╟ ╞ diameter, morphology transition of eutectic from faceted and club-shaped to separate eutectic.

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MICROSTRUCTURE OF $AL_{88}NI_7Y_5$ ALLOY SOLIDIFIED UNDER HIGH PRESSURE

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The microstructure of $Al_{88}Ni_7Y_5$ solidified under 6.0GPa has been analyzed by X-ray diffraction, metallograghy and SEM. The results show that the melted temperature of alloy can increased more than 400□ and the grains and the secondary phase are remarkably fined after high pressure treatment.

KEY WORD $Al_{88}Ni_7Y_5$ alloy; high pressure; solidification microstructure; melt temperature

SUPERCONDUCTING MgB_2 THIN FILMS BY HOT FILAMENT CHEMICAL VAPOR DEPOSITION

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A new method for preparing superconducting MgB_2 thin films has been introducted. MgB_2 films have been prepared on (110) Al_2O_3 single crystal substrates by *in-situ* and *ex-situ* hot-filament chemical vapor depositions. For the *ex-situ* process, amorphous boron film grown by hot-filament chemical vapor deposition was encapsulated in a evacuated quartz tube with excess Mg and annealed at 820□ for 1.5h. For the *in-situ* process, B_2H_6 gas was decomposed at the hot-filament and reacted with Mg vapor, and then formed MgB_2 films on the substrates. The structural properties of the films were examined by X-ray diffractometry, indicating that both the *in-situ* and the *ex-situ* processed films are [101] oriented. The superconducting critical transition temperatures of the thin films were determined by magnetization measurements, indicating that the *ex-situ* processed film shows a zero-resistance transition temperature (T_{c0}) of ~37K, while the *in-situ* processed film shows T_{c0} of ~35K.

IMPURITY DIFFUSION OF MO IN $ZR_{57}NB_5CU_{15.4}NI_{12.6}AL_{10}$ BULK METALLIC GLASS

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Impurity diffusion of Mo in $Zr_{57}Nb_5Cu_{15.4}Ni_{12.6}Al_{10}$ Bulk Metallic Glass is studied by ion implantation combined with secondary ion mass spectroscopy (SIMS). Activation enthalpy Q and pre-exponential factor D_0 of diffusion are obtained to be 1.95 eV and $D_0=1.13\times10^{-5}$ m^2s^{-1}., respectively. The viscosity of $Zr_{57}Nb_5Cu_{15.4}Ni_{12.6}Al_{10}$ Bulk Metallic Glass is investigated below the glass transition temperature. The result shows that the viscosity coefficients decreases with the increasing of temperature from 1.07×10^9 poise at 593 K to 1.42×10^7 poise at 673 K.

PRESSURE DEPENDENCE OF CRYSTALLIZATION, PHASE TRANSFORMATION AND MICROSTRUCTURE OF $ZR_{41}TI_{14}CU_{12.5}NI_{10}BE_{22.5}$ BULK METALLIC GLASS

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High pressure can induce atomic rearrangement in metallic glasses and alter most of their physical properties. It is also powerful tool for modifying and controlling the nucleation and growth in metallic glasses. For examples, pressure is an effective in influencing the relaxation and crystallization process of amorphous solids induced by thermal annealing; by controlling the crystallization, bulk metallic glasses could crystallized to very fine-grained nano-structural material under high pressure..

Ingots with nominal composition of $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$ were prepared by melting a mixture of elements in a Ti-gettered arc furnace, and remelted in a vacuum-sealed quartz tube, then quenched in water to obtain rods with diameters of 12 mm. High pressure was performed in a six-anvil apparatus. NaCl powder was as the solid pressure transmitting medium. A NiCr-NiAl thermocouple was mounted near sample to measure temperature within ±2K. HRTEM observation was

performed in a JEOL-2010 operating at 200kV.The DSC measurements were carried out under a purified argon atmosphere in a Perkin-Elmer DSC7 device at a heating rate of 10 K min^{-1}.

The glass transition, crystallization and supercooled liquid region ($\Delta T=T_x-T_g$) are different for the three alloys after a various treatment. The obtained parameters of *Tg, Tx, Tpi* andΔT arelist in Table 1. From the results, it can be seen that the first crystallization peak is more sensitive to the annealing and high pressure: it shrinks after preannealing and disappears when annealed under high pressure.

Table 1. Thermofynamic and kinetic parameters of the as-prepared $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$ BMG (alloy A) and BMG annealed at 623 K for 2 h (alloy B) and at 572 k, 3 GPa for 1 h (alloy C). Tg, Tx and Tp2 are measured at a heating rate of 20 K/min.

sample	T_g (K)	T_x (K)	T_{p1} (K)	T_{p2} (K)	ΔT (K)	E_g (KJ/mol)	K_{og} (s-1)	E_{p1} (KJ/mol)	E_{p2} (KJ/mol)	K_{0p2} (KJ/mol)
Alloy A	629	710	723	741	81	559.1	$1.41x10^{45}$	192.6	272.5	$2.56x10^{17}$
Alloy B	631	681	707	730	50	453.3	$1.47x10^{36}$	256.7	317.1	$4.07x10^{20}$
Alloy C	687	731		750	44	200.4	$3.52x10^{13}$		378.3	$6.0x10^{24}$

From the DSC traces of the BMG annealed at high pressure at different heating rate, the significant structure relation induced by preannealing and high pressure annealing has been observed. The experimental results indicate that the BMG contains a large amount of vacancy-like free volume. The relaxation results in microstructureal transition from short-range order to medium-range order and significant effects on the subsequent glass transition and crystallization.

The pressure dependence of crystallization of the BMG reveals that high pressure markedly decreases the crystallization temperature. It is deduced that high pressure annealing can promote crystal nucleation by decreasing the work of formation of the critical nucleus, but it also restrains crystal growth by decreasing the diffusion velocity of atoms.

EPITAXIAL $TL_2BA_2CACU_2O_8$ SUPERCONDUCTING FILM GROWTH BY *EX SITU* RF MAGNETRON SPUTTERING

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Epitaxial superconducting $Tl_2Ba_2CaCu_2O_8$ thin films were successfully deposited on single crystal (001) $LaAlO_3$ and (001) $SrTiO_3$ substrates. Precursor films made by rf magnetron sputtering were thalliated at high gas pressure.

The obstained Tl-based superconducting films are characterized by X-ray diffraction(XRD) θ-2θ scans, ω scans and φ scan. Scanning electron microscopy (SEM) is used to observe film morphology. Energy dispersive X-ray analysis (EDX) is used for compositional analysis. Transmission electron microscopy (TEM) is used for microstructure analysis. The electrical property was determined by the four-probe method.

The morphology and the property of the film are related with post-annealing temperature and the duration. By optimizing the method of preparation, highly *c*-axis oriented and epitaxial films were obtained. The rocking curve of the (0,0,12) reflection had a FWHM of 0.29°. X-ray φ scans and TEM revealed better epitaxial growth. No reaction layers are observed between superconducting thin film and substrate. The highest zero resistance temperature T_{c0} reached 108K.

RESISTANCE TO WEAR OF $ZR_{41}TI_{14}CU_{12.5}NI_{10}BE_{22.5}$ BULK METALLIC GLASS

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Behavior of resistance to wear for $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$ bulk metallic glass (BMG) is investigated. It is found that three stages are involved in the wear loss-operating time curves in the as-quenched and annealed samples. They are running-in, steady-state and severe wear stages respectively. An increase of the wear resistance ability is observed in an order: crystallization state, as-prepared state and relaxation state. Besides, no sliding wear-induced crystallization is observed in both as-prepared and relaxed samples, indicating good thermal stability of the BMG

PROBLEMS OF DESIGN AND SEARCH OF NEW ACENTRIC OXIDE CRYSTALS FOR OPTOELECTRONICS

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The family of the «acentric» oxide crystals plays an important role in the development of optoelectronic devices. In the past twenty years, about fifty new efficient non-linear optical (NLO), piezoelectric and electrooptic crystals have been found and several novel self-frequency doubling (SFD) laser media have been created by using of ones. There are some approaches for search and properties prediction of such materials, including a computer-assisted materials design. The phenomenological model of classification and search for new NLO crystals have been early suggested by us [1]. The combination of chemical bond lengths for all components of crystal is a first criterion, which determine the structure, properties and chemical systematic of material.

In this report such approach is continued, the list of acentric crystals is extended and more detailed analysis is presented for polar, pure piezoelectric, enantiomorphic and optical active binary oxide crystals. It is shown that a formation of acentric binary oxide crystals is represented with rosette of two ellipses, plotted on plane of the oxide bond lengths, and acentric ternary oxide crystals – with rosette of two ellipsoids. The polar crystals are arranged near ellipse lines and piezoelecrical ones – more uniformly inside these ellipses. The crystals having all mentioned properties arranged inside of two separate truncated ellipses. The dependence of «acentric» properties on chemical bond length is non-monotonic and it divides the oxides in some typical groups. In view of this phenomenological model is valuable how for the evolution of theory, so and methodology classifications, of search and the synthesis of novel promising materials for use in optoelectronics.

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THEORETICAL ANALYSIS OF FORMATION OF STABLE AND METASTABLE PHASES AND COMPOUNDS IN BINARY OXIDE SYSTEMS

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Many complex oxides ($ma_kO_l{\cdot}nb_pO_r$) can dissociate at melting and then crystallize at deep supercooling with formation of different metastable compounds or eutectics. The calculation of liquidus lines of solid compounds in bi_2O_3 - geO_2, li_2O - b_2O_3 systems have been carried out in subregular solutions model and then the extents of dissociation (α) of complex compound have been calculated in melting point (t_m) by the method of work [1].

The qualitative theoretical analysis of nucleation kinetics in such systems has been carried out. The complex binary compound ($ma_ko_l \cdot nb_po_r$) is really nucleating in melts of virtual ternary system $(\mathbf{1-\alpha}) \cdot (ma_ko_l \cdot nb_po_r) + \boldsymbol{\alpha} \cdot (ma_ko_l) + \boldsymbol{\alpha} (nb_po_r)$. The kinetics of the association $(ma_ko_l) + (nb_po_r) = (ma_ko_l \cdot nb_po_r)$ in supercooled melt can be a limitative stage of the nucleation process. So, the energy of formation of critical nucleus in virtual melt (Δg_c) can be written at first approximation as:

$$A_N = \Delta G_C = 1/3 \cdot \sigma S_C = 16\pi/3 \cdot \sigma^3/[RT_L LN(C_\alpha / C_L)]^2 \qquad (1)$$

$$C_\alpha = (1-\alpha)/[1+\alpha(M+N-1)] \qquad (2)$$

$$C_L = (1-\alpha_L)/[1+\alpha_L(M+N-1)] \qquad (3),$$

Where - $\mathbf{c_\alpha}$, $\mathbf{c_l}$, $\mathbf{c_\alpha}'$ and $\mathbf{c_\alpha}''$ is compound concentration in virtual melt and one at melting point, at overheated and undercooled state correspondingly ($c_\alpha' < c_l(c_\alpha) < c_\alpha''$), σ - interface «solid-liquid» tension.

The experience is shown that possible melts supercoolings ($\mathbf{\Delta t}$) is nearly proportional to dissociation extent $\boldsymbol{\alpha_l}$, ($\mathbf{\Delta t} \approx k\boldsymbol{\alpha_l}$) in these systems. Besides, at deep supercoolings the field of crystallization of low dissociated compounds can be more then one for strong dissociated compounds and metastable eutectic crystallization is possible in case of high $\boldsymbol{\alpha}$ and $\mathbf{\Delta t}$. Other peculiarities of crystallization of complex oxides have been discussed more detail.

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DESIGN OF CRYSTAL GROWTH TECHNOLOGY FROM AQUEOUS SOLUTIONS

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The explanation of the large diversiform of minerals, the diversity of types of crystallization processes is needed for the «first principle» knowledge about basic laws of crystal formation [1]. The system studies of the nucleation kinetics in many salt aquosystems have been carried out by statistical method of many samples. The interrelation into crystallization and thermodynamic parameters of solutions has been established by plotting of various dependencies: solubility product (**SP**), the enthalpy of dissolution ($\mathbf{\Delta H_s}$) and the solution supercooling ($\mathbf{\Delta T}$) (supersolubility $\mathbf{-x_{ss}}$) on ionic salt radii ($\mathbf{R_i}$); the deviation extent from an ideal Debay-Hückel model of electrolyte solution (**q**) on **SP** and $\mathbf{R_i}$. It is shown, that **SP**, $\mathbf{\Delta T}$, $\mathbf{\Delta H_s}$ and types of solution crystallization are changing periodically due to an increasing of ionic dimensions of salts. It is stipulated by the simultaneous changing of a crystal lattice, a crystal lattice energy and a solute hydration energy for solutions of I-I and others types of electrolytes. It is known that the surface entropy factor $\boldsymbol{\alpha}$ ($\boldsymbol{\alpha} = \xi\{(\mathbf{\Delta H_s}(T, x)/kT_m) - \ln \mathbf{x_s}(T)\}$) predetermines the law of defect or perfect crystal formation [1].

In this work it is shown that the salts solutions of all types divide into three main groups, having large, middle and small supercooling. On this bases the certain correlation into **SP**, $\mathbf{\Delta T}$, crystallization salt types and methods of crystal growth from solution has been established [2]. Consequently, it is possible approximately a priory predict an optimal method and condition of perfect crystal growth for new promising materials by estimation of dimensional factors of salts.

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DISLOCATION PROCESSES AND PHASE TRANSITION AT A HIGH-TEMPERATURE CREEP OF ALLOYS

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The methods of a diffraction electronic microscopy and X-ray diffraction analysis the examinations of a phase composition and thin structure of an alloy VKNA - 1B were carried out, which were prepared by of a directional crystallization. Then the heat treatment of the samples were sent so: 1).annealing at T = 1150^0C, 1 hour; 2) annealing at T = 1100^0C of various time; 3) agings at T = 800^0C, 50 hours. The subsequent trials for a creep were carried out at T = 11000C at a loading 100 МПа. The time of trial varied from 3 to 77 clocks.

There are phases γ and γ' as main on the basis of fcc lattice. The β-phase having vcc a lattice had place only sometimes. γ'-phase has ordered location of atoms with superstructure $L1_2$. At all heat treatment γ' is the basic phase. The fraction of γ-phase (solid solution on a basis nickel, having the short-range order) does not exceed 20%.It was established, that after a directional crystallization samples consist of major areas (γ'+ γ) phases and separate coarse particles γ' - phase.

The particles γ' - phase are classified by their sizes: 1) greatest sizes (20-90μm) have separately located round shape particles γ'_1; 2) much smaller sizes (on the order) - particle of γ'_{II}; taking place inside two-phase area (γ+γ'); 3) still smaller sizes have particles γ'_{III}, taking place inside an mixture (γ+γ'_{III}), located in large particles γ'_1; 4) most small size (~ 0,05 microns) have particles γ'_{IV}, taking place in interlayers (γ+γ'_{IV}), bordering γ'_{II} in two-phase areas (γ+γ').

Concentration inhomogeneities, phase composition, morphology of phases in γ'-phase quantitatively were investigated. On the basis of it the mechanisms of a creep were analysed. It was established, that the basic contribution to a creep is imported by a dislocation creep in volume of a γ'-phase. The considerable role of a diffuse creep is detected at a phase transition γ→γ'→γ. The estimation of a role of the contribution of a diffusion creep inside γ'-фазы, stipulated by shaping of concentration inhomogeneity is carried out. Is shown, that the structural modification of a phase γ'_I is labile at all actions near temperature 1100^0C. On the contrary, in these requirements the phase γ'_{II} - inconvertible.

LEGITIMACIES OF THE DISSIPATION OF ACOUSTIC ENERGY AT THE CYCLING OF MARTENSITIC TURNING INTO ALLOY TINICU

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In alloy $Ti_{50}Ni_{40}Cu_{10}$ the first stage of martensitic transformations (MT) at cooling B2□B19 (B2 - a superstructure such as CsCl, B19 - the trimetric martensite) proceeds according to a microexplosive kinetics. A microexplosive kinetics of occurrence, and it is equal also disappearances of martensitic crystals represents spontaneous reducing (cutting) a martensitic crystal up to the terminating sizes. It is considered, that such process of travel of martensitic boundary is carried out with rate not below rate of reducing of elastic waves in the given crystalline environment.

Both at direct B2 □ B19, and at revertive B19 □ B2 transformation it is observed produced acoustic radiation. Acoustic radiation is unsymmetrical - radiant energy at direct transformation surpasses radiant energy at revertive. Cycling martensitic transformations feebly influences a type of asymmetry, lowering energy of acoustic radiation produced at direct transformation however is observed. Annealing (heating up to 600 ^{0}C) of previously nanocycled material reduces starting relations of a radiation energy at direct and inverse.

The situation essentially varies at carrying out of cycles B2 □ B19 and B19 □ B2 of transformations at an application of an exterior mechanical load. The consecutive stage high of an exterior mechanical loading in cycles of a MT up to some limit results in lowering, and then high of energy of acoustic radiation produced at direct B2 □ B19' transformation. At revertive B19' □ B2 transformation the level of acoustic energy does not change.

The cycling of martensitic transformations at a stationary value to an external loading is accompanied produced acoustic radiation which unsymmetrical character decreases with propagation of quantity of a loading. And the level of radiated energy grows at inverse, and at direct - remains to stationary values.

These data testify, that introduction in the energy balance of martensitic transformation of an exterior mechanical energy changes character of an acoustic dissipation of energy. As the factor of pinch of a share of a heat of dissipation at direct transformation amplification of a correlation may act in spontaneous travels of martensitic boundaries at formation of system of martensitic crystals under influence of an external load.

ATOMIC STRUCTURE OF SPECIAL TILT GRAIN BOUNDARIES IN METALS AND THEIR INTERACTION WITH THE VACANCIES.

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In this work, tilt grain boundaries in nickel and aluminium were computer simulated. Symmetric GBs (special boundaries) with reverse density of coincidence sites 9 and 11 with an axis of turn [110] and with reverse density of coincidence sites 5 with an axis of turn [100] were studied. The atomic interactions were described by Morse semi-empirical central-force potentials. The stability of atomic structure of GBs was analyzed by the method of energy surface construction using rigid two-dimensional relaxation where the atoms at shift one grain relative to another are in sites of corresponding lattices and full atomic relaxation by molecular static method.

The calculation showed that GBs in coincidence site lattice model were unstable. Stabilization was achieved by an additional displacement at some vector. The directions and values of these vectors were determined. The investigated GBs had several states - stable state having minimum energy and metastable ones. The variants of reorganization of GBs from one stable state to another were investigated. The directions and values of potential barriers of GB sliding were found. The relaxation along the normal of GB plane was the reason of origin of excess volume on the GB. The values of GB excess volume were determined for each point of an energy surface.

Interaction of vacancies with symmetric grain boundaries with an axis of turn [100] in pure Al were computer simulated. The energy of GB-vacancy interaction was determined as the difference of energies of a crystal, containing the vacancy near GB and crystal, containing vacancy separately of GB (with identical quantity of atoms). Both crystals (with and without GB-vacancy interaction) were relaxed using full atomic relaxation. The initial structure of the GB was coincident with GB given by the coincidence site lattice model. The vacancy was generated in each of several GB-adjacent planes. Simulations showed that the energy of GB-vacancy interaction had negative quantity, thus vacancy generation near special GB was profitable.

COMPUTER SIMULATION OF ELECTRONIC DISTRIBUTIONS IN ATOMS CU, NI AND AL AND POTENTIAL CONSTRUCTION OF INTERATOMIC INTERACTION OF IT ALLOYS

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We suggest electronic density of external shells of each atom was approximated spherical Gauss function as follows:

$$\rho(\vec{r}) = -Ze\left(\frac{\alpha}{\sqrt{\pi}}\right)^3 \sum_j \exp\left[-\alpha^2(\vec{r}-\vec{r}_j)^2\right].$$

Here $\vec{r}-\vec{r}_j$ - distance to j atom, α, Z - parameters.

One use the assumption that atoms cooperate only by means of coulomb forces. Then the potentials, described the interactions of atoms of different sort (A and B) in alloys, are easy constructed by using elaborated methodics:

$$\varphi(R) = \frac{Z_A Z_B}{R}\left[2\mathrm{erfc}(\alpha' R) - \mathrm{erfc}\left(\frac{\alpha' R}{\sqrt{2}}\right)\right].$$

Here R- interatomic distance, $\alpha' = \dfrac{\alpha_A \alpha_B}{\sqrt{\alpha_A^2 + \alpha_B^2}}$.

Parameters of distributions α_A and α_B obtained by condition crystal stability of pure metal using given size of the elementary cell and the sublimation energy.

The calculated values of elasticity modules of metals correspond with the experimental values. The calculated values of defects formation energies of ordered alloys NiAl (B2) and Ni_3Al ($L2_1$), calculated within the framework of model, are about 1,0 ÷ 1,3 eV.

LONG-PERIOD STRUCTURES IN AL_3TI ALLOY

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It is well-known, that in Cu-Au, $Cu_{3-x}Pd_{1+x}$, $Cu_{3-x}Pt_{1+x}$, $Ag_{3-x}Mg_{1+x}$ and other systems very intriguing ordered phases – long-period superstructures (LPSs) are formed. The existing electronic theory of long-period states attributes these to the Paierls instability of the electronic spectrum of the initial disordered state consisting in opening of an energy gap on the nesting patches of the Fermi surface (FS). LPSs are formed not only in noble metal alloys but also in other systems, in particular Al_3Ti.

LPSs in a Al_3Ti system are very much similar to that in Ag_3Mg (a comparatively short period compared to that in Cu-Au, stability at all temperatures, and commensurability of an average period with respect to the basis $L1_2$-superstructure). In spite of the similarity of their behaviour, some authors assume that the nature of the LPSs in Al_3Ti is different from that in noble metal alloys and in Ag_3Mg. The present work is devoted to investigating this assumption. With this aim an attempt is being done to find the FS nesting patches that may be responsible for the LPS formation in Al_3Ti.

Ab initio calculations and analysis of the electronic spectrum and electronic susceptibility of ordered Al_3Ti have pointed to existence of some FS nesting patches directly connected to the observed LPSs formations in this alloy. Distinctive feature of this system from noble-metal alloys is a considerable dependence of the antiphase domain value on the thetragonal degree *c*/*a* of the basis crystalline cell.

PHASE COMPOSITION AND DIFFUSION LAYER FORMATION MECHANISM IN THE PROCESS OF CARBON STEELS TITANIZING BY THE POWDER MIXTURES CONTAINING THE SPECIAL ADDITIONS OF NICKEL AND COPPER

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The influence of different elements and chemical compounds upon the nature of carbon steels diffusion strengthening was studied. The composition of diffusion titanizing saturant mixture providing a high saturation rate of titanium into steel surface was presented. The structure, phase composition and carbon steel diffusion case formation mechanism in titanizing process by saturant powder, consisting of Ti – Ni and Ti – Cu alloying compositions as well as K_2TiF_6 allying composition was learned.

Investigation of the saturating capacity of saturant medias that was studied brought to conclusion that Ti – Cu alloying composition used as powdered saturant media is effective. Application of it as the addition to known media for aluminum-thermal titanizing gives considerable effect: on the surface of low carbon steel the case to be formed contains a large amount of intermetallic particles and the case of a high carbon steel contains the intermetallic and carbide particles.

Powdered Ti - Ni alloying composition is the perspective saturant media to obtain intermetallic coverings. K_2TiF_6 compound is the effective activator of diffusion in titanizing process.

THE DETERMINATION OF MELTING TEMPERATURE, LATENT MELTING HEAT AND TEMPERATURE COEFFICIENT OF LINEAR EXPANSION BY THE METHOD OF MOLECULAR DYNAMICS

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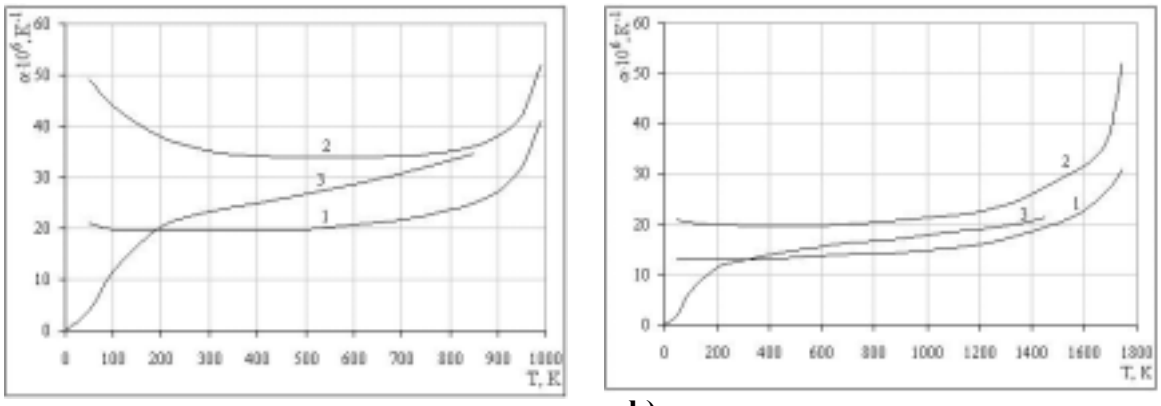
It is important to know such characteristics as melting temperature and temperature coefficient of linear expansion for solving the problems, connected with amorphous state and melting of simulating materials, by the method of molecular dynamics. The determination of these values is necessary for the approbation of using potentials of interatomic interaction and for proof of the simulation method, in particular the method of determination of the initial temperature and the initial parameter of the lattice of the simulating metals.

The methods of determination of the mentioned values by the method of molecular dynamics are shown in this work. The method of determination of melting temperature is based on the phenomena of the destruction of crystal structure, it needs some energy, called latent melting heat. The atoms of two-dimensional metals Ni and Al, described by two types of the potentials: Morse and Lennard-Jones, are considered as the examples. It is found, that the values of melting temperatures and temperature coefficients of linear expansion of the simulating two-dimensional metals at the usage of Morse potentials are well agreed with the values, corresponding to the real three-dimensional metals. Melting temperature, obtained by the method of molecular dynamics, has the value 1750 K for two-dimensional Ni (known experimental value is 1726 K for three-dimensional Ni), 1000 K – for two-dimensional Al (known experimental value is 933 K). The dependence graphs of temperature coefficient of linear expansion on temperature for two-dimensional Al and Ni, determined by two different methods, are presented in Pic.1 (a, b). The dependencies, corresponding to real three-dimensional materials, are also shown here.



a) **b)**

Pic.1. Temperature coefficient of linear expansion of two-dimensional Al (a) and Ni (b) in the dependence on temperature: 1 – determined by the first method; 2 – determined by the second method; 3 – experimental data for real three-dimensional metals Al and Ni.

COMPUTER SIMULATION OF PHOTOCONDESATION

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Photocondensation of vapor Br_2 and SF_6 on the glass surface were investigated by computer simulation. Recently Galashin and co-authors experimentally obtain drop of iodine in the center of laser beam on a glass surface. At a later time Petrov's group made more detail investigations of this phenomenon with Br_2 and SF_6.

We used pressure vapor Br_2 and SF_6 in the range 30-100 Torr. System were irradiated by resonant laser field. Intensity of the laser irradiation were above 100 watt/cm^2. The results are presented as distribution of density of condensate as function of distance between molecule and surface.

In the range of low intensities the increase of intensity of irradiation lead to growth the number of layers. We explained it by increasing of dispersion interaction. At a later time growth of number of layers lead to warming-up of condensate. As a result appeared a desorption.

Both processes condensation by light and thermal desorption are equilibrium.

We obtain four layers in system gas+surface+light: 1) condensate, 2) transitive superficial layer of condensate, 3) dense layer of gas, 4) free gas.

LEGITIMACIES OF AN ACOUSTIC EMISSION AT MARTENSITIC DEFORMATION IN ALLOYS WITH THERMOELASTIC MARTENSITIC TRANSFORMATIONS

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To apply of a mechanical loading in a cycle of thermoelastic martensitic turning into alloys on the basis of an intermetallic compound gives nickel of titanium in accumulation of deformation at direct transformation and a deformation relief at revertive. The simple thermal cycle in the interval of temperatures containing an interval of reversible martensitic transformations is accompanied essentially unsymmetrical acoustic radiation, and the radiant energy, produced at direct transformation considerably exceeds the radiant energy, produced at revertive. During such repeated cycles of martensitic transformations energy of acoustic radiation at direct transformation the level drops exponentially before saturation. At inverse radiant energy remains to a stationary value.

Opposite, at carrying out of the composite thermomechanical cycles of martensitic transformations when serially incremental loading is enclosed only at direct transformation, the monotonic propagation of energy of acoustic radiation is observed. At inverse radiant energy is constant. That is asymmetry of an acoustic emission amplifies.

If serially incremental loading is enclosed only at inverse acoustic radiation at direct transformation degrades, and at revertive is confidently fixed. Thus, inverse of asymmetry of an acoustic emission is observed.

If serially incremental loading is enclosed both at direct and at revertive transformations energy acoustic radiation at direct transformation grows only in some interval of loadings, at revertive radiant energy is constant.

THE EVOLUTION OF GRADIENT STRUCTURE-PHASE STATES AT CRYSTALLIZATION OF FERRIT STEEL WELDING SEAMS

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The purpose of the present work is the research of structure and phase composition of a welded seams of steel 09G2S with thickness >30 mm, used in casings of blast furnaces.

The metallographic researches of structure and the phase composition of a welded seams have shown, that a method and a way of welding in a melted zone form the gradient structure having following characteristic features. In the centre of a seam the biphase structure consisting of grains of ferrite and pearlite is forming. The grains of ferrite have the anisotropy with factor of anisotropy k=L/D~2.

The layer, adjoining to the given one, has similar phase composition, however the morphology of pearlite in it changes strikingly. The lamellar structure pearlite does not come to light, the pearlite grains are broken into colonies of the submicronic sizes. The interphase boundaries have a gear (fragmentary) structure. The grains of ferrite thus change a little bit. The revealed features of a structure-phase state of the given layer allow to voice the assumption about the incompleteness of phases division and process coagulation.

The further structure formation of the steel seam is carried out by recrystallization of grain structures. The nuclei of steel recrystallization are formed along boundaries of initial grains. In process of removal from the centre of a seam the volume fraction of recrystallization a material grows, the formed grains are increased in the sizes.

The transitive zone forming in the field of contact of melting with solid material, is characterized by the third type of structure consisting of large grains, with plates. Such structure due to the morphological attribute may be referred as widmannstatten ferrite.

THE ANALYSIS OF THE DISLOCATION SUBSTRUCTURES EVOLUTION DURING FATIGUE OF AUSTENITE STEEL

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The problem of fatigue fracture of steels and alloys is important despite a young history of investigations. The vast literature about dislocation substructures being formed during fatigue refers to pure metals.

In this work such a problem was being solved for austenitic steel 45G17Yu3 (0,45%C, 17%Mn, 2,74%Al) undergone the fatigue tests before fracture.

The analysis of dislocation substructure of steel was being carried out by methods of electronic diffraction microscopy of thin foils.

The quantitative analysis of steel dislocation substructure in its initial state showed that the largest density of dislocations spreaded along the volume is fixed by net-shaped substructure; the maximum level of curvature-torsion of the crystalline lattice is in fragmented substructure. Here, in fragmented substructure the elastic constituent of material curvature-torsion is maximum.

The fatigue tests of steel ($N=7\cdot10^4$ cycles) brings to the evolution of dislocation structure – substructure of dislocation chaos is transformed into net-shaped dislocation substructure. The deformation of steel is accompanied by an increase of scalar density of the dislocations from $1,3\cdot10^{10}$ to $1,8\cdot10^{10}$ cm^{-2} in net-shaped substructure and from $0,5\cdot10^{10}$ to $1,1\cdot10^{10}$ cm^{-2} – in fragmented one.

In steel structure undergone the tests for fatigue, in small quantities there are the deformation microtwins. The test of steel for fatigue is accompanied by essential increase of curvature-torsion amplitude of the crystalline lattice in fields with net-shaped dislocation substructure. The cyclic deforming of steel fields with fragmented substructure is accompanied by some other processes despite that the scalar density of dislocations located inside of fragments essentially grows (more than in two times), the curvature-torsion of crystalline lattice of these fields material is decreased.

THE EVOLUTION OF MESOSCOPIC SUBSTRUCTURE AND ELECTROIMPULSE SUPPRESSION OF FATIGUE FAILURE OF AUSTENITE STEEL

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The problem of the fatigue failure of steels and alloys is actual now inspite of its long history of research. It is connected with that, many constructions and products of crucial purpose are used in such modes, but their failure occurs suddenly without marked previous signs.

The change of structure, phase composition and failures of steel 08X18H10T subjected to low-cycle fatigue has been studied by methods optic, rastered and transmission electron diffracting

microscopy on mesolevel. The reasons of resource increase and suppression of fatigue failure by electroimpulse treatment in a moment of transition to the third critical stage of the dependence of ultrasound speed on a number of cycles loading have been found out.

Firstly, the electrostimulation brings to slowing-down the process of self-organization of dislocation substructure, i.e. in zone of fracture in initial sample there is a cell substructure, but in electrostimulated one there is a transition of grid substructure to cell remained unfinished. Secondly, the electrostimulation suppresses the process of martensitic $\gamma \rightarrow \varepsilon$ transformation occurring in zone of fracture of research material. The suppressing of $\gamma \rightarrow \varepsilon$ transformation plasticizies the steel. Since in electrostimulated sample ε martensite is in smaller quantities and in the background of cell-grid dislocation substructure, the stability to nucleation of microcracks in the latter is higher than in initial material. Thirdly, the electrostimulated sample is failed in higher values of scalar density of dislocations and density of curved extinctional contours, in smaller quantity of microcracks and smaller value of torsion curvature of the crystalline lattice in comparison with initial sample.

THE PROPERTIES AND STRUCTURE DEGRADATION OF BOILER ELEMENTS AFTER LONG OPERATION

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In this work the change of mechanical properties and structures of boiler pipes from steel 10 (0,13%C; 0,44%Mn; 0,23%Si; P, S≤0,02 %) after 50 years of operation at working pressure ≤ 1,5MPa and temperature ≤250^{0}C were investigated.

As a result of operation there was a change of all basic mechanical characteristics. The yield stress and tensile stress have decreased accordingly on 27,5 % and 16,5 %, and specific elongation before break and reduction of area – have increased by 15,7 % and on 9 %.

Table 1.

Material	$\sigma_т$, MPa	$\sigma_в$, MPa	δ, %	ψ, %	Velocity of ultrasound, m/s
Steel 10 in a condition of delivery	364	510	25,4	56	2851±2
Steel 10 after operation (50 years)	264	426	29,4	61	2865±0,2

In an initial condition steel has the ferrite-pearlite structure where the pearlite volume fraction does not exceed 15%. The boundaries of the ferrite grains are thin and precise. The precipitations of carbide phases are absent both in the body of ferrite grains, and on the boundaries. After the long operation the structure becomes a very non-uniform. The alongside with sites where it has remained practically former, there are the zones of local recrystallization where the average size of a grain has increased from 17,6 microns up to 22,2 microns. In these zones there is no the pearlite component. On the other hand, the increased content of pearlite is observed on the edges of such zones. Obviously, the strong disorder of microhardness from 1430 up to 1700 MPa is connected with these facts. Also it is important to note, that the fracture of the samples took place in area of such recrystallization zones.

DISLOCATION SUBSTRUCTURES EVOLUTION OF STEEL 45G17YU3 DURING ELECTROSTIMULATED FATIGUE TEST

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In this work the influence of impulse electric current on dislocation substructure being formed in austenitic steel 45G17Yu3 as a result of fatigue tests.

Steel 45G17YU3 is the polycrystalline GTsK – solid solution on the basis of iron. There are chaotic, net-shaped and fragmented dislocation substructures. Their volume fractions are correlated as 1:2:7.

The treatment of steel having passed the fatigue tests by low-frequency electric current (electrostimulation) results in proceeding the relaxation processes in material. The grain structure is reconstructed by nucleation and growth of recrystallization grains (found by us for the first time in this work). The new grains are being form near the boundaries of the old grains or their joints. The dislocation substructure is reconstructed partially: substructure of dislocation chaos is formed (~0,05 of steel structure), the scalar density of dislocations in this case is guite low than in chaotic structure, appearing during hot rolling of steel; the volume fraction of net-shaped structure (upto ~0,4) is decreased and of fragmented substructure (~0,55) is increased. The processes of return run in two channels: annihilation of dislocation results in reconstruction of net-shaped substructure into chaotic one; the creeping of dislocations, i.e. the net-shaped dislocation into fragmented one. The process of microtwinning is initiated as a rule in net-shaped dislocation substructure.

The action of electric current on steel results in decrease of scalar density of dislocations located in fragmented and increase of dislocations density placed in net-shaped substructure.

FORMATION OF GRADIENT STRUCTURE–PHASE STATES AT ROLLING OF BIG DIAMETER ARMATURES

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The purpose of the present work is the investigation of the laws of plastic deformation and fracture of armature of big diameter from steel 18G2S (0,18%C, 2%Mn, <1%Si) alongside with detailed research of their defect structure and phase composition.

The armature of low-alloy steel of various diameters strengthened by a method of interrupted quenching in a stream of high-speed mills of West-Siberian Metallurgical Works.

The researched material at the certain way of etching of face section of rod reveals the concentric zones differing by a degree of etching and the various colors. The macrostructure and the amount of zones and their parameters depend on the diameter of armature. Zones are not equivalent on the sizes. As a rule, the greatest volume is occupied by the intermediate zone. The central and undersurface zones are rather insignificant and have the similar character.

The metallographic structure analysis revealed the qualitative and quantitative distinctions in the structure of zones. The etching picture of undersurface zones is characteristic for the martensitic similar structure. In the central zone the areas of the pearlite structure are observed and we can see also the structure characterized by the fine undergraine chaotically located particles of carbide phases. The intermediate zone contains elements the both zones considered above.

The analysis of grain structures has revealed two types of grains: the large grains with the sizes of 30-40 microns, having an equilibrium configuration of boundaries and the fine grains having sizes of 3-5 microns and located along boundaries.

The structure formed on martensitic mechanism concerns to the massive matrensite. It represents the crystals of α-iron parallel located to each other. The average cross sizes of crystals are 1,5-2 microns.

The bainite structure is close to structure of the above described martensite according the mechanism of formation and to morphological attributes. The bainite has the form of crystals (lenses) having units of microns in cross sizes the longitudinal – the tens of microns.

CONCENTRATION VARIATION OF ADDITION AT LATERAL BOUNDARIES OF GRAINS UNDER ELECTRONIC EXPOSURE

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The experimental investigation of additive re-distribution under electronic beam revealed a recovery of the additive at grain boundaries. Additive accumulation mainly takes place at the boundaries that are perpendicular to material surface, whereas there is no an observed recovery of additive at the boundaries that are parallel to the surface.

The additive recovery is caused by spot fault gradients near the grain boundary. The grain boundary is an intensive run-off region of vacancies. Therefore, the average vacancy distribution profile near the grain boundary changes its pattern.

The above case indicates that there are two additive fluxes. One of them is vectored perpendicular to the surface, and the other one is parallel to it, i.e. it is vectored to the grain boundary. A study of the perpendicular and parallel boundaries shows that there is no additive settling at the boundaries that are parallel to the surface, since the general flux is vectored to the parallel boundaries. There is no such kind of phenomenon at the grain boundaries that are perpendicular to the surface. Besides, the perpendicular boundaries are more effective run-off regions for vacancies, since there is a slower build-up of the region with vacancies due to displacement of the vacancies to the surface.

To compute concentration of vacancies we will consider a grain on the surface as a model. The computations indicate the presence of vacancy gradients vectored to the surface and grain boundaries, which are perpendicular to the surface.

Comparison of the experimental and theoretical outcomes shows a good agreement between the theoretical model and actual processes occurring under the exposure. This theory discloses wide potentials for application of diffusion processes in alloys.