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Аннотации на английском языке

Review

Review article

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The decisive role of biological factors in the corrosion of the D16T alloy. Review

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Abstract

The biocorrosion of duralumin grade D16T has been studied and a mechanism has been proposed according to which the initiators of initial corrosion damage are reactive oxygen species (ROS) produced by micromycetes. An assumption was made about the participation of hydrogen peroxide in the mycological corrosion of the D16T alloy, which is formed both during the life of micromycetes and during the activation of oxygen by zero-valent aluminium (ZVAL). The mechanisms of intergranular, pitting and pitting corrosion of duralumin under the influence of microscopic fungi are proposed. Purpose: determination of the main biological factor initiating biocorrosion of the D16T alloy; assessment of the biological impact of the association of microscopic fungi on the alloy in order to develop scientifically grounded and effective methods of protecting aluminium and its alloys from biocorrosion by micromycetes.

The object of the study was an aluminium alloy D16T in accordance with state standard (GOST) 4784–2019 after hardening and natural ageing, which is widely used for the manufacture of load-bearing elements of structures and equipment of fuel systems of aircraft, car bodies, parts of various machines and assemblies operating at low temperatures, and in the food and pharmaceutical industries. The stages of initiation and development of biocorrosion of the D16T alloy under the influence of a consortium of moulds have been studied using a scanning electron microscope. The phase composition of the D16T corrosion products has been studied.

In the process of vital activity of microscopic fungi, reactive oxygen species are formed, initiating the biocorrosion of the D16T alloy. The initial stage of biocorrosion is caused by hydrolysis of the protective passive aluminium film. At the stage of intense biocorrosion, oxygen-containing aluminium compounds are formed in the form of a water-saturated gel. Further, as this corrosion product accumulates, its water permeability decreases. The gel undergoes “ageing” and turns into crystalline products. Conidia and hyphae of microscopic fungi adhere, are mechanically fixed on the metal surface and penetrate into the surface layers and deep into the metal, causing its corrosive destruction in the form of pitting, ulcers, and cavities. It is possible that the initiation of metal biocorrosion is a consequence of the hyperproduction of reactive oxygen species by the cells of micromycetes as a result of oxidative stress. This may be their defensive strategy aimed at destroying xenobiotic material.

The development of intergranular and pitting corrosion of the D16T alloy under the action of micromycetes occurs at the sites of contact with the exudate, which, due to a cascade of reactions with the participation of ROS, is locally enriched in hydroxide ions. The origin and development of pitting on the duralumin surface occurs in defects of the passive oxide film due to the displacement of oxygen-containing surface aluminium compounds and their interaction with corrosive OH⁻ and ROS anions. Hydrogen peroxide, as an intermediate product of the metabolism of micromycetes, on the surface of the D16T alloy can participate in the Fenton process or decompose heterogeneously, also provoking the development of aluminium biocorrosion.

Keywords: Biocorrosion, Mycological corrosion, Duralumin, D16T, Zero-valent aluminium, ZVAL, Micromycetes, Microscopic fungi, Reactive oxygen species, ROS, Superoxide anion radical, Hydrogen peroxide, Intergranular corrosion, Pitting corrosion

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Original articles

Research article

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The quasi-binary Cu₃In₅S₉ – FeIn₂S₄ section

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Abstract

The Cu₃In₅S₉–FeIn₂S₄ section was studied by methods of physicochemical analysis; differential thermal (DTA), X-ray phase (XRD), microstructural (MSA) and microhardness measurement. Based on the results of the obtained data, a phase diagram of the Cu₃In₅S₉–FeIn₂S₄ section of the Cu₂S–In₂S₃–FeS ternary system was constructed. It was established that the Cu₃In₅S₉–FeIn₂S₄ section is a quasi-binary section of the ternary Cu₂S–In₂S₃–FeS systems and is eutectic by type with limited solubility based on both initial components. The liquidus of the system consists of two branches of primary crystallization of σ₁ (solid solution based on Cu₃In₅S₉) and σ (solid solution based on FeIn₂S₄)

phases. The eutectic point has coordinates: 1150 K temperature and composition 42 mol% FeIn_2S_4 . The boundaries of the solid solutions were also determined. The region of solid solutions based on $\text{Cu}_3\text{In}_3\text{S}_9$ extends to 3 mol. % FeIn_2S_4 , the region of solid solutions based on FeIn_2S_4 extends to 5 mol. % $\text{Cu}_3\text{In}_3\text{S}_9$ at room temperature.

Keywords: Microhardness, Phase diagram, System, section, Quasi-binary, Eutectic, Solid solution

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Research article

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Calorimetric determination of phase transitions of Ag_8BX_6 (B = Ge, Sn; X = S, Se) compounds

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Abstract

Differential scanning calorimetry (DSC) was used to study ternary Ag_8GeS_6 , Ag_8GeSe_6 , Ag_8SnS_6 , and Ag_8SnSe_6 compounds which undergo polymorphic transformations at relatively low temperatures. Two samples of each compound with different masses in the range of 20–40 mg were examined and three DSC heating curves were taken for each sample. The DSC curve data were used to determine the temperatures and enthalpies of the phase transitions of the studied compounds from a low-temperature rhombic modification to a high-temperature cubic modification. The difference in the DSC data between all samples and all heating curves did not exceed 2%. The obtained data were used to calculate the entropies of phase transitions. It was shown that these values are abnormally high. The study also involved a comparative analysis of the obtained thermodynamic data for the Ag_8GeSe_6 and Ag_8SnSe_6 compounds and the results obtained by the method of electromotive forces.

Keywords: Ag_8GeS_6 , Ag_8GeSe_6 , Ag_8SnS_6 , Ag_8SnSe_6 , phase transition, thermodynamic functions, enthalpy, entropy, differential scanning calorimetry

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Research article

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Sorption of 3-glucosides of six common natural anthocyanidins on anatase

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Abstract

In this study, the sorption of 3-glucosides of six common natural aglicones: delphinidin, cyanidin, petunidin, pelargonidin, peonidin and malvidin, on the surface of anatase was studied in comparison with sorption on the surface of silica gel, as a result, a different order of change in the sorption activity of anthocyanins depending on their structure was found. The structure of the (001) face of the surface layer of anatase crystals due to the ololation and oxolation of the initial $[\text{Ti}(\text{OH})_4(\text{H}_2\text{O})_2]$ octahedra upon condensation into three-dimensional grids was proposed.

The mechanisms of sorption of anthocyanins on the surface of sorbents are proposed. Delphinidin derivatives have the highest sorption activity on anatase.

Keywords: Anthocyanins, Sorption, Sorption mechanisms, Anatase, Surface layer structure, Silica gel

For citation: Deineka V.I., Salasina Ya. Yu., Deineka L. A. Sorption of 3-glucosides of six common natural anthocyanidins on anatase. *Condensed Matter and Interphases*. 2022;24(2): 196–203. <https://doi.org/10.17308/kcmf.2022.24/9259>

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Research article

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Surface-active and chemical properties of alkylbenzenesulfonic acid – nitric acid – water composites

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Abstract

Industrially produced anionic surfactant alkylbenzenesulfonic acid is proposed as a reagent for the ionic flotation of metals from acidic media. To establish the possibility of its application using this method, it is necessary to study the surface-active (surface tension, adsorption, cross-sectional area of a molecule in the adsorption layer) and colloidal (particle size, critical micelle concentration, solubilisation) properties of its aqueous and nitric acid solutions.

In this study, a series of solutions with various concentrations of alkylbenzenesulfonic acid and containing various amounts of nitric acid (from 1 to 10 wt%) were prepared. The surface tension of the obtained solutions was determined by the hanging drop method using a DSA

25E tensiometer. The introduction of HNO_3 led to a decrease in the surface tension of alkylbenzenesulfonic acid solutions and in its CMC value in comparison with aqueous solutions. On surface tension isotherms with a nitric acid content of 5 and 10 wt%, the presence of several inflections was found, which indicates a stepwise micelle formation. The values of surface activity and Gibbs energies of micelle formation of alkylbenzenesulfonic acid in aqueous and nitric acid solutions were calculated. Adsorption isotherms were constructed from the results of processing the curves of the surface tension of alkylbenzenesulfonic acid solutions. With small amounts of HNO_3 (1 and 2%), the limiting adsorption value of the anionic surfactant significantly increased as compared to the aqueous solution. A further increase in the acidity of the medium led to a decrease in the maximum on the adsorption isotherm. In the presence of an inorganic acid, the monomolecular layer of the surfactant first significantly loosened and then gradually became denser with an increase in acidity. The values of the limiting adsorptions, the adsorption equilibrium constants and the Gibbs energies of adsorption at the liquid-gas interface were calculated using the obtained isotherms. The solubilising ability of alkylbenzenesulfonic acid in relation to the Sudan I dye was determined photometrically using a UNICO 1201 spectrophotometer. With an increase in the solution acidity and the surfactants content the amount of solubilised dye increased.

Keywords: Alkylbenzenesulfonic acid, Surfactant properties, Nitric acid, Adsorption, Solubilisation

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Research article

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Substances and the transformations they undergo: basic concepts

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Abstract

We formulated the specific features for the notions of substances and transformation of substances. A substance is a set of interacting particles characterised by the following parameters 1) composition, or the type and ratio of amounts of particles that form the substances, 2) the energy of their interactions, 3) their structure and, finally, 4) the size of particles (dispersion). Transformations of substances occur when these properties change. Such processes are called chemical reactions. To control the transformation of a substance from the thermodynamic point of view, we need to evaluate: 1. The possibility of spontaneous processes (without energy consumption). 2. The thermal effect of the chemical reaction. 3. The equilibrium composition of the reaction medium.

We solved these problems using a mathematical model based on the improved notions (substance, energy, work, supersaturation) and the known laws of thermodynamics.

Keywords: Substances, Transformation of substances, Thermodynamics, Energy, Work, Chemical reactions, Chemical equilibrium, Spontaneous process, Thermochemistry, Supersaturation

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Research article

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Electrocrystallisation of Cu-Sn-TiO₂ composite coatings in sulphuric acid electrolytes

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Abstract

The aim of the article is to determine the peculiarities of electrochemical production of Cu-Sn-TiO₂ composite coatings in sulphuric acid electrolytes with intermittent agitation under stationary and pulsed modes of electrolysis.

Linear voltammetry and static and pulsed chronopotentiometry were used to study the kinetic features of electrocrystallisation of Cu-Sn-TiO₂ composite coatings in a sulphuric acid electrolyte with intermittent agitation. When the electrolyte was stirred, the cathodic potential shifted towards electropositive values. It was shown that after switching the agitation off, the value of the cathodic potential at which the copper-tin alloy forms at a cathodic current density of -0.013 A/cm^2 was reached within 70 s and when using pulsed electrolysis, it was reached within 80 s. Scanning electron microscopy established that the most homogeneous and uniform Cu-Sn-TiO₂ coatings were formed when pulsed electrolysis was used.

Intermittent agitation of the sulphuric acid electrolytes led to the formation of ordered multilayer structures consisting of microlayers of the Cu-Sn alloy and copper due to the intermittent elimination of diffusion limitations for the discharge of copper(II) ions when agitation was switched on, which resulted in suppression of the process of the underpotential deposition of tin.

Keywords: Electrocrystallisation, Formation of alloys, Composite coating, Pulsed electrolysis, Structure

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Research article

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Theoretical and experimental investigation on ADT organic semiconductor in different solvents

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Abstract

The purpose of this work is to investigate experimental and theoretical methods for the properties of (ADTs) organic semiconductors. The effect of solvent on optical and electrical on Anthradithiophene (ADT) characteristics was investigated. The optoelectronic properties associated with experimental work consists of bandgap energy, Tauc plot, transparency, electrical and optical conductance and dielectric properties calculated. For theoretical calculations, firstly, HOMO and LUMO have been used for the computation of the bandgap energy. The average bandgap energy between HOMO and LUMO is found to be 2.84 eV by using five basis sets in gas phases. After that, the FTIR has been elucidated. In addition, to determine the functional group, and determined the important region did not take place absorption. In general, this region did not occur absorption which is around between 1650 cm⁻¹ and 3200 cm⁻¹ by using five basis sets. The UV-Vis spectroscopy was elucidated. Furthermore, to determine the energy band-gap, the average energy band gap was found to be 2.59 eV, and it was determined the correct transition type. The ADT molecule exhibited the indirect allowed transition.

Keywords: UV-visible spectroscopy, FTIR, HOMO, LUMO, HF and DFT

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Research article

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Preparation and characterization of Ge-Ni-Te nanocomposite

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Abstract

Ni_xGe_{50-x}Te₅₀ with x = 2, 4, 6, 8, 10, 15 and 20 at% ternary nanocomposite prepared using multistage solid-state direct reaction. Nanocrystalline nature was studied by X-ray powder diffraction, results revealed that, the main phase is rhombohedral GeTe polymorph, and the second major phase is hexagonal Ni₃GeTe₂. The calculated average crystallite size of the whole constituents in prepared samples is within the range of 47.3–83.8 nm. Optical properties evaluated from diffuse reflection measurements and the calculated bandgap of all samples are nonmonotonically changes with Ni content from 1.45 to 1.62 eV with the direct allowed transition.

Keywords: Ni-Ge-Te, Nanocomposite, Structural and optical properties, Diamagnetic

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Research article

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Growth of InGaAsSb/GaSb compound for infrared optoelectronic devices

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Abstract

In this study, we report on the synthesis of InGaAsSb epi-layer for optoelectronic devices in short infrared wavelengths (SWIR) at room temperature (RT).

The InGaAsSb with lattice matched to GaSb substrate was grown by the molecular beam epitaxy (MBE) using the strain engineering. The structural and optical properties of InGaAsSb layer was investigated by high resolution X-ray diffractometer (XRD), and photoluminescence (PL). Devices with a 400×400 μm of size were fabricated using traditional photolithography and inductively coupled plasma etching. The spectral response of InGaAsSb photodetector with a 90% cutoff wavelength and electroluminescence spectra of light emitting diode (LED) obtained at 2.38 μm at an applied bias of –0.1 V and 2.25 μm with $I_{ic} = 500$ mA, respectively at room temperature. Also, the spectral response of the detector indicates an increasing intensity and low noise when the temperature is high.

Keywords: InGaAsSb; MBE, Optoelectronic device, SWIR

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Research article

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Kinetics of the cathodic evolution of hydrogen on alloys of the $Mo_xW_{1-x}Si_2$ system in an alkaline electrolyte

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Abstract

The kinetics and mechanism of the hydrogen evolution reaction on alloys of the $Mo_xW_{1-x}Si_2$ system ($x = 1.0; 0.68; 0.41; 0$) in a 1.0 M NaOH solution have been studied by the methods of polarization and impedance measurements. The cathodic polarization curves of silicides were characterized by the Tafel plots with constants a and b , equal to 0.47–0.49 and 0.068–0.076 V, respectively. The impedance spectra of $Mo_xW_{1-x}Si_2$ electrodes in the Tafel region are a combination of a capacitive semicircle with a displaced centre at high frequencies and an inductive arc at low frequencies. In the region of the highest frequencies on the impedance plots a straight-line section with a slope slightly higher than 45° was recorded, indicating the presence of pores in the surface layer of the electrodes.

To describe the hydrogen evolution reaction on silicides an equivalent electrical circuit was used, the Faraday impedance of which consisted of series-connected charge transfer resistance R_1 and a parallel R_2C_2 -chain (at $R_2 < 0$, $C_2 < 0$), which corresponded to the atomic hydrogen adsorption on the electrode surface. The impedance of the double layer capacitance was modelled by the constant phase element CPE_1 .

The results of polarization and impedance measurements for the investigated silicides were in satisfactory agreement with the discharge – electrochemical desorption mechanism, in which both stages are irreversible and have unequal transfer coefficients. The limiting stage is the electrochemical desorption. The Langmuir isotherm for adsorbed atomic hydrogen was fulfilled. It was concluded that $Mo_xW_{1-x}Si_2$ alloys in an alkaline electrolyte are promising electrode materials that are active in the electrolytic hydrogen evolution reaction.

Keywords: Molybdenum and tungsten silicides, Hydrogen evolution reaction, Electrocatalysis, Self-propagating high-temperature synthesis

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Research article

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TEM and XPS studies of bio-nanohybrid material based on bacterial ferritin-like protein Dps

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Abstract

The work is related to the research of a biohybrid nanomaterial formed on the basis of protein molecules of bacterial origin recombinant ferritin Dps.

To obtain recombinant protein, *Escherichia coli* cells were used as producers, and purification was carried out chromatographically. The source of iron atoms for the formation of the biohybrid nanomaterial was the Mohr salt. The possibility of the hybrid particles formation, the shape and size of their inorganic core were studied experimentally by high-resolution transmission electron microscopy. The composition and specificity of hybrid particles inorganic core physico-chemical state were studied by X-ray photoelectron spectroscopy, including the use of focused ion etching.

It is shown that using the chosen method of nanomaterial formation, the internal cavities of protein molecules deposited inorganic nanoparticles. The sizes of these nanoparticles formed in hollow protein molecules averaged 2 nm. A complex composition of particles has been established, mainly including oxides of the iron-oxygen system. Inclusions of metallic iron are also possible.

The results obtained show the possibility of smooth properties control of the biohybrid nanomaterial through their composition. This makes it extremely attractive for the implementation of modern technologies tasks such as spintronics or targeted delivery of functional nanoparticles.

Keywords: Nanostructures, Biomolecules, Hybrid materials, Developed surface, Recombinant ferritin-like Dps protein, Transmission electron microscopy, Combination, X-ray photoelectron spectroscopy

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Research article

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Liquid-vapour phase equilibria of three-component systems formed by *n*-propanol, *n*-butanol, and *n*-alkylethanoates

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Abstract

The production of *n*-alcohols and ethanoic acid esters involves solving problems regarding the rectification of solutions of multicomponent systems. The main achievements related to the methods of calculating the phase equilibria in multicomponent systems have been associated with the development of equations based on local compositions. Equilibrium in multicomponent systems is predicted using data about the binary components of these systems. The most common local composition models are the Wilson and NRTL equations. Liquid-vapour equilibria of binary systems formed by aliphatic alcohols and esters of organic acids have been already studied. Liquid-vapour equilibria of the studied binary systems have been described by the Wilson and NRTL equations.

Boiling points (the pressure of saturated vapour) of solutions of three-component systems formed by *n*-propanol, *n*-butanol, *n*-propylethanoate, and *n*-butylethanoate were measured under various pressure values using the ebulliometric method. The activity coefficients of the solution components of the three-component systems were calculated using the Wilson and NRTL equations. The parameter values in the Wilson and NRTL equations for the binary systems were calculated by nonlinear regression methods. The results of the calculations were verified experimentally.

It was found that the values of the activity coefficient of *n*-propanol and *n*-butanol increase with a decrease in their concentrations in the solutions of the systems. Similar changes in the values of the activity coefficients of the components in the solutions of the systems were observed for the molecules of *n*-propylethanoate and *n*-butylethanoate. In the case of solutions of the *n*-butanol – *n*-propylethanoate – *n*-butylethanoate system, there is a predominance of the values of the *n*-propylethanoate activity coefficient. With an increase in the molar mass (molecular sizes) of *n*-alcohol, the values of its activity coefficient in solutions of the systems decrease. The Wilson model more accurately describes the vapour-liquid equilibrium of the solutions of the studied three-component systems. The obtained data are necessary for technological calculations and can be used to further improve the methods for calculating the liquid-vapour equilibrium of multicomponent systems.

Keywords: Liquid-vapour phase equilibria of three-component systems, Wilson and NRTL equations

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