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MODELING AND QUANTITATIVE ANALYSIS OF CONNECTIVITY AND CONDUCTIVITY IN RANDOM NETWORKS OF NANOTUBES (p. 4-12)

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The work describes the framework that allows performing a computer simulation of complex random networks of conducting nanotubes embedded in the dielectric medium. The representative volume element filled with a large number of interconnected nanotubes is modeled and the tunneling conduction mechanism between adjacent tubes is considered. The principal goal is to develop a computational approach for the three-dimensional multielement structure simulation, which will be relatively simple, yet capable of producing realistic results.

The connectivity formation processes among nanotubes in random nanotube networks are studied using the elements of graph theory. All stages of the modeling process are discussed in details. The system conductivity model with taking into account the tunnel effect and intrinsic nanotube conductivities is formulated. The random resistor model is used to calculate the total equivalent conductivity of the network.

The results of the computer experiments on electrical conductivity simulations for different systems are presented. The dependencies of the electrical conductivity of nanotube networks in the insulating medium on the concentration of nanotubes, geometric parameters and properties of tunneling conductivity between individual tubes are investigated. It is found that the percolation threshold corresponds to the nanotube loading of 0.5 % when the aspect ratio of nanotubes is 160. Non-linear dependence between the aspect ratio and the percolation threshold was established. The analysis of computational complexity and calculation time is performed for quad-core computing systems.

Computer experiments carried out in a systematic fashion within the proposed framework can be useful when designing novel CNT-polymer composites for state of the art electronic applications. By following the predictions of the proposed model, tailoring of electrical properties of such composites can be made easier when adjusting the parameters of nanotubes and their concentration during the fabrication of the nanocomposite samples.

Keywords: statistical modeling, random resistor networks, percolation, tunneling conductance, nanotubes, nanocomposites.

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COMPARISON OF OXYGEN EVOLUTION PARAMETERS ON DIFFERENT TYPES OF NICKEL HYDROXIDE (p. 12-19)

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A simple method for determining the oxygen evolution parameters; that uses step-wise potentiostatic regime was proposed. The proposed method was used to study the oxygen evolution on the nickel hydroxide samples that were prepared using different methods and had different grain size. The samples used in the research were studied using Scanning Electron Microscopy, X-ray diffraction, IR-spectroscopy, and Energy Dispersive X-ray analysis. It was demonstrated that the used $\text{Ni}(\text{OH})_2$ samples have different morphology, structure and composition. The industrial $\beta\text{-Ni}(\text{OH})_2$ sample has a

shard-like structure, high degree of crystallinity and no intercalated anions. The electrochemically prepared sample has a low degree of crystallinity and has a structure that is composed of α and β -forms that contain carbonate and sulfate ions. It had been demonstrated that polarization of oxygen evolution depends on the methods of nickel (II) hydroxide synthesis and its grain size. The effective constants of the Tafel equation had been determined, which for industrial Ni(OH)₂ samples are $a_{eff}=0.383$, $b_{eff}=0.055$ (0–70 μm grain size) and $a_{eff}=0.414$, $b_{eff}=0.067$ (0–40 μm grain size), for the electrochemically prepared sample – $a_{eff}=0.451$, $b_{eff}=0.089$ (0–70 μm grain size). It was also demonstrated that polarization of oxygen evolution is affected differently by high current densities for different powders.

Keywords: oxygen evolution, side-process, nickel hydroxide, Ni(OH)₂, cyclic voltamperometry curve.

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**RESEARCH INTO SURFACE PROPERTIES OF
DISPERSE FILLERS BASED ON PLANT RAW
MATERIALS (p. 20-26)**

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The properties of the dispersed fillers are investigated based on the agricultural and wood industry wastes: buckwheat and oats husk, wood and pine-needle flour. We experimentally determined structural-rheological characteristics, morphology and acid-base properties of the surface. By applying a potentiometric determining of hydrogen indicator of aqueous suspensions pH_{susp} , we studied the qualitative and quantitative characteristics of acid-base active centers on the surface of the particles of fillers. It was revealed that the surface of buckwheat husk is dominated by two types of active centers: weakly-acidic ($pK_a \approx 5.53-5.83$) and close to neutral ($pK_a \approx 6.16-6.30$). The surfaces of wood flour and pine-needle flour are characterized as the weakly-acidic with centers $pK_a \approx 5.29-5.52$ and $pK_a \approx 5.02-5.36$, respectively. Based on sources from the scientific literature, we compiled a comparative characteristic of the chemical composition of the examined fillers. A correlation is established between chemical composition, physical-chemical and surface properties. It is shown that the total mass content of cellulose and lignin can be one of the criteria for evaluating resistance of the fillers to high temperatures and acidic-base properties. A decrease in the sum of mass content of cellulose and lignin in the composition of fillers results in the improved thermal resistance while the surface acidity decreases. The results obtained allow us to predict behaviour of the fillers in compositions and control performance characteristics of composite materials.

Keywords: disperse filler, plant raw materials, composite material, surface active centre, acid-base properties.

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SYNTHESIS AND CHARACTERISATION OF DYE-INTERCALATED NICKEL-ALUMINIUM LAYERED-DOUBLE HYDROXIDE AS A COSMETIC PIGMENT
(p. 27-33)

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Dye-intercalated layered double hydroxides (LDH) are modern promising pigments for paint and cosmetics industry. For the preparation of high-quality cosmetic pigments, particularly for nail polish, it was proposed to use not only intercalation but also chemisorption. For the pigment synthesis, Ni-AL LDH was chosen, along with murexide (Ammonium (purpurate) 2,6-dioxo-5-[(2,4,6-trioxo-5-hexahydropyrimidinylidene)amino]-3H-pyrimidin-4-olate), in which colored purpurate anion is able to form complex compounds with Ni²⁺. The murexide-intercalated (murexide amount for intercalation only) and murexide-intercalated-chemisorbed (murexide amount for Ni²⁺) Ni-Al LDH pigments were synthesized and used for the preparation of nail polish samples. The crystallographic composition was studied by means of XRD analysis. The color parameters (coordinates of color and chromaticity, dominant wavelength and color purity) of pigment powders and nail polish samples with these pigments have been studied using a color comparator. Organoleptic characteristics of pigment and nail polish samples were studied. The positive influence of chemisorption was shown: murexide-intercalated-chemisorbed pigment is easily ground, with the formation of highly dispersed powder, which during the preparation of nail polish was easily dispersed with the formation of stable yellow samples (dominant wavelength 583 nm) with high color purity of 43 %. Also, high covering ability of the murexide-intercalated-chemisorbed pigment was shown: high-quality, opaque, colored nail polish coat was formed at the pigment content of 45 %, 30 % and 15 % (wt.). For the synthesis of such pigments, it was recommended to choose anionic dyes that can form coordination bonds with LDH cations.

Keywords: cosmetic pigment, murexide, Ni-Al LDH, chemisorption, intercalation, nail polish.

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RESEARCH INTO SPECIFICS OF RECYCLING THE SCALE OF NICKEL-MOLYBDENUM CONTAINING PRECISION ALLOYS BY THE METHOD OF HYDROGEN REDUCTION (p. 34-38)

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We explored kinetic patterns of hydrogen reduction of the scale of a nickel-molybdenum containing precision alloy at a temperature of 673–1573 K over the interval from 0 to 360 min. The largest degree of reduction is achieved after thermal treatment at 1273 K – 99 %. This is due to the intensification of reduction processes and a sufficient level of porosity, which enables a satisfactory gas exchange. It was discovered that the starting scale consists mainly of Fe₂O₃ and Fe₃O₄ with the atoms substituting their alloying elements, as well as MoO₃. The target product of metallization had a sponge microstructure and consisted of γ -Fe, FeNi, the phase of Mo, and the remaining non-reduced Fe₃O₄ and FeO.

The resulting phases do not demonstrate a noticeable inclination to sublimation. This ensures a reduction in the losses of alloying elements when obtaining and using the highly-alloyed metallized scale, which was confirmed by the experimental- industrial tests. At the same time, disposal of industrial wastes provides a reduction in the technogenic load on industrial regions and improves ecological situation.

Keywords: scale, precision alloy, hydrogen reduction, phase analysis, microstructure, resource saving, alloying.

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**RESEARCH INTO CORROSION AND
ELECTROCATALYTIC PROPERTIES OF THE
MODIFIED OXIDE FILMS ON TiN (p. 39-44)**

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Oxide films on tin, modified by titanium compounds, are non-toxic and serve as anticorrosion protection, material for gas sensors, photo- and electrocatalysts. We investigated the process of anodic tin treatment in the presence of potassium metatitanate. It is shown that the two-stage technique for the formation of an oxide film at the electrode potentials of –0.3 V and 3.0 V makes it possible to substantially increase the content of titanium oxide compounds in the oxide mixture. The content of Ti(IV) reaches values of 14–15 % (mol). Films with a maximum content of titanium compounds and the largest corrosion resistance are formed at a concentration of potassium metatitanate above 1·10⁻³ mol/l. The time of self-activation of such films is 10 times longer than that of the unmodified films.

We explored catalytic properties of the obtained films with mixed composition SnO_x(TiO_y). It is shown that an increase in the content of titanium oxide compounds in the film contributes to the acceleration of anodic oxidation of MTBE. It was established that

this process takes place directly on the surface of the oxide film rather than during interaction with oxygen formed on the anode. The modified oxide films $\text{SnO}_x(\text{TiO}_y)$ on tin with maximal corrosion resistance and electrocatalytic activity are formed from the solutions that contain 0.5M KOH.

Keywords: modified oxide films, titanium oxide compounds, tin, corrosion resistance, electrocatalytic activity.

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A STUDY OF THE INFLUENCE OF ADDITIVES ON THE PROCESS OF FORMATION AND CORROSIVE PROPERTIES OF TRIPOLYPHOSPHATE COATINGS ON STEEL (p. 45-51)

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The anodic behavior of cold-rolled low-carbon steel in the aqueous STPP solution with aluminum hydroxide, borax, and glycerin additives at room temperature has been studied.

It was revealed that the potentiodynamic curves that characterize the anodic behavior of steel st05kp samples shows up to three passivation plateaus. Additionally, the anodic curve ends with the complete passivation plateau with an anodic current density equal to zero. The obtained results demonstrate realization of the step-wise formation mechanism of tripolyphosphate coat in the 12 % aqueous STPP solution with additives.

It was found that with the addition of 2 % $\text{Al}(\text{OH})_3$, a narrowing of the first passivation plateau is observed. The addition of glycerin shifts the potential of passivation plateau formation toward negative

values by about 150 mV. When borax was added, only the complete passivation plateau is present on the anodic curve.

It was established that in the STPP solution with the addition of aluminum hydroxide, glycerin, and especially borax, steel passivation occurs earlier than in the solution without additives. This indicated the acceleration of tripolyphosphate coat formation when additives are used. The absence of the first two passivation plateaus on the anodic curve that describes the coat formation in the STPP solution with the borax additive indicated that formation occurs at the highest rate.

In the process of studying the anodic behavior of steel st05kp with the formed coats, in 0.1 N Na₂SO₄, it was found that the coats formed in the aqueous sodium tripolyphosphate solution with additives possess protective properties. The greatest positive effect on protective properties of the coats is provided by aluminum hydroxide.

Based on the results of combined studies, it was established that aluminum hydroxide can be recommended as the most effective additive for improving protective properties of tripolyphosphate coats. Borax can be recommended as an additive that accelerates coat formation.

Keywords: steel, corrosion, tripolyphosphate coat, additives, anodic behavior, potentiodynamic curves, passivation, acceleration, composite structure, protective properties.

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THE INFLUENCE OF THE CONDITIONS OF MICROPLASMA PROCESSING (MICROARC OXIDATION IN ANODE-CATHODE REGIME) OF ALUMINUM ALLOYS ON THEIR PHASE COMPOSITION (p. 52-57)

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Investigations have been performed on the effect of microplasma oxidation regimes in electrolytes with activating additives on the phase-structural state of coatings formed on the basis of aluminum. In microarc oxidation (MAO), the surface layer of the processed aluminum-based alloy was converted to a coating consisting of aluminum oxides with increased hardness. Such a modification of the surface layers makes it possible to use the properties of base materials and modified layers most rationally, sparing expensive and rare metals and alloys.

The study has revealed the formation of intermediate phases (multistage) during the formation of coatings on aluminum alloys in the alkali-silicate electrolyte and the anode-cathode mode of microplasma oxidation. The main intermediate phases are γ -Al₂O₃ and 3Al₂O₃·2SiO₂.

The composition of the electrolyte has a significant effect on the initial stages of the process during which strong passivating layers are formed on the metallic surface. These layers determine the possibility of spark explosions of sufficient intensity and, thus, the

implementation of the MAO process. The obtained results indicate that during the oxidation process, the γ -Al₂O₃ phase is alloyed with the base components and the electrolyte components to form solid substitutional solutions. The change in the lattice period in this case will be determined, on the one hand, by the difference in the ionic radii of atoms in the lattice and, on the other hand, by the difference in valence.

The paper discloses the influence of the crystal-chemical characteristics of the cations of the processed alloy and the cations that make up the electrolyte on the γ -Al₂O₃→ α -Al₂O₃. The absence of the hardest phase of α -Al₂O₃ (corundum) in the coating is explained by the low power of microdischarges, at which the temperature of the polymorphic γ → α transformation is not ensured. Pilot-industrial tests were performed on friction pair parts, and recommendations have been given on the change in the composition of the electrolyte and the parameters of electrolysis that ensure an increase in the content of the α -Al₂O₃ phase in the coating composition.

Keywords: structural engineering, microplasma treatment, anode-cathode regime, phase composition.

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DESIGN OF THE THERMAL INSULATION POROUS MATERIALS BASED ON TECHNOGENIC MINERAL FILLERS (p. 58-64)

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We report results of research into processes of formation of porous structure by the method of thermal bloating of the gel-like mixture of raw materials. Regularities of the course of physicochemical transformations are considered in the material when it is heated; as a result, we established the initial water content in the raw mixture, optimal for the formation of xerogel, and the residual water content in gel, sufficient for effective bloating. We proposed the optimized composition of the raw mixture that employs maximally permissible amount of ash as a mineral filler; the thermal modes of bloating are studied. Based on the data obtained, a new technology for the production of porous thermal insulation materials is created. New porous thermal insulation materials were obtained using soluble glass as a binding component; foaming agent; regulator of hardening rate of the mixture. The basic thermophysical properties were determined.

A study of physicochemical phenomena occurring during thermal bloating of analogous compositions allowed us to predict the course of the processes in the case of using additional chemical elements and techniques. It was established that ash can be effectively utilized when creating an efficient raw material mixture. The results obtained could be useful for the production of effective porous thermal insulation materials for various purposes. In addition, the task is resolved on the disposal of ash from coal-based thermal power plants.

Keywords: fly ash, soluble glass, alkaline silicate composite thermal insulation materials, thermal bloating.

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EFFECT OF FLAME RETARDANT FILLERS ON THE FIRE RESISTANCE AND PHYSICAL-MECHANICAL PROPERTIES OF POLYMERIC COMPOSITIONS (p. 65-70)

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An effect of copolymer of ethylene with vinyl acetate of the polymeric matrix and flame retardant fillers on the fire resistance of composite materials was studied. We used of ethylene-vinyl acetate copolymer in the research. The content of vinyl acetate is 18 % and 28 %; melt flow index is 1.8 g/10 min and 2.5 g/10 min, respectively. The flame retardant fillers are aluminum oxide trihydrates with an average diameter of particles of 1.5 μm and 3 μm; magnesium oxide dihydrates – 3.0 μm and 3.7 μm; hydromagnesites – 1.5 μm.

The fire resistance of polymeric compositions was determined using a method of Oxygen Index. It is shown that in order to achieve Oxygen Index larger than 27 %, the degree of filling of the polymeric compositions based on EVA 1 and EVA 2 has to reach 40–60 % depending on the chemical composition and properties of the fire retardants. At the same time, applying EVA 2 makes it possible to achieve this indicator at smaller values of the filling.

We established regularities in the effect of the nature of a polymeric matrix and flame retardant fillers on the physical-mechanical

properties of compositions before and after ageing. An increase in the content of fillers in the polymeric composition results in reduced destructive stress and relative elongation at breaking, while the modulus of elasticity at stretching increases.

The results obtained could be applied when designing the formulations of polymeric compositions, which do not support combustion, for cable products, and which allow control over operational characteristics.

Keywords: fire resistance, ethylene-vinyl acetate copolymer, flame retardants, physical-mechanical properties, Oxygen Index.

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