

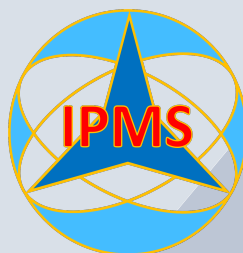


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ADVANCED COMPOSITE MATERIALS

KEYNOTE: Fabrication of B₄C-SiC ceramic composites prepared by ultra-high pressure sintering

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Composite materials based on boron carbide (B₄C) and silicon carbide (SiC) were intensively studied in the past decades because of their high usage potential in structural applications at both low and high temperatures. However, the B₄C and SiC are highly covalent bonding compounds which possess a low self-diffusion coefficient impeding massive grain-boundary movement. These inherent properties induce very poor sinterability, as well as a very high sintering temperature of these materials. To obtain a fully dense pure B₄C-SiC ceramic composite an alternative ultra-high pressure sintering technique is necessary. This process reduces the sintering temperature and simultaneously reduces the sintering time. The objective of this work was to rapidly densify the B₄C-SiC ceramic composites without the usage of sintering additives, by applying the ultra-high pressure (4 GPa) and to investigate the influence of the B₄C and SiC ratio in the initial compounds mixture on the densification behavior, microstructural development and some mechanical properties of the resulting composites. Additive-free boron carbide (B₄C) - silicon carbide (SiC) ceramic composites with different B₄C and β-SiC powders ratio were densified using the high-pressure “anvil-type with hollows” apparatus at 1500 °C under a pressure of 4 GPa for 60 seconds in air. Also starting compounds, B₄C as well as SiC powders were densified by using the same technique in the range of 1500-1900 °C. The effect of starting powders ratio on the composites sintering behavior, relative density, microstructural development, and thermomechanical properties was studied. The sintered samples hardness was found to be in the range from 24 to 31 GPa. The thermal conductivity measurements, conducted in the temperature range from room temperature to 1000 °C, showed that the thermal diffusivity of sintered samples was between 6 and 9.5 mm²/s whereas the thermal conductivity was in the range from 16 to 28 W/(m·K). The results of this study show that the high-pressure sintering can be a very effective low-temperature densification method for the obtainment of additive-free B₄C - β-SiC ceramic composites. Moreover, the process can be up-scaled for producing large size (16 mm diameter) composites required in various cutting tools and other application in extreme conditions.

KEYNOTE: Nanocomposites: Paths to Perfection of Materials

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Present lecture is about manufacturing of the ceramic nanocomposites through various experimental approaches as a modern art in materials science. In the world of bulk nanomaterials the bound between structure and properties is becoming more meaningful as compared to conventional materials of the same composition. The size effects in properties appear due structure refining down to 20-50 nm. The advanced consolidation methods for manufacturing of ceramic nanocomposites maintaining such a small grain size will be considered in details. The competition between shrinkage and grain growth is the natural phenomenon for these methods and the control over this competition is the main force of the art and the path to perfection of nanomaterials.

The impact of high voltage electric discharge treatment on the properties of Ti - TiC system metal-matrix composites

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Problem statement and objective Properties of metal-matrix composites (MMC), obtained by powder metallurgy, are largely dependent both on the method of powder mixture preparation and on the technology of their consolidation. Technology of the preparation of powder mixtures for MMC by their treatment with high voltage electric discharge (HVED) in hydrocarbon liquid was developed at the Institute of Pulse Processes and Technologies of NASU. In order to preserve disperse structure and phase composition of the powder mixture in the consolidated MMC, method of spark plasma sintering (SPS) was used. The objective of the present study is the research of the impact of HVED treatment and subsequent SPS on the properties of Ti - TiC system MMC. Methods Studies were performed by experimental treatment of Ti - TiC powder system in hydrocarbon liquid, subsequent consolidation of MMC specimens from treated powders and determination of their composition, structure, hardness and wear resistance. Two different types of electrode systems, namely "point - plane" (P - P) and "3 points - plane" (3P - P), were used. Ti - TiC system MMC were consolidated using SPS with the temperature of 1100 °C and holding time of 180 s. Main results and Conclusions The consolidation of Ti - TiC powder mixture after HVED treatment in kerosene with specific energy of $W_s=20$ MJ/kg and P - P electrode system allows increasing TiC content from 21 % up to 87 %, which indicates the presence of residual carbon, that enters carbidization reactions with TiC particles during the consolidation. The consolidation of Ti - TiC powder mixture after HVED treatment in ethanol with $W_s=20$ MJ/kg using P - P electrode leads to ~ 2 times TiC content increase. The use of 3P - P electrode system for HVED treatment of Ti powder in kerosene does not lead to increase of TiC content after consolidation. This allows increasing wear resistance from 1.39 m/mg to 1.7 m/mg as well as increasing hardness from 3.6 GPa to 4.8 GPa.

Investigation of the wear resistance of instrumental composites based on a hybrid organic-inorganic polymer binder in the processing of super alloys

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Hybrid organic-inorganic oligomeric systems are perspective materials for the manufacture of abrasive composites filled with cubic boron nitride (CBN). The aim of the paper was to investigate the application of the developed hybrid organic-inorganic composite materials based on organic complexes of polyphenylene with vanadium, iron and copper for creating grinding tool for processing samples of nickel super alloys. The materials developed by us contained layers of graphene and graphane grown as part of polymer structure. The conditions for obtaining the materials were selected for achieving the maximum content and the maximum degree of ordering of graphene-graphane layers in the material. To create the tool, cubic boron nitride powders were used, which were introduced into the material before polymerization at a concentration of 25% vol. Studies of the process of obtaining the material made it possible to optimize the composites according to the criterion of the specific consumption of CBN and showed a high level of durability of bonds in an optimal design. With a change in the temperature and pressure of polymerization of instrumental composites based on hybrid polymers, it was possible to reduce the consumption of cubic boron nitride. The parameters at which the minimum consumption of the abrasive material was achieved are close to those at which the maximum amount of graphene-graphane layers and the maximum degree of their ordering are achieved. It is possible to formulate a regularity that with an increase in the content of graphene and graphane structures in a grinding tool based on the developed bonds by 1.1-1.2 times, the consumption of cubic boron nitride decreases by 2.3-3.5 times. A qualitative relationship between the durability of retention of grains of abrasive material and the number of free volume elements in the composite material was also shown.

Peculiarities creation of glass-metal composites with superhard materials adhesive-active to metal and polymeric binders for abrasive-cutting tools production

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Creating abrasive-containing glass-metal composite materials for tooling based on superhard materials (SHM) powders seek to development coatings that play the role of a transition layer between the grains of the abrasive and the abrasive layer binder of the tool, and have high adhesion both to the surface of the abrasive, and to the binder, helping to increase the strength of the abrasive grains fixing in the tool matrix, and accordingly increase its wear resistance in the viscous materials processing, especially without the lubricating and cooling fluids. The glass-metal tool composites from SHM with high performance characteristics were developed. Technology for applying of glass coating SHM with metal and polymer coatings in the form of thin films to increase adhesion in the SHM system with glass coating-binders for tool making were developed. It increases the strength of diamonds and cBN in binder and reduces the tool wear of viscous materials. A study of the peculiarities of the interfacial boundary formation between cubonite-glass aggregates with metal (Ti, Ni, Cu) coatings and metal binders were shown that the mutual diffusion occurs at the contact boundary at $T_{sint} = 600\text{ }^{\circ}\text{C}$ leads to glass-metal unit - binder system with the formation of intermetallics and new crystalline phase of aluminum silicate. This increases the adhesion at the interface and ensures a strong fixation of both the metal coating on the glass unit and the glass unit itself in the metal binder. The developed glass-metal composites provide increase in wear resistance of circles on a metal binder at grinding of difficult-to-process materials without cooling in 3.2 times and in 5 times in comparison with serial analogs (without a covering) by increasing the strength of the units and increase the adhesion at the interface of the coating with the binder.

Influence of the manufacturing technology of metal-ceramic WC-8%Co on its physical and mechanical properties

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A comparative study of the effect of the method of manufacturing metal-ceramic WC 8%Co on its properties is performed. Samples were made using three technologies. The initial powder mixture was the same in all cases. The first technology is a uniaxial pressing and sintering in vacuum. The second technology is a uniaxial pressing, vacuum sintering and thermocompression treatment (TCT). The third technology is a uniaxial pressing, cold isostatic pressing (CIP) with a pressure of 0.2 GPa and sintering in vacuum. Then after sintering, grinded and polished samples were measured for density, coercive force, the structure was studied using SEM and XRD, residual stresses were measured, and the three-point bending strength and Rockwell hardness were measured. The study of the structure showed that the average WC grain size in the samples that passed CIP is 0.292 μm , in the samples that passed TCT is 1.396 μm , and in the samples without additional processing is 1.315 μm . The measurement of residual stresses showed that in the samples that passed CIP, compressive stresses are present in WC and in Co, and in the samples that passed TCT, they are both in WC and in Co are tensile. It was found that the hardness of the samples that passed the preliminary CIP treatment is 92 HV100, the samples that passed TCT is 87 HV100, and the samples without additional treatment are 88 HV100. It is also established that the strength of samples that have passed preliminary CIP is 2040 MPa, samples that have passed TCT is 2090 MPa, samples without additional processing is 1880 MPa. During the analysis of the obtained results, information about the relationship between mechanical properties and structure from previously published experimental works about the effect of high isostatic pressure on the destruction of single crystals and the crushing of large single-crystal WC particles during quasi-isostatic compression of the powder during CIP was used [1, 2].

Obtaining composite powders for WC-Ni for manufacture of hard alloys

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The development of superhard ballistic products from frame metal-ceramic composites by using nickel-plated tungsten carbide powders to improve the structure and complex physical and mechanical characteristics of sintered composites, which is ensured by uniform distribution of metal bonds is a promising and relevant approach. The use of mechanical mixtures of hard alloys has certain disadvantages associated with both the high cost of the latter and the uneven distribution of alloying elements during mechanical mixing. The aim of this work is to study the modes of the plating process on the physical and technological characteristics of nickel-plated tungsten carbide powders. The process of obtaining nickel coatings on tungsten and tungsten carbide particles using acidic and alkaline media has been studied. It is established that when carrying out the process in an acidic environment where the supplier of nickel is nickel sulfate, the optimal pH value in the working bath should be in the range of pH = 4.0-4.5 and can be correlated by adding 2% sodium hydroxide solution. Studies have shown that the nickel plating reaction should be carried out in a narrow temperature range equal to 90-92 °C. A study of the process of obtaining nickel coatings using an alkaline medium, which was provided by adding to the working solution 25% ammonia solution in a working solution containing nickel chloride (as a source of nickel). The particle size distribution of the clad powder was studied, which showed the difference in the coating thickness on the tungsten powder particles. This is due to the fact that the uniformity of the deposition of the coating depends on the shape and morphology of the original tungsten particles. In this case, as shown by metallographic studies, almost all particles are covered with a layer of nickel with a thickness of 8-12 μm, which confirms the spectral chemical analysis of clad powders. Acknowledgements This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0108).

Effect of cobalt additive on boron carbide matrix ceramics phase (B4C, ZrB2, W2B5) formation process

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Development of methods of introducing of WC-Co or metallic Co nanoparticles into the boron carbide matrix to improve material physical-mechanical properties is an actual problem. Work aims to compare processes of low-temperature synthesis of B4C-ZrB2-W2B5 and B4C-ZrB2-W2B5-Co matrix ceramic components. Usually, ceramics of similar composition are obtained by high-temperature (>1600°C) synthesis. Here, ultrafine powders of B4C-ZrB2-W2B5 and B4C-ZrB2-W2B5-Co were synthesized in two stages: low temperature pyrolysis of initial compound at 600°C and thermal treatment of preceramic precursors to form intermediate (WC-Co, WO₃, a-C) and basic phases (B4C, ZrB₂, W₂B₅) at 600-1200°C. The starting compounds were ZrO₂ and ammonium paravolframate-sucrose-a-B. WC-Co phase was obtained from ammonium paratungstate-sucrose-cobalt acetate at >800°C. Full phase formation performed by SPS at 1300, 1500 and 1700°C. During the annealing B4C-ZrB₂-W₂B₅ and B4C-ZrB₂-W₂B₅-Co ceramic precursors the formation of ZrB₂ observed at 800°C, when B4C and W₂B₅ not yet formed. When annealing at 1000°C, the influence of cobalt on main phases formation was clearly visible. Powders containing B4C, ZrB₂, W₂B₅ and WC phases were obtained from cobalt containing precursors. Average content of Co approached 0.79-2.13% (it should be 4.0% in mixture). After annealing of non-cobalt precursors at 1000°C, no B4C or WC forming was observed. No WC phase was visible in XRD pattern, presumably due to overlapping of the components diffraction maxima. However, authors previous studies have established that at this temperature WC is formed from ammonium paratungsten-sucrose system. It can be concluded that the presence of cobalt in the process of obtaining ultrafine powders of multicomponent boron carbide matrix ceramics contributes to the low-temperature formation of B4C and W₂B₅ phases and can be considered as a catalyst for their synthesis.

New method of synthesis of boron carbide matrix ceramics ultra-dispersive powders

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Boron carbide B₄C has unique complex of physical-chemical properties, but it also characterized by low strength and fracture toughness. Overcoming these disadvantages became possible by production boron carbide based matrix ceramics. Addition of some borides TiB₂, ZrB₂ and W₂B₅ are often used to increase sinterability and improve mechanical properties compared to B₄C ceramic. Currently the main method of obtaining B₄C-W₂B₅, B₄C-TiB₂-W₂B₅, B₄C-TiB₂-W₂B₅-Co and B₄C-W₂B₅-SiC-Co type matrix ceramic powders is high-temperature synthesis from B₄C, WC, SiC, W, Co and C powders. Previously, authors obtained B₄C, B₄C-TiB₂, B₄C-TiB₂-Co and WC-Co nanocomposites powders from liquid charge. But, there is no information on obtaining TiB₂, W₂B₅, and Co containing powders by wet method. Here a new method of synthesis B₄C, TiB₂, W₂B₅ and Co phases in single technological cycle is discussed. Precursors are obtained by pyrolysis of a paste made from ammonium parasulfide, zirconium and titanium oxides, cobalt salts, sucrose and amorphous boron at 200-600°C. By the proposed method it is possible to obtain B₄C, TiB₂, W₂B₅, and Co phases at low temperatures (200-1000°C). So far 1000°C was the lowest temperature, at which the W₂B₅ phase formation was detected. By hot pressing at 1300°C boron carbide matrix ceramic of composition (60-70%)B₄C-30%(ZrB₂-W₂B₅)-2%Co was obtained. WC and Co, the effective growth inhibitors for B₄C grains, are homogeneously distributed. SEM micrographs confirm that particles size was 0.4-1µm in the samples obtained by SPS sintering at 1500°C. When the sintering temperature increases to 1700°C, grains size ranges within 0.5-2µm and they are characterized by more uniform distribution. Maintaining the powders grain size during high-temperature sintering demonstrates the method advantages. Proposed method allows obtaining of multicomponent ultra-dispersive powders for different boron carbide matrix ceramics. The ratio between phases can vary over wide limits.

Metal-ceramic composites based on reinforced ceramics

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Today, the development of materials that would have low diffusion activity during cutting and retain a range of mechanical properties at elevated temperatures (ductility, strength, hardness) is promising. Currently, a huge amount of work is being done on the introduction of high-entropy alloys (HEA) as a matrix phase. As refractory inclusions, instead of tradition carbides we proposed used reinforced carbide or boride ceramics (WC-W₂C and B₄C - TiB₂), which has higher values of hardness and crack resistance in comparison with tungsten carbide. Of particular interest in this regard are the WC-W₂C and B₄C - TiB₂ systems. The composites were sintered by the of spark-plasma sintering (SPS) at temperatures of 1000 - 1600 °C and holding time of 0-30 minutes. The initial mixture of 10-30 wt.% of the matrix phase were used. In order to establish kinetic and thermomechanical compatibility the studies of the microstructure and chemical composition of the phase interface were performed. Thus, metallographic analysis of the obtained composites showed that in the system (B₄C-TiB₂) -HEA intensive interphase interaction begins at 1400 °C and increases significantly at 1500 °C, contributing to the compaction of the formed composite. Instead, in the system with WC-W₂C there is no such critical interaction of HEA components with the refractory component. This correlation is related to the nature of the starting components, boron carbide, which is part of the composite is an excellent donor of boron and carbon, which leads to the active formation of carbide, boride and possibly even carbo-boride phases. In the (B₄C-TiB₂)-Ti system, the formation of a complex hierarchical structure due to the intense interaction of titanium with carbon and boron was observed. As in the case of using HEA, the interaction of the boron carbide phase of the eutectic particles B₄C-TiB₂ leads to the formation of a reinforced boundary, because the titanium boride fibers do not interact with the binder (Ti). Acknowledgements This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0108).

Directionally solidified eutectic alloys based on boron carbide

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Materials based on boron carbide are increasingly used in industry due to its unique complex of physical and mechanical properties. Due to the specific configuration of boron bonds in the crystal structure, B₄C has high values of strength of chemical bonding and as a consequence, high hardness, elastic modulus and melting point. However, a significant drawback of B₄C and materials on its base is high brittleness and low strength. One of the most effective ways to improve the strength of the ceramic material is a fiber reinforcement of refractory compounds, which is realized in the directional solidification of eutectic alloys melts of quasi-binary systems B₄C-RC (where RC - TiB₂, ZrB₂, HfB₂, SiC, etc.). The directionally solidified B₄C-based eutectics (B₄C-MeB₂, B₄C-MeB₂-SiC, B₄C-(Ti_xZr_{1-x})B₂) were prepared by the floating zone method based on the crucible-free zone melting of compacted powders. B₄C, SiC and powders of transitional metals diborides with technical purity were used as the initial materials. The microstructure of all as prepared alloys consists of B₄C matrix reinforced by diborides and/or silicon carbide. The formation of eutectic structure and phase compositions of the directionally solidified B₄C-based eutectics were discussed. The Vicker's hardness and fracture toughness of the composites reach 45 GPa and 7 MPa•M^{1/2}, respectively. The bending strength of the eutectic alloys was evaluated in the temperature range of 25-1600 °C. The temperature dependence of the bending strength is associated with the temperature variation of the thermal expansion coefficients and with the increasing plasticity of the phase components. Acknowledgements This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0108).

Phase relations and properties in the CeO₂-La₂O₃-Dy₂O₃ system at 1500 °C

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Materials based on cerium oxides and lanthanides are widely used in high-tech industries. In recent years, cerium dioxide has been used as a protective coating that absorbs UV radiation, as the main component of polishing mixtures and abrasives, in sensor devices that allow to determine the minimum amount of impurities in gas mixtures, solid electrolytes for fuel cells and others. Physico-chemical design of new materials can not be performed without basic fundamental information about the original components and their interaction under different conditions. The state diagram of the CeO₂-La₂O₃-Dy₂O₃ system is a physicochemical basis for the creation of materials for structural and functional purposes. Present work is about phase equilibria in the ternary CeO₂-La₂O₃-Dy₂O₃ systems at 1500 °C in air in the whole concentration range. X-ray diffraction, petrography and electron microprobe X-ray diffraction were used to determine phase contents. The microstructures of the sintered ceramic samples were examined by using the scanning electron microscopy (SEM). To study the phase equilibria in the CeO₂-La₂O₃-Dy₂O₃ system, the following experimental parameters were selected to elucidate location of the three lines: La₂O₃ - (50 mol % CeO₂ - 50 mol % Dy₂O₃), CeO₂ - (50 mol % La₂O₃-50 mol % Dy₂O₃) and Dy₂O₃ - (50 mol % CeO₂ - 50 mol. % La₂O₃). It was established that in the system there exist fields of solid solutions based on hexagonal (A) modification of La₂O₃ and cubic with fluorite-type structure (F) modification CeO₂, cubic (C) modification Dy₂O₃ and monoclinic (B) modification Ln₂O₃. The cubic ceria-based solid solution has a fluorite-type structure and homogeneity field shows the maximum extension. It forms solid solutions of substitution type with phases of binary systems. The systematic study that covered whole composition range excluded formation of new phases.

Creation full-composite fuel tanks for launch vehicles cryogenic propellants

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The development of rocket and space technology is possible only with the creation of competitive means of launching a payload. They must meet modern requirements for energy and economic performance. Reducing the launch mass of disposable launch vehicles with payloads or using reusable space transport systems can improve energy performance, reduce economic costs and ensure competitiveness. The use of materials with the highest specific strength values minimizes the weight of fuel tanks, main lines and pressurized cylinders. Currently, carbon plastics based on high-strength carbon fibers provide the maximum value of the specific strength. The use of high-strength carbon fibers makes it possible to significantly reduce the thickness of the power shell of the fuel tank, but due to the peculiarities of the layered structure of the composites, the problem of ensuring the tightness of the thin-walled shell. This is especially important when operating in cryogenic environments under cyclic loading. The most rational solution is the creation of a without liner fuel tank, in which the tightness is ensured by the binder, on account of the implementation of multiple overlapping of the composite layers. To confirm the efficiency of using new materials, technologies and design features of the fuel tank, a number of unique tests were carried out. The study of full-scale structures was carried out during tests with excess water pressure and in a liquid nitrogen environment. At the same time, deformations and changes in the geometric parameters of the structure were recorded at characteristic points. As a result of the research, new scientific results were obtained in the direction of creating rocket and space technology from composites with high mass perfection. During the development and manufacture, a number of unique design solutions for a full composite without liner fuel tank, including those with a small pole hole, which have no analogues in the world, were implemented.

Influence of carbon nanostructures on the mechanical characteristics of a composite based on solid polymers for 3D printing technology (FDM)

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This paper presents the results of the technology for creating 3D products by 3D printing (FDM) from ultra-strong composites based on solid polymers filled with carbon nanostructures (CNS). The paper did not study or apply post-shaping processes to provide 3D printed products with additional performance characteristics or additional properties. Purpose: To study the effect of CNS on the mechanical characteristics of a composite based on hard polymers for 3D printing technology (FDM). In this work, for the synthesis of the carbon nanostructures was used: pyrolytic method, the electric arc method in a gas medium and liquid phase, and the treatment of the synthesis product was carried out using ultrasound, Raman spectroscopy, transmission and scanning electron microscopy and other hard polymer composite analysis methods. Key words: Additive technologies, 3D printing from carbon nanostructures, composite, nanotubes, pyrolysis, electric arc synthesis, polymers, technology FDM. This paper presents the results of the technology for creating 3D products by 3D printing (FDM) from ultra-strong composites based on solid polymers filled with carbon nanostructures (CNS). In this work: 1. Created products by 3D printing from a composite material (hard polymer with carbon nanostructures); 2. 3D products from a composite material (polymer and carbon nanostructures) has porosity, which increases with an increase in the concentration of carbon nanostructures in a solid polymer (from 0.05% to 25%); 3. The optimal percentage of carbon nanostructures (CNS) in solid polymers is about 15%, which allows 3D products to acquire the maximum mechanical compressive strength; 4. It was found that the mechanical strength of 3D products made of composite material increases in direct proportion to the increase in the dispersion of carbon nanostructures that were used in the manufacture of the working composite.

Influence of carbon nanostructures on the electrical conductivity of ceramics (Al₂O₃) for 3D printing technology (CJP)

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One of the promising areas of materials science is the formation of various composites containing carbon nanotubes (CNTs) in order to increase their thermal and electrical conductivity, as well as strength and tribological characteristics. Main purpose: Creation of electrically conductive ceramics and study of the effect of carbon nanostructures on the electrical conductivity of ceramics (Al₂O₃) using 3D printing technology (CJP). In this work, for the synthesis of the carbon nanostructures was used: pyrolytic method, the electric arc method in a gas medium and liquid phase, and the treatment of the synthesis product was carried out using ultrasound, Raman spectroscopy, transmission and scanning electron microscopy and other ceramic composite analysis methods. Key words: Additive technologies, 3D printing from carbon nanostructures, composite, nanotubes (NT), pyrolysis, electrical conductive ceramics, Al₂O₃, technology CJP. Carbon-ceramic composites were obtained by mechanical mixing (in a planetary ball mill) powders of Al₂O₃ and CNTs in different weight proportions (1%, 2%, 3%, 4% and 5% of the CNT mass), and by the synthesis of CNTs in the bulk of the Al₂O₃ powder, which ensured a more uniform distribution of the tubes in the bulk. Such carbon-ceramic composites are well suited for use in CJP 3D printing technology. At a low CNTs content (1-2wt.%) In the composite, the specific electrical conductivity practically does not change and is about 5×10^{-8} siemens/centimeter (S/cm). An increase in the content of NTs to 5 wt.% leads to a sharp increase in specific electrical conductivity up to 3×10^{-4} S/cm. Conclusions: Using the CJP 3D printing technology, a ceramic material was obtained, into which CNTs were introduced, which increased the electrical conductivity of Al₂O₃ by more than 4 orders of magnitude. A sharp rise in the bending strength of the sintered specimen was also recorded, depending on the amount of CNTs in the composite.

Influence of nickel boride and titanium diboride additives on corrosion properties of chromium carbide steels

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The corrosion resistance of carbide steels largely depends on the chromium content in the solid solution of ferrite or austenite. It is known that the corrosion resistance and scale resistance of steels is provided only when the solid solution contains at least 7.5–8% Cr. Corrosion media for the study were selected based on the corrosion resistance of the source components of materials and possible areas of their application. The corrosion resistance of materials alloyed with nickel boride and titanium boride (65Fe-35FKh800 - 3,5-8,7 Ni₃B and 65Fe-35FKh800-0,38-2,2TiB₂) in 3% NaCl solution, 30% NaOH solution and 20% HNO₃ solution at room temperature was investigated by the accelerated method. The highest corrosion resistance was shown by materials alloyed with 5.2 and 6.9 (% wt.) nickel boride, in 30% NaOH solution. The results can be explained by the increased density of samples of these materials, which is 7.3-7.4 g/cm³, as well as the fact that nickel, as an austenitic element increases the solubility of carbon (chromium carbides) in austenite, which leads to an increase in chromium content in solid solution and improves the corrosion resistance of the alloy. Corrosion resistance of carbide steels alloyed with nickel boride in 20% HNO₃ solution, and in 3% NaCl solution corresponds to 4-5 points (stable). By increasing the amount of TiB₂ additives from 1.48 to 2.2 (% wt.) significantly improves the corrosion resistance of materials in 30% NaOH and 20% HNO₃. Samples with 1.48 and 2.2 (% wt.) TiB₂ with 1-point resistance (completely stable) have the best corrosion resistance in 30% NaOH solution. The 2% of Ti in the composites alloyed with TiB₂ dissolves in austenite and ferrite increases the corrosion resistance of carbide steel. This has been confirmed by the results of local X-ray spectral analysis.

Study of the physical and mechanical properties of aluminum matrix composites hardened with nano-quasicrystals

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The main aim of the study was to obtain composite materials based on aluminum alloys of the Al-Fe-Cr system using nanocrystalline hardening particles obtained by powder metallurgy technology. To studying the structure of the composites, we used the methods of optical and electron microscopy, as well as X-ray spectral and X-ray phase analysis. Mechanical properties were determined by standard tensile and indentation test methods in the temperature range 20-300 °C. The most promising aluminum matrix composites were Al₉₄Fe_{2.5}Cr_{2.5}Ti_{0.7}Zr_{0.3} alloys (nanos-structured Al matrix reinforced with nanocrystalline particles), Al₉₄Fe₂Cr₂Ti₂ (the same matrix hardened with nanocrystalline particles and intermetallic particles). To compare the hardening effect, the Al₉₄Fe_{4.1}Cr_{1.3}Zr_{0.6} alloy was chosen, in which the Al matrix is hardened only by intermetallic compounds within the same percentage. It is known that if the hardening particles are in a crystalline state, then the content of such particles in the composite should not exceed 20%, since an increase in the content of particles leads to embrittlement of the alloy. Hardening of alumomatrix materials with nano-quasicrystals makes it possible to increase the percentage of particles up to 40%. Herewith increase the strength and maintains sufficient plasticity at 20 °C. For the first time the expediency of hardening with nanoparticles with insignificant additions of intermetallic compounds is shown in this study. The physical nature of the increase in the plasticity of aluminum-matrix alloys by nanosized quasicrystals is due to the phase transition of the surface layers of these particles into the crystalline phase. Composites with increased strength up to 330 MPa at 300 °C and plasticity range of 8-10% at room temperature were obtained by extrusion.

Influence of the reinforcing component of experimental inserts made of a composite diamond-containing material on the characteristics of the products of destruction of rocks

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The efficiency and wear intensity of a diamond-bearing tool for the destruction of rocks, with inserts made of composite diamond-containing material (CDM) is ensured by the use of high-strength heat-resistant diamond powders and appropriate bonds. The aim of the present work is to study the dependences of the influence of the degree of reinforcement of the working surface of the insert with diamond powder in elements with CDM on a metal bond (Ni 94.0% -Sn 6.0%) on the characteristics of rock fracture products. The results of the study of the influence of the CDM structure obtained by the method of resistive electric sintering under pressure up to 400 MPa on the intensity of its wear during turning of the sandstone of the Torez deposit are presented. The sludge was investigated by the granulometric method, the chemical-gravimetric method, the X-ray fluorescence spectrometry method, the magnetic fractional analysis, the system-analog method. It was found that a decrease in the size and concentration of grains of the reinforcing component leads to a decrease in the average particle size of the sludge. The sludge contains elements: Si, Cl, K, Ca, Ti, Fe, Ni, Zn, Sn, Zr. The total content of Ni and Sn ranges from 0.048 to 0.741 vol.%. Specific magnetic susceptibility of sludge varies within $(1.81-72.57) \cdot 10^{-8} \text{ m}^3 / \text{kg}$. The effect of changes in the concentration and grain size of the reinforcing component correlates with changes in the magnetofractional and elemental composition and the intensity of bond wear. Thus, the wear rate of CDM can be determined as the ratio of the insert mass loss relative to the cutting path length, and as the ratio of the content of binder particles (taking into account the change in the chemical composition of the cuttings) to the mass of the formed cuttings. This fact makes it possible to evaluate the wear resistance of a composite diamond-containing material directly with varying degrees of reinforcement of its working surface.

Synthesis and properties of MgH₂-based nanocomposites

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MgH₂-based nanocomposites were synthesized by the reactive ball milling using 3-5 wt.% of various catalytic additives (TiO₂, TiN, ZrN, ZrVN_x and carbon nanotubes). The starting components for the preparation of hydride nanocomposites were magnesium powder, nanopowders of oxides, nitrides and hydrides of subnitrides. After desorption of hydrogen from the hydride composites, they were rehydrogenated at 1 MPa H₂ pressure and 150...300 °C temperatures. It has been shown that the TiO₂, TiN, ZrN, ZrVN_x additives facilitate the hydrogenation of magnesium during grinding and significantly improve further hydrogen absorption and desorption kinetics. The influence of the above-mentioned additives on the hydrolysis of MgH₂ as materials for hydrogen generation has been studied. This hydrogen producing method is of great interest as an environmentally friendly and safe technology, which is especially important for the development of portable power supply systems. In such systems the hydrogen is used to power the fuel cell. The synthesized nanocomposites were tested by hydrolysis in pure water. It has been shown that the reactive ball milling of Mg with nanoadditives improves the rate of hydrolysis reaction and hydrogen yield. However, this reaction is rapidly interrupted by passivation (formation of a layer of magnesium hydroxide). Therefore, hydrolysis in aqueous solutions with the addition of metal chlorides and in citric acid was also investigated. In such solutions, the degree of MgH₂ conversion is significantly improved. The efficiency of mechanochemical grinding with the addition of various catalysts for the hydrolysis of MgH₂ will be the subject of detailed analysis.

Effect of heat treatment on the properties of a hydrothermal powder 90 (wt.%) Al₂O₃ – 10 (wt.%) ZrO₂ (Y₂O₃, CeO₂)

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ZTA-ceramics belongs to the disperse-toughened materials where α -Al₂O₃ - matrix is toughened by pure ZrO₂-particles, or ZrO₂-based solid solutions. The introduction of ZrO₂-based solid solutions particles, complex stabilized with Y₂O₃ and CeO₂, into a brittle α -Al₂O₃ matrix allows changing the toughness characteristics of ZTA-composites. ZTA-composites are promising for the creation of materials for various purposes: structural, functional and medical. It is known that the microstructure and properties of ZTA-composites are largely determined by the characteristics of the starting powders. Nanocrystalline ZTA-powder with a 10% (wt.) ZrO₂ (Y₂O₃, CeO₂) was obtained by hydrothermal synthesis in an alkaline medium. To study the change patterns of physicochemical properties, the obtained powder was heat treated in the range of 400–1450 °C with a 2-hour exposure at each temperature. According to XRD, in the process of heat treatment, phase transformations of ZrO₂-based solid solutions and boehmite occur according to the following schemes: F-ZrO₂ → F-ZrO₂ + T-ZrO₂ → T-ZrO₂; γ -AlO(OH) → γ + δ -Al₂O₃ → δ -Al₂O₃ → Θ -Al₂O₃ → α -Al₂O₃. The formation of γ -Al₂O₃ from boehmite is accompanied by decreasing in the size of primary Al₂O₃ particles by almost three times (from 15nm to 5 nm). The increasing of primary Al₂O₃ particles accelerates during the phase transformation: δ -Al₂O₃ → Θ -Al₂O₃ → α -Al₂O₃, and almost does not change after its completion. The growth of primary ZrO₂ particles begins after the completion of the phase transformation F-ZrO₂ → T-ZrO₂. In the process of thermal treatment, the effect of topochemical memory of ceramics appeared: the powder morphology varies topologically continuously. General changes regularities of physicochemical properties of nanocrystalline powders with different composition in the Al₂O₃-ZrO₂ (Y₂O₃, CeO₂) system open the ways to create materials with required microstructure and complex properties at a fairly low (1450 °C) sintering temperature.

Boroncarbide- and aluminum-dodecaboride- based lightweight composite materials with enhanced characteristics

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The actual scientific and technical problem connected with establishment of regularities of structure formation of refractory-borides-based composite materials on (a-AlB₁₂, AlB₁₂C₂, AlB₁₂C₂-TiB₂, B₄C, B₄C-SiC) in thermobaric conditions (30 MPa and 2 GPa, in the temperature range 1200-2200 °C) has been solved, resulting in the development of new lightweight impact-resistant materials for personal protective equipment, protection of helicopters and aircrafts, where the weight of protective elements is one of the determining factors, as well as structural ceramics for nuclear power plants, abrasive nozzles, ceramic bearings, friction pairs operating in aggressive environments, etc. The study of the regularities of C, TiC and SiC additives influence on the structure and properties of materials based on a-AlB₁₂ and B₄C allowed to create composites with mechanical characteristics that exceed or are at the level of hot-pressed boron carbide, with following compositions:(1) B₄C-22 wt.% SiC (with approximate stoichiometry B_{3.64}C_{Si0.01} of matrix phase and SiC_{1.07} of inclusions) specific density $\rho = 2.63 \text{ g/cm}^3$, with Vickers microhardness HV (49 N) = $34.6 \pm 0.5 \text{ GPa}$, fracture toughness K_{1c} (49 N) = $5.4 \text{ MPa}\cdot\text{m}^{1/2}$, K_{1c} (with three-point bending) = $7.4 \text{ MPa}\cdot\text{m}^{1/2}$, bending strength R_{bm} = 474 MPa, compressive strength R_{cm} = 1878 MPa and ultimate tensile strength R_m = 386 MPa, logarithmic decrement L = 1,45 % and Young's modulus E = 521 MPa; (2) AlB₁₂C₂-22 wt.% TiB₂-4 wt.% Al₂O₃ (with approximate stoichiometry Al_{0.17}B_{4.55}C₂O_{0.04}N_{0.21} - matrix phase and TiB_{2.58}C_{0.8}Al_{0.02} and Al₂O_{3.79}B_{2.04}C_{0.8} inclusions) with $\rho = 3.2 \text{ g/cm}^3$, HV (49 N) = $37.7 \pm 6.7 \text{ GPa}$, K_{1c} (49 N) = $6.9 \pm 0.6 \text{ MPa}\cdot\text{m}^{1/2}$, K_{1c} (by three-point bending) = $6.1 \text{ MPa}\cdot\text{m}^{1/2}$, R_{bm} = 646 MPa, R_{cm} = 1143 MPa, R_m = 515 MPa, L = 1,44 % and with Young's modulus E = 509 MPa. A high level of mechanical properties was achieved due to the formation of solid solutions. This work is supported by the NATO SPS Programme, Project G5773.

Composite ceramics for ZrO₂-based thermal barrier coatings

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The creation of new materials for thermal barrier coatings for hot zones of gas turbine engines, in particular blades, is an urgent task of modern materials science. ZrO₂-based materials stabilized with REE oxide mixtures are expected to have higher operating temperatures (up to 1300 °C) and lower thermal conductivity due to a more defective coating material structure. In addition, doping ZrO₂ with a mixture of REE oxides should increase the heat resistance of coatings. The forecast of the phase diagrams of Y₂O₃ - Ln₂O₃ systems, where Ln = Tb - Lu, and LnI₂O₃ - LnII₂O₃, where Ln = Tb - Lu, indicates the expected complete solubility of the components of binary systems in the liquid and solid states. Below 1850 °C regions of solid solutions of cubic C-structure are formed in the whole range of concentrations in the systems. To study the effect of HCS content on the stabilization of zirconium dioxide, a concentrate of rare-earth elements oxides of the yttrium subgroup with composition, % (wt.): 13.3 Y₂O₃; 1.22 Tb₄O₇, 33.2 Dy₂O₃; 8.9 Ho₂O₃; 21.8 Er₂O₃; 1.86 Tm₂O₃; 12.5 Yb₂O₃; 0.57 Lu₂O₃; the total content of other oxides is 6.65 (including 3.2 Al₂O₃), as well as zirconium oxide powder of monoclinic modification (M-ZrO₂) of pure grade CRO-1 were used. The samples were formed with the addition of 5% aqueous solution of polyvinyl alcohol by uniaxial double-sided pressing in steel molds on a hydraulic press grade P-125 and annealed at a temperature of 1600 °C for 2 hours. The test mixtures contained 10, 20, 30 and 40 wt.% of HCS. According to the results of X-ray diffraction, the phase diagram element of the system ZrO₂ - heavy complex stabilizers was constructed. The obtained diagram shows that the optimal composition of targets for TBC deposition is the composition ZrO₂ + 30 wt.% HCS, located at the boundary of the M + T- and T-phase regions. As the content of HCS increases, traces of the δ-phase, the Zr₃Y₄O₁₂ superstructure, appear.

Promising composite material based on Ti-Si-C for SOFC interconnect application

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Modern interconnect of solid oxide fuel cell (SOFC) materials are Crofer ferritic stainless steels developed in Germany. Crofer has chromium content up to 25%. Chromium contributes to the degradation of the cell electrodes properties during long-term operation and reduces the overall efficiency of the SOFC stack as result. The work proposes a new solution of the SOFC chromium poisoning problem. The composite material based on Ti-Si-C was synthesized and its properties were studied. The composite powder based on the MAX phase Ti₃SiC₂ was synthesized and the dense material was compacted by spark-plasma sintering (SPS) at different temperatures in a range of 1200-1400 °C and was processed with chemical and thermal treatments that have simulated the SOFC operation conditions. The samples were exposed in hydrogen and air at 700 oC for 3 hours. As result, it was found that the SPS sintering of Ti-Si-C composite material in argon at 1300 oC followed by exposure in hydrogen at 700 oC results in the best combination of mechanical strength $\sigma = 359$ MPa, specific electrical conductivity $\lambda_p = 22.6 \times 10^6$ (Ohm · m)⁻¹ and porosity $\theta = 0.47$ % that meets the requirements for the SOFC interconnect. The thermal expansion coefficient (TEC) in the SOFC operation temperature range from 20 to 800 oC for Ti-Si-C composite material sintered via SPS at 1200 and 1400 oC are equal to 8.5-12 and 9-11 $\times 10^{-6}$ K⁻¹, respectively. These TEC values are very close to the CTE values for the zirconia electrolyte material 8YSZ - 11 $\times 10^{-6}$ K⁻¹ and Crofer APU - 10-12 $\times 10^{-6}$ K⁻¹ widely used in SOFC energy systems. It was found also the Ti-Si-C composite material developed is almost twice lighter than Crofer APU. Please compare their specific densities: $\rho_{\text{Ti-Si-C}} = 4.5$ g/cm³ against $\rho_{\text{Crofer 22APU}} = 7.7$ g/cm³. The obtained data indicate that the Ti-Si-C composite material is promising to be applied in mobile power systems for the aerospace.

Biogenic hydroxyapatite/glass/carbon nanofiber composites for bone tissue engineering

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A lot of various composites with different physical and chemical properties are developing in modern materials science for targeted use in medicine. These are, for example, bioactive calcium phosphate composites based on hydroxyapatite and bioglass, the use of which is aimed primarily for bone tissue treatment. Carbon fibrous nanostructured materials also take a special place in medical practice due to their capillary-porous structure and biocompatibility. The aim of the work is to create composite materials based on hydroxyapatite glass ceramics and carbon nanofibers promising for bone tissue engineering. Carbon nanofibers and hydroxyapatite glass ceramics based biogenic hydroxyapatite were used as starting materials. For composites preparation carbon nanofibers were covered by hydroxyapatite glass ceramics slurry followed by drying and sintering at 800 °C. According to X-ray diffraction data for biogenic hydroxyapatite/glass/carbon nanofiber composites it was established that prepared materials is characterized by the presence of only the hydroxyapatite phase and a slight halo in the region characteristic of carbon nanofibers. The obtained results are in a good agreement with the IR spectroscopy results. Analysis of the IR spectra showed that composites are characterized by absorption bands that are characteristic for hydroxyapatite, sodium boron-silicate glass and carbon nanostructures. The study of the microstructure and morphology of fracture of obtained composites showed the formation of a porous amorphous-crystalline microstructure with a complex specific relief, presence of long tubes of carbon nanofibers with a diameter of several microns and a developed system of micro- and macropores. In general, it was established the preservation of the phase composition and nanostructure of starting materials in biogenic hydroxyapatite/glass/carbon nanofiber composites.

Modelling of processes for creation new porous permeable materials with adjustable properties

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Sustained modern trends in industrial development are increasing requirements for the quality of all types of wares. To receive new porous permeable materials with guaranteed adjustable properties possible with using traditional powder metallurgy technology and it is necessary to predict and control the parameters of their structure in the manufacturing process, which include: granulomere composition of the charge, the form of particles, the density of the molded work piece, the quality of the contacts, the diagram of pressing, porosity, density and their volume distribution. The aim of our research is a decision of the important scientific and applied problem of optimization the technology of manufacturing porous permeable materials with regulated properties from waste of machine-building production on the basis of computer-information technologies for their forecasting and modeling. Methods. However, methods of powder metallurgy do not always ensure the homogeneity of properties within the materials and do not give the opportunity to obtain structural characteristics of materials on a qualitative level increase the efficiency of traditional technologies, and also introduce non-waste production of products of a wide-scale purpose, save energy, increase labor costs and control the parameters of the structure of porous powder materials in the process of their manufacturing possible through modeling with the using of computer-information technologies. Main results and Conclusions. Modeling the properties of porous structures of a concrete PPM from steel powder BBS15 (wastes of industrial production) was carried out in the package of applications MATLAB. According to the method described above, the author of the article developed software in the language C++, that and gave an opportunity to model the process of the radial-isostatic pressing with the set porosity of PPM. The practice of the use of new porous materials based on metal powders shows that realization in full volume of their strength and performance characteristics requires a significant increase in the level of prediction of physical and mechanical properties of materials and the development of new methods of modeling. The patterns of distribution of density along the radius of each layer of PPM at different time of deformation are established. Distribution of porosity is uneven - 0,55 and 0,64. The radial velocity makes it possible to control the distribution of porosity in PPM.

Effect of nano additive on physical and mechanical properties of refractory composite

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The present work investigate alumina cement based refractory composite modified by graphene oxide. For the evaluation of graphene oxide (GO) effect on the hydration kinetic and structure of the composite, the SEM and XRD analyses along with calorimetry measurements were performed. The study included thermal cycling and mechanical testing as well. It was found that the addition of GO changes the hydration of aluminate cement and the structure of cement stone: the peak intensities corresponding to CAH10 hydrates were found to be higher and those of unreacted CA and CA2 - lower, as compared with unmodified samples; the duration of the hydration induction period was shortened and formation of new crystallization centers were observed. The addition of GO effects the physical and mechanical properties of composite: regardless of the heat treatment temperature, which varied from to 110 °C to 1200 °C, the density of the specimens does not change but the compressive strength increases by ~ 4%, thermal shock resistance increases ~2 time.

METALS AND ALLOYS

KEYNOTE: Reaction Synthesis Mechanisms in Binary Metallic Systems under Intense Shock Loading

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Because the strength, toughness and other key engineering properties of heterogeneous materials are strongly dependent on their grain size and density, the quest to achieve simultaneously dense and fine, ultrafine, and nanostructured grain size materials has been one of the most important and difficult challenges in materials science and engineering. In this research we explore novel approaches for producing dense and fine, ultrafine, and nanostructured heterogeneous materials. Typical approaches consist of reaction synthesis, sonochemistry, combustion synthesis and shock wave synthesis followed by dynamic and static consolidation and densification pre and post reaction synthesis. Typical heterogeneous materials covered in this research consist of tungsten heavy alloys, coated graphite powders, metal silicides, aluminides and multiphase, multi microstructural constituent ceramic armor materials. The synthesized and densified materials are fully characterized by OM, SEM, TEM, STEM, EDX analysis, quantitative image analysis, X-Ray diffraction and Mechanical Testing. This paper focuses and discusses the mechanisms of reaction synthesis in binary metallic systems and the effect of reaction and processing parameters on the microstructure and densification of typical materials under intense shock loading.

KEYNOTE: Determination of new plasticity characteristic of alloys in mechanical compression and tension tests, and the influence of structural factors and alloying on plasticity

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In physics and mechanics, plasticity is defined as the ability of a material to irreversible (plastic) deformation. However, the plasticity characteristic corresponding to the scientific definition of this property has been absent for a very long time, and in most cases, the plastic strain at fracture in tensile tests δ is used as a plasticity characteristic. But, δ does not meet the scientific definition of plasticity and the theories of the influence of structural factors and temperature on the δ were not elaborated over many decades, that hindered efforts to control and to increase the plasticity of materials. The plasticity characteristic, corresponding to the scientific definition of this quantity ($\delta^* = \text{plastic strain } \epsilon_p / \text{total strain } \epsilon_t$), was proposed in the article [Yu.V.Milman et al. Acta metal. mater., 1993]. In the present work, a technique for the determination of the plasticity characteristic δ^* in mechanical compression and tensile tests of metallic alloys has been firstly developed. In this case, δ^* is determined more precisely than by indentation, and the second deformation curve $\delta = f(\epsilon_t)$ is constructed. The present work is devoted to the development of the technique for the determination of the plasticity δ^* of metallic alloys in standard mechanical tensile and compression tests and the elaboration of the theory of the dependence of δ^* on the structural factors (grain size, dislocation density, disperse particles of the second phase etc.) and the alloying by the substitutional elements. The deformation curves in tensile and compression tests of four steels with different level of strength and four aluminum alloys with different level of strength were obtained. The discovered correlation of the values of δ^* and δ for steels and for aluminum alloys made it possible to use the developed theory to calculate the influence of the structural factors and alloying on δ for these materials as well.

Phase Diagram of the Al-Cr-Co System

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Alloys of ternary Al systems with Cr and d metals of the VI-VIII groups are promising for practical applications in various fields of modern technology. In particular, the Al-Cr-Co alloys are becoming increasingly important in high-temperature applications where combined oxidation and hot corrosion resistance are required. Information about phase equilibria may serve as a basis for search of new materials. Data on the solidus and liquidus surfaces up to beginning of our investigations were almost absent. The alloys of the Al-Cr-Co system of 19 compositions are prepared from components Al, Cr and Co (purity of 99.995%, 99.93% and 99.9%, respectively) by arc melting. The alloys are investigated in as-cast and annealed at sub-solidus temperatures states by optical microscopy, scanning electron microscopy, electron microprobe analysis, differential thermal analysis and X-ray diffraction techniques. On the basis of the obtained experimental data in the range of 0-70 at.% Al solidus and liquidus surfaces, a melting diagram as their superposition, a Scheil diagram for solidification as well as series of isopleths were constructed for the first time. Solid solutions based on Cr, Co, Cr₅Al₈ (γ_3 and γ_1 phases), CoAl, Co₂Al₅ binary compounds and the ternary compound τ_5 take part in equilibria. The monoclinic ternary compound τ_5 forms by peritectic reaction at 1065 °C. Four invariant four-phase reactions and one invariant three-phase reaction involving liquid take place at 1280, 1175, 1110, 1065 and ~1480 °C, respectively. Series of isopleths demonstrate peculiarities of the phase diagram. Based on experimental data of B. Grushko, W. Kowalski, S.B. Mi. // *J. Alloys Compd.* — 2018. — 739. — P. 280-289) and constitution of the boundary binary systems it was predicted by us that in the range 70-100 at. % Al solid solutions based on Al, binary Al-Cr and Al-Co compounds and four ternary compounds (τ_3 to τ_6) will take part in equilibria with liquid phase.

Constitution of the Liquidus and Solidus Surfaces of the Al-Ti-Cr System in the Range of Compositions 45-100 at.% Al

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Alloys of ternary Al systems with Ti and d metals of the VI-VIII groups are promising for practical application in various fields of modern technology. Addition of a third alloying element, such as Cr, can improve the low temperature ductility and the oxidation resistance. In order to develop new functional materials, an understanding of the phase equilibria in this system is essential. Earlier we studied experimentally the Al-Ti-Cr system at 45 to 75 at.% Al. In this study we represent the liquidus and solidus surfaces at 45-100 at.% Al taking into account the data from new thermodynamic assessment of [V.T. Witusiewicz et al. // J. Alloys Compd. — 2015. — 644. — P. 939-958]. The alloys of the Al-Ti-Cr system of 28 compositions are prepared from components Al, Ti and Cr with purity of 99.995%, 99.8% and 99.93%, respectively by arc melting. The alloys are investigated in as-cast and annealed at subsolidus temperatures states by optical microscopy, scanning electron microscopy, electron microprobe analysis, differential thermal analysis and X-ray diffraction techniques. As a result of the study, it is shown that the solidus surface of the Al-Ti-Cr system in the range of compositions 45-100 at.% Al is formed by 10 single-phase surfaces corresponding to solid solutions based on components, binary compounds and the ternary compound tau. The constituent parts of the surface are also 19 linear surfaces limiting the two-phase volumes as well as 13 isothermal planes. The highest temperature on the solidus surface corresponds to the temperature of congruent melting of pure Cr (1863 °C), the lowest (660.452 °C) — to the temperature of congruent melting of pure Al. The components of the liquidus surface of the Al-Ti-Cr system at 45-100 at.% Al, in accordance with the solidus surface constitution, are 10 primary solidification surfaces. The primary solidification surface of (betaTi, Cr) extends deep into the ternary system to 60 at.% of the aluminum content from the Al-Cr side.

Nanostructured AlNiCoFeCrTiMo high entropy alloy synthesised by mechanical alloying and pressure sintering

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Recently, the development of multicomponent alloys, known as high-entropy alloys (HEAs) with extraordinary properties and applications are of growing attention for researches. HEAs are promising new class of materials and candidates for many potential applications at room temperature as well as at high temperature. High homogeneity and nanocrystalline structure of HEAs can be achieved by mechanical alloying (MA) synthesis with next sintering under pressure at the low temperatures. Equiatomic nanocrystalline AlNiCoFeCrTiMo HEA was synthesised by MA with following sintering under high pressure and characterized by XRD, SEM and mechanical testing. The elemental powders were milled in a planetary ball mill with tungsten carbide grinding media in petrol for 30 hours. The consolidation of synthesised AlNiCoFeCrTiMo HEA powder was carried out at the 900 °C for 30 min at a pressure of 5 GPa using hydraulic press D 0044. From the XRD results it is clear that the alloy formation is completed after 30 h of MA with the formation of bcc supersaturated solid solution with nanoscale structure and tungsten carbide impurities. Significant broadening of the XRD peaks and disappearance of all the peaks of the solid solution except the most intense one has been observed. The XRD patterns of the consolidated MA powder confirm retain of the AlNiCoFeCrTiMo HEA phase composition without any phase transformation. After sintering under pressure, the AlNiCoFeCrTiMo alloy remains in a nanocrystalline state with a crystallite size about 50 nm, and the porosity of the sample doesn't exceed 1 vol. %. The Vickers microhardness and yield strength of the sintered AlNiCoFeCrTiMo alloy are 14.0 GPa and 3.87 GPa, respectively. Sintering under high pressure at a relatively low temperature was found to contribute to the maintenance of the nanostructured state of alloy obtained during MA. Also AlNiCoFeCrTiMo alloy exhibit extremely high Vickers microhardness and yield strength. Acknowledgements This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0108).

Manufacturing of complex-shaped products consisting of several metal-powder elements

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The article's primary purpose is to give a technological assessment of the process of manufacturing complex-shaped parts by means of powder metallurgy. The process is considered in the example of a complex-shaped product consisting of several elements manufactured separately from Fe-C-Cu powder mixture and then combined into a single structure. The joining was carried out by impregnation of porous structural elements with the fusion of copper-containing material. It has been demonstrated that the infiltration process is affected by many factors: porosity of structural elements, wettability of their pore channels, fluid flowability of the infiltrating material and other factors. The research was carried out on the mass products - centrifugal pump stages for oil production. The elements compaction was carried out on hydraulic press at a pressure of 500 MPa, which ensured average density of the parts after sintering up to 7.8-8.4 g/cm³. During sintering and impregnation, various types of defects of the pieces were detected, which were caused by the excessive thickness of the infiltrating material, different density of the walls and insufficient wettability in the connection zones of the elements. The investigations have shown that the method of manufacturing complex components by prefabricating single elements and their subsequent sintering combined with infiltration is feasible. It can be done in a chamber furnace as well as with belt sintering. However, it is necessary to prepare the mould thoroughly before sintering, choose the infiltrating agent carefully, and analyse possible disadvantages.

On the kinetics of isothermal sintering of powder Fe-20% (mas.) Mo

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Formation of intermediate phases during sintering of multi-component powder causes a complex phase and structural inhomogeneity including diffusion pores. This leads to technological problems and determines the relevance of the topics. The features of phase transformation in the powder Fe-20 mas. % Mo during isothermal sintering at 920 °C was studied. The microstructure (SEM (EDS) Selmi 106И) and phase composition (diffractometer Rigaku Ultima IV) were identified. Results. 1. The polymorphic transformation $\alpha\text{-Fe} \rightarrow \gamma\text{-Fe}$ (during heating) and $\gamma\text{-Fe} \rightarrow \alpha\text{-Fe}$ (during saturation of Fe with Mo) causes appearance of an disordered zone of Fe atoms with increased diffusion mobility. This is evidenced by the formation of a wide hill of diffusion X-ray scattering. 2. The mass of the intermediate phases (Fe_7Mo_6 , Fe_3Mo , FeMo) is abnormally rapidly increasing up to 30 minutes exposure. This can be explained by powerful pumping of Fe atoms, caused by the reverse phase transformation $\gamma\text{-Fe} \rightarrow \alpha\text{-Fe}$, from disordered zone of Fe crystals to Mo crystalline pattern. 3. Extreme changes both specific fraction of the phase constituents and the density of the samples during isothermal exposure were shown. 4. At long exposure, the spherical pores formed during 15 min. exposure are completely replaced by crack-like pores generated by effect of Kirkendall - Frenkel and localized at interfaces of $\alpha\text{-Fe}$ with intermediate phases. So the pores are an active constituent of phase transformations as source or stock of vacancies. Crack-like pores to some extent isolate $\alpha\text{-Fe}$ grains from peritectoid constituent and these two structural constituents begin to behave as two isolated subsystem that have little mutual influence. Thus the paradox is discovered: non-equilibrium structure is formed during long-term exposure. Acknowledgements This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0108).

A study of damping capacity in magnesium and Mg-Al alloys

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The low density of magnesium alloys has motivated the development of structural Mg alloys for automobiles, where weight reduction is needed to achieve high fuel efficiency. Polycrystalline magnesium samples with purity 99.9% and 99.95% and alloys Mg-Al systems with 3, 6, 9 wt.% of Al contents were fabricated by casting at cooling rate about 50-70 °C/s. The high damping capacity of pure Mg can usually be ascribed to the extremely low critical resolved shear stress of basal slip (≈ 0.6 MPa) as compared to that of non-basal slip systems (>38 MPa). The aim of the work is to study the damping capacity of Mg with a purity of 99.9% and 99.95% and the Mg-Al system alloys with different aluminum contents using four independent measurement techniques: mechanical spectroscopy (reverse torsional pendulum, dynamic mechanical analysis, electrodynamic resonant vibrations with 500-700 Hz frequency), as well as dissipation of elastic energy in cycles of unloading - loads during tensile tests. This approach made it possible to reveal the various mechanisms (elastic, anelastic and plastic) of the elastic energy absorption depending on the vibration amplitude (from 10^{-6} to 10^{-1}). The relationship between the damping characteristics and the realization of various mechanisms depending on the stresses (magnitudes of vibration amplitudes) for Mg and Mg-Al alloys is established. In particular, for magnesium polycrystals, it was found that dislocation mechanisms of elastic energy absorption prevail in the stress range up to 2.5-2.8 MPa, and above this value, the effect of the twinning mechanism increases and reaches a maximum at stress range of the order of 20 MPa. At the same time, the purity of the metal does not significantly affect these values. The characteristic intervals and the damping value in the Mg-Al system alloys shift to the region of higher stresses and depending on the structural state (the concentration of Al in the solid solution, the presence of the Mg₁₇Al₁₂ phase).

Computer simulation of the temperature field during electron beam heating of porous body

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The temperature field and its gradient are the determining factors of the sintering process. This factor plays a special role in technological processes that use local high-speed heating from point energy sources - electron or laser beam. Earlier we substantiated the application of the finite element method for predicting the specific thermal conductivity of a porous product under conditions of high-speed electron beam heating. The purpose of this work is to calculate the temperature field in a porous product. We used computer simulation by the finite element method of heating the porous product. The computer model is implemented as a non-stationary thermal problem. ANSYS Workbench 2020 Academic edition was used as a calculation environment. We used two geometric schemes: 1) heating of the vertically placed cylindrical porous sample, energy flow to the upper plane of the cylinder; radiation from the side surface to the protective screen and from the upper surface into space; 2) heating a horizontally placed sample rotating about its axis. In both cases, the computation predicts "temperature saturation" - for each power of radiation there is an average temperature of the sample, which does not increase with increasing exposure time. As the porosity of the sample increases, the thermal conductivity decreases, and the values of the temperature gradient increase accordingly. For the heating scheme 1) the temperature field is homogeneous: the maximum temperature is observed in the zone of direct influence of the electron beam. The maximum temperature gradient depends on the porosity and reaches values greater than 100°C/mm. For the heating scheme 2) the temperature field is more complex. It is in constant motion. The maximum temperature is observed on the surface of direct exposure to the electron beam, while minimum temperature - on the surface that has passed the path about 270 ° after direct exposure to the beam. The maximum temperature gradient is about 70°C/mm. Acknowledgements This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0108).

Structures and properties of BCC HEAs formed by 3d- and 4d-metals of IV-VI groups with Ta and Al

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The goal of the present work is to search HEA alloy compositions with low density ($\sim 8 \text{ g/cm}^3$) based on 3d- and 4d-metals, in particular at the expense of Al and Ta additions, suitable for high-temperature applications. 19 alloys were experimentally investigated, $\text{Ti}_{20}\text{V}_{20}\text{Nb}_{20}\text{Cr}_{20}\text{Mo}_{20}$, $\text{Ti}_{33}\text{V}_{27}\text{Nb}_{12}\text{Cr}_{20}\text{Mo}_8$, $\text{Ti}_{20}\text{V}_{20}\text{Nb}_{10}\text{Cr}_{20}\text{Mo}_{20}\text{Ta}_{10}$ and $\text{Ti}_{40}\text{Nb}_{20}\text{Cr}_{25}\text{Mo}_{15}$, as well as the alloys with Al and/or Ta additions. These alloys (HEAs) were produced by arc-melting from pure metals. Aluminium from 15 to 75 at. % or/and tantalum (no more 17 at. %) were added to some of them. As found density of the alloys did not exceed 8.3 g/cm^3 . Temperatures of incipient melting and completion of melting for as-cast and annealed alloys were measured by DTA. The alloys began to melt mainly at 1600-1800 °C and melting intervals were within the range of 50-200 °C. According to full profile analysis of diffractograms after Rietveld, all the alloys contain the mainly BCC phase. Diffraction peaks are sharp in spite of the fact that the SEM microstructure of the HEAs is dendritic and looks as heterophase. Examination of distribution of the components carried out by EDX-grid analysis and study of microstructure in characteristic X-ray radiations establish that the cores of dendrites are enriched with Mo, Nb and Ta and depleted in Ti, V and Cr. Measurements of Vickers hardness for selected alloys were performed in the interval from room temperature to 800 °C. As revealed the temperature of sharp softening caused by diffusion mechanism of deformation was not reach up to 800 °C for the alloys $\text{Ti}_{25}\text{Nb}_{25}\text{Cr}_{25}\text{Mo}_{25}$, $\text{Ti}_{40}\text{Nb}_{20}\text{Cr}_{25}\text{Mo}_{15}$ and $\text{Ti}_{16.7}\text{V}_{16.7}\text{Nb}_{16.7}\text{Ta}_{16.7}\text{Cr}_{16.7}\text{Mo}_{16.7}$. The hardness of all the studied alloys is high (2.7-4.25 GPa at room temperature) and remains quite high even at 800 °C (1.5-2.5 GPa).

Comparison of mechanical characteristics of thin sheet structures made of dispersed-hardened Ni-based alloys produced by brazing and laser welding in vacuum

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The results of a comparison of the mechanical characteristics of integrated ultralight heat-shielding structures made of heat-resistant dispersion-hardened Ni-20Cr-6Al-Ti-Y₂O₃ alloys of increased strength, obtained by brazing using filler powders based on Ni and laser vacuum welding, are presented. Features of the design of heat-insulating elements, which are a cellular (honeycomb) structure, consisting of two plates with a thickness of 0.1 to 0.14 mm, inside which there are fillers, are considered. It has been determined that the small thickness of the plates and the complexity of the design significantly complicate the possibility of a strong connection of such elements and do not allow the use of known methods of diffusion welding or soldering in a vacuum. It is shown that an alternative to known methods can be laser welding, which provides satisfactory structural strength. Local heating at certain points prevents deformation of the parts to be joined during the welding process. The use of a pulsed Nd-Yag laser with a power of 400–500 W, operating in the frequency range of 50–200 Hz, allows welding with and without filler metal. It has been established that the use of filler metal practically does not affect the mechanical properties of the welded joint, however, it significantly reduces the melt zone, while increasing the density of the welded joint. Based on the results obtained, it was concluded that the increase in bond strength is achieved due to the high cleanliness of the vacuum chamber, low vacuum (less than 10–2 Pa), and optimization of the welding process. The use of brazing in vacuum using filler powders makes it possible to obtain high-strength joints, provided that the contacting surfaces have a sufficient area. The ultimate strength of the joint under linear loading is 320 MPa. Acknowledgements This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0108).

Peculiarities of crystalization of Hf-Ru-Rh-Ir alloys

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The Hf-Ru-Rh-Ir system is of interest both from a scientific point of view and regarding the possible use of its alloys as heat-resistant structural materials, ultra-high temperature coatings, in semiconductor technology. In the literature there are no experimental data about this system; the boundary ternary systems were studied by us earlier [1]. Hf-Ru-Rh-Ir alloys of 10 compositions were prepared from components by arc melting and investigated in the as-cast state by electron microprobe analysis, differential thermal analysis and X-ray diffraction technique. It was established that a continuous series of solid solutions between isostructural (CsCl-type) phases based on the compounds HfRu and high-temperature modifications of the Hf(Rh, Ir) (δ phase) exist in the Hf-Ru-Rh-Ir system. Phase equilibria in this system are formed by the above-mentioned δ -phase and solid solutions based on β -hafnium, ruthenium, isostructural rhodium and iridium, as well as based on compounds Hf₂(Rh, Ir) (Ti₂Ni-type, the γ phase), Hf₅Ir₃ (Mn₅Si₃-type, the η phase), Hf₃Rh₅ (Ge₃Rh₅-type, the θ phase) and Hf(Rh, Ir)₃ (AuCu₃-type, the ε phase). As a result of the research of processes occurring during the crystallization of alloys were studied for the first time. The processes are realized along the curves, which are directed from one boundary ternary system to another: $L \leftrightarrow \delta + \gamma$, $L \leftrightarrow \delta + \varepsilon$, $L + \eta \leftrightarrow \delta + \gamma$, $L + \delta \rightleftharpoons \theta + \varepsilon$ and $L + \langle \text{Ir, Rh} \rangle \leftrightarrow \delta + \varepsilon$, which transforms to the $L + \langle \text{Ir, Rh} \rangle + \varepsilon$. 1. Structure and phase constituents of as-cast alloys of the Hf-Ru-Rh-Ir quaternary system / Kriklya L.S., Korniyenko K.Ye., Levchenko P.P., Tikhonova I.B., Samelyuk A.V.// 7th International Samsonov conference «Materials science of refractory compounds» (MSRC-2021). May 25-28, 2021, Kyiv, Ukraine, p. 130.

Storage of hydrogen in a duralumin vessel with metal hydride

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Purpose: Creation of a modern ultra-light high pressure cylinder with increased heat transfer for storage of hydrogen in the metal hydride. After smelting the metal hydride, its Mechano-chemical activation was carried out in a ball mill in a hydrogen atmosphere. After that, the work body was analyzed for hydrogen capacity on hydrogen volumetric installations. **Key words:** Hydrogen materials science, hydrogen energy, hydrogen storage, Metal hydrides, hydrogen, duralumin, alloys. In this work to create a functioning hydrogen storage, a high-pressure cylinder made of duralumin with a capacity of 45 cm³ was made. **Conclusions:** Developed radiator system improves heat exchange with the environment during operation; The hydrogen storage device is machined from duralumin, and this makes it lighter (the cylinder weighs 70 grams compared to 240 grams of a stainless steel cylinder of the same capacity) ; The pressure gauge, in addition to its main function, acts as a safety valve, which increases the safety level of the hydrogen storage; The duralumin cylinder has a high thermal conductivity, which is especially important in the processes of hydrogenation and dehydrogenation of the hydrogen storage.

High Young's modulus magnesium alloy strengthening by icosahedral quasicrystals

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One of the important tasks in the development of magnesium alloy technology is to increase the absolute value of Young's modulus E , which currently does not exceed 44-46 GPa. Despite the huge advantages of commercially available composites such as Mg (Al)/SiC and Mg(Al)/Al₂O₃ used in the automotive and aerospace industries, several disadvantages prevent their widespread use. These include degradation of their properties at high temperature, low tolerance to damages, low resistance to settling and processing difficulties. In addition, the integrity of composites is critically dependent on the wettability between the particles and the matrix. Since, as is known, quasicrystals have a low interfacial energy, because they have a good potential for being used as a strengthening phase in composite materials. It is known that, in addition to high hardness, quasicrystals also have a high Young's modulus; therefore, the use of quasicrystalline nanoparticles to strengthen magnesium ones seem promising. To implement the idea of strengthening the industrial alloy AM50, the Mg₈₀Cd₁₅Ca₅ alloy was chosen, which contains stable icosahedral quasicrystals. According to the data of nanoindentation, the Young's modulus of the quasicrystalline alloy was about 62-70 GPa. It should be noted that, based on the distribution of hardness values over the surface, the alloy is sufficiently homogeneous and the volume fraction of the quasicrystalline phase is significant. Using a quasicrystalline alloy as a master alloy, the AM50 10% Mg₈₀Cd₁₅Ca₅ alloy was prepared by standard casting technology. The results of investigations showed that the average value of Young's modulus of the modified alloy exceeds 50 GPa. In addition, given the mechanical properties comparable to the AM50 alloy, the modified alloy due to the high Young's modulus can be used in die casting technology for producing car parts.

Thermokinetics of titanium oxidation

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The study of the dynamics of high-temperature oxidation of titanium is important both for a specifically enhance the heat resistance of titanium alloys and for the rational use of titanium as an alloying element in heat-resistant nickel and cobalt alloys. Earlier the autocatalytic reaction of decomposition of molecular selenium was investigated. Oxygen, as an analogue of the group with selenium, can also form dissipative structures when interacting with metals. Therefore, the problem of the stability of the protective oxide film is directly related to the problem of the nonlinear interaction of oxygen with transition metals, in particular, with titanium. When constructing thermokinetic model, a synergistic approach was used. Thermokinetics of oxidation was studied experimentally using high-speed recording of the temperature of porous titanium oxidized upon heating. The thermokinetic model of the open system included six reactions describing, in particular, the direct interaction of atomic and molecular gases with titanium and the reactions of molecular oxygen dissociation and atomic oxygen recombination. The thermokinetic behavior of the open reaction system was studied in a wide range of control parameters. An experimental study of the thermokinetics of the oxidation process of porous titanium has shown that the temperature rise at the initial stage of oxidation corresponds to the above theoretical calculations. At temperatures close to 873 K, titanium begins to oxidize and the temperature rises within 0.02 sec to 1273 K. The temperature growth rate is about 20,000 K/sec. At this stage, most likely, the formation of titanium oxide occurs. At the next stage, nonlinear oscillations appear. It should be noted that the proposed model describes the initial stage of the process and does not take into account the above-mentioned oscillations. The results obtained make it possible to control the oxidation process by suppressing the catalytic reproduction of atomic oxygen.

Electronic structure of Tl₄CdI₆: First-principles calculations and X-ray photoelectron spectroscopy measurements

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Ternary thallium cadmium iodide, Tl₄CdI₆, is a representative member of a family of halides with a common formula Tl₄BX₆ (B = Cd, Pb; X = Cl, Br, I) that attract essential attention of scientists and engineers in the recent two decades due to their essential physicochemical properties which induce these compounds to be considered as very attractive materials for the use in non-linear optical devices, for production of X-ray detectors, ionic conductors, sensors of measuring temperature, ion-selective electrodes, etc. These ternary halides are transparent in near- and mid-infrared regions being very attractive semiconductors for production of optical parametric generators. In addition, they possess big enough radiation damage thresholds and birefringence coefficients. In the present work we report on XPS measurements of the Tl₄CdI₆ alloy. These experimental studies indicate low hygroscopical ability and high stability with respect to 3 kV Ar⁺-ion-bombardment. The XPS measurements reveal the existence of high covalent Tl-I and Cd-I bonds in Tl₄CdI₆ that is in agreement with the present first-principles calculations carried out within density functional theory (DFT) framework. The calculations are made using full potential linearized augmented plane wave (FPLAPW) method as implemented in the WIEN97 package. The present DFT FPLAPW calculations indicate that the total valence band region of Tl₄CdI₆ alloy can be considered as consisting of three sub-bands: the upper and central sub-bands are formed mainly from I 5p states, while the lower sub-band is dominated by Tl s states. However, significant contributions of Tl s and Cd d states in the upper sub-band, Tl p and Cd p states in the central sub-bands, while Cd s and I p states in the lower sub-band of the valence band of Tl₄CdI₆ are also observed in our calculations.

The thermodynamic properties of ternary Ag-Ca-Ge liquid alloys

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The study of Ag-Ca alloys is a part of a global trend in the development of science aimed at “green” technologies, such as hydrogen energy in the context of its application in the automotive industry and in the creation of environmental energy sources. The partial enthalpies of mixing of components in liquid Ag-Ca-Ge ternary alloys were determined over a wide range of compositions by means of isoperibolic calorimetry in a high temperature solution calorimeter in purified helium atmosphere at 1300–1550 K. The experimental method is based on measurement of the temperature difference between the sample and the reference specimen (a crucible contained W), plotted as a function of temperature relaxation time. The integral enthalpies of mixing for the ternary system were calculated from partial enthalpies of components by the Darken method. Partial and integral enthalpies of mixing of the ternary Ag-Ca-Ge melts were determined for the first time. The enthalpies of mixing in this ternary system are exothermic values which increase in absolute value from the Ag corner of the concentration triangle towards the constituent binary Ca-Ge system. The minimum value of the integral enthalpy of mixing was obtained for Ca_{0.6}Ge_{0.4} composition of the Ca-Ge binary system (about -58.00 kJ mol⁻¹). The enthalpies of mixing of the ternary Ag-Ca-Ge melts are calculated for the whole concentration triangle by the Redlich-Kister-Muggianu method, taking into account the term of specific ternary interaction defined from our experimental data. The topology of the isoenthalpies of mixing is determined. The excess Gibbs energies of mixing for Ag-Ca-Ge melts were calculated using these parameters of the ternary interaction.

Thermochemical properties of ternary Al-Gd-Mn melts

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Physico-chemical properties of Al alloys with transition metals are being studied increasingly. The intermetallic compounds of the Al-Gd-Mn ternary system are of particular importance, since they exhibit superconducting properties, related to the formation of a stable compound $\text{GdMn}_2\text{Al}_{20}$. Alloys of this ternary system also can display promising magnetic properties in amorphous state combined with excellent mechanical and corrosive characteristics. There are no calorimetric data for the enthalpies of mixing in the ternary Al-Gd-Mn system in the literature. The partial enthalpies of mixing of components in this ternary alloys were determined over a wide range of compositions by means of isoperibolic calorimetry along five sections with a constant ratio of two components up to the molar fraction of the third component equal to 0.3. The experiments were carried out in a high temperature solution calorimeter in purified helium atmosphere at 1650 K. The integral enthalpies of mixing for the ternary system were calculated from partial enthalpies of components by the Darken method. The enthalpies of mixing in this ternary system were found to be exothermic and steadily increasing in absolute values from Mn corner towards the Al-Gd constituent binary system, reaching the minimum value of approximately $-37 \text{ kJ}\cdot\text{mol}^{-1}$ in the vicinity of the $\text{Al}_{0.6}\text{Gd}_{0.4}$ composition, evidently related to the formation of stable Al_2Gd phase. The topology of the isolines of enthalpies of the Al-Gd-Mn alloys indicates the predominant influence of short-range order in the Al-Gd and Al-Mn binaries on the energetics of alloy formation in the ternary system. The line of maximum interaction in this system connects the compositions of the Al-Gd and Al-Mn systems at which the corresponding binary interaction maxima is observed.

Ab initio study of high pressure-induced structural transitions in SnTe.

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Tin telluride is a narrow band-gap semiconductor which has many unusual properties. In particular, it is expected to pass into a superconducting state at the temperature of 7.1 K under compression [1]. In order to understand the mechanism of superconductivity, the detailed information about the crystal structure of SnTe in the wide pressure range is needed. As has been reported in a number of experimental researches, with increasing pressure, SnTe undergoes a series of structural transitions from NaCl-like to intermediate rhombic phases with Cmc₂m and Pnma symmetries and then to CsCl-like phase [2]. However, there is a discrepancy between the results of different studies in identification of transition points and crystal structure. In particular, the possibility of GeS-like structure is considered as well. The purpose of this work is to examine theoretically different structural phases observed in experiments with tin telluride at elevated pressures, namely, to establish the ranges of thermodynamical stability of these phases, localize the transition points, and investigate the associated changes in mechanical and electronic properties. The study is based on the first-principle density functional approach by using the PBE PAW pseudo-potentials with generalized gradient approximation for the exchange-correlation energy. In computer simulations, there were monitored and analyzed the thermodynamical and mechanical properties of SnTe samples with different structure subjected to progressively increasing hydrostatic compression. The obtained theoretical results on the structure of tin telluride correlate well with the available experimental data within the pressure range of 1-30 GPa. 1. Dan Zhou, Quan Li, Yanming Ma, Qiliang Cui, and Changfeng Chen, J. Phys. Chem. C 2013, 117, 23, 12266-12271 2. А. Г. Иванова, И. А. Троян, Д. А. Чареев и др., Письма в ЖЭТФ том 106, вып. 10, с. 637 - 641

Formation of the structure of Al-15Fe alloys during sintering of products from them

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The current state of science and technology poses a wide range of tasks for materials scientists to develop multifunctional materials with low density and high physical and mechanical properties. In this regard, dispersed-reinforced powder composite materials based on iron-alloyed aluminum are promising. In such a system, a number of intermetallics are formed. But in the manufacture of products from such alloys by classical casting methods under conditions of relatively low cooling rate of castings, their structure contains a phase of intermetallics, the crystals of which range in size from 200 to 1600 μm have a developed dendritic, needle shape. However, if we ensure the presence in the structure of Al - Fe alloys of the intermetallic phase in the dispersed state with a size of less than 3-5 μm , it can act as a disperse-strengthening phase. The aim of our work was to establish the influence of sintering conditions of compresses obtained by spraying melts of Al + 15% Fe alloy at the cooling rate of dispersion products 1×10^{-6} deg./s with a structure consisting of an aluminum-based matrix and dispersed inclusions smaller than 3-5 μm of intermetallics of iron Al_xFe_y . Samples were pressed from the initial powders at pressures of 500, 600, 700, 800 MPa, which were sintered at temperatures from 500 to 800 ° C, with an isothermal holding time of 30 minutes. The microstructure of the samples sintered at temperatures of 500 and 600 ° C in the solid phase is almost identical to the structure of the initial powders. Increasing the sintering temperature to 700 ° C, at which the liquid phase appears due to the melting of the aluminum phase, leads to the enlargement of the intermetallic phase. Small inclusions of intermetallics disappear with simultaneous aggregation of large ones with the formation of large crystals of intermetallics. Increasing the sintering temperature to 800 ° C intensifies these processes.

Finding simple regularities in the hydrogen occupation of voids in Mg₂NiH hydride from ab-initio calculations

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Theoretical methods are widely used to find the ways to improve properties of hydrogen storage materials. Calculations help to direct and optimize experiment. Therefore, finding regularities of the occupation of sites by hydrogen in disordered structures can help to decrease number of ordered models to calculate. An effort has been made to find the distance dependence of H-H interactions in Mg₂NiH compound. The models of cubic modification of Mg₂NiH were created on basis of str. type K₂PtCl₆ with 4 of 24 sites, occupied by H. 119 independent models were generated by program Supercell. The calculations were performed using program JDFTx (PBE functional) for optimized Mg₂Ni, models of Mg₂NiH, and H₂ in order to obtain energies of reactions. The H-H interactions $E_{hh} = \sum (X_i/R^i) + X_{13} \cdot \exp(-R)$ were fitted against DFT data, where $i=4-12$, R - H-H distance, X_i - coefficients. The dependence of energy of hydrogenation reaction $Mg_2Ni + 1/2H_2 = Mg_2NiH$ was studied in order to develop simplistic method of search of the most stable configuration of hydrogen positions. The energies of interactions depend on both distances and angular positions of neighboring atoms, with dominating contribution of the first coordination sphere. The following approximation of energy of hydrogenation was proposed: 1) fixed term, describing structure transformation and H insertion; 2) distance-dependent interactions between H-atoms, belonging to far coordination spheres of each other. The interactions of all H-atoms of one unit cell were described as the sum of interactions between: 1) H inside single unit cell; 2) H inside single unit cell and all H outside with $R \leq 100 \cdot a(Mg_2NiH)$ (650 Å); 3) residuals. The expression with 7 parameters $i=4,6,7,11,12,13$ predicted energies with correlation 0.74 and was enough to select the most favorable model.

Mechanical Performance of Aluminium Foam Fabricated by Melt Processing with Different Foaming Agents: Comparative Analysis

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Closed-cell aluminum foams are in focus for different engineering application due to outstanding combination of low density, physical and mechanical properties [1]. Herewith, stiffness/mass ratio for the foams superiors to that of dense aluminium alloys. The foams demonstrate capability to undergo large strains (up to 60–70%) under almost constant stress in compression, providing remarkable absorption of mechanical energy. So, they are efficient in lightweight crashworthy structures such as integral ceramic/metal/synthetic fibre composites against ballistic impact and blast protection used for defence of terrestrial and marine vehicles. Because of theoretical models based on an idealized representation of cellular structure do not represent the actual profile of mechanical properties for real aluminium foams the experimental verification of compression response the foams using normalized test procedure is strongly required. The study presents the comparative analysis of compressive response for experimental aluminium foams of different parent alloys fabricated by melt processing with/without Ca additive and conventional TiH₂ blowing agent or CaCO₃. It was recognized that response of the foams is significantly depended on the foaming agent and Ca additive due to the presence in wall material the undesirable low ductile and brittle side products formed at foaming. Eutectic domains and particles/layers of Al₃Ti, residues of partially decomposed TiH₂, Ca bearing compounds, etc. results in reducing the compressive strength of the foams and deviation of their mechanical profile from theoretical predictions. Application of cheap CaCO₃ offers indisputable advantages compared to TiH₂, resulting in enhancing energy absorption. [1] M. F. Ashby, A. G. Evans, N. A. Fleck et al.// *Metal Foams: A Design Guide*, Butterworth Heinemann, Boston, USA, 2000, 521 p.

Gas and electrochemical hydrogenation properties of new RT3 phases

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Since Kohno et al. [1] reported that the discharge capacity of the La_{0.7}Mg_{0.3}Ni_{2.8}Co_{0.5} alloy reached 410 mAh/g, which was 25 % higher than that of commercial AB₅-type alloys, La-Mg-Ni-based hydrogen storage alloys have gained increasing interest as one of the most promising materials for negative electrodes in Ni-MH batteries [2,3]. Much attention has been concentrated on the alloys with PuNi₃ structure type. It was found that these materials, which are mainly based on the La₂MgNi₉ intermetallic compound, possess high hydrogen storage capacity, high discharge capacity and low production cost. However, the poor cyclic stability (degradation during the cyclic process) is the main problem, which hinders its practical application. Several methods were adopted to improve their cyclic stability. Elemental substitution is one of them. In present work, we investigated the influence of composition of the PuNi₃ structure type phases on the gas and electrochemical hydrogenation properties. The RT₃ (R = La, Y, Mg; T = Ni, Co, Cu) samples were prepared from the metal powders by sintering/annealing. Gas hydrogenation curves were obtained by using a Sieverts type apparatus. Electrochemical charging-discharging properties were studied by galvanostatic measurements. Powder X-ray diffraction and microprobe analysis were used for the sample characterization. Single phase samples with PuNi₃ structure type (R-3m space group) were obtained. Upon hydrogenation the structure of parent compounds was preserved. Values of the maximum discharge capacities (C_{max}) and cyclic stabilities (S₅₀) were obtained from the experimental data. The best electrodes composed by PuNi₃ type structure phases exhibit C_{max} more than 400 mAh/g and S₅₀ near 95 %. [1] T. Kohno, H. Yoshida, F. Kawashima, et al. J. Alloys Compd. 311 (2000) L5-L7. [2] Yu.V. Verbovytskyi, I.Yu. Zavaliy, Mat. Sci. 51 (2016) 443-456. [3] Yu.V. Verbovytskyi, I.Yu. Zavaliy, Mat. Sci. 52 (2017) 747-759.

The nature of the heat resistance of nano-dispersion hardened nichrome in atmospheric conditions

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When solid state sintering the composition retains the effect of the inheritance of the powder system. At the Frantsevich Institute for Problems of Materials Science of the National Academy of Sciences of Ukraine, a new technology for the consolidation of powder pressing has been developed [1]. Due to the high crystallization rate during reacting synthesis, the powder system loses its heredity. The standard nichrome with 20% Cr was chosen for further use as parts of thermal protection against aerodynamic heating of aircraft [1]. In this case, it is necessary to preserve the heat resistance of the nichrome up to 1200 0C. The aluminum content varied up to 6%. Sintering was carried out at temperatures of 1275- 1300 0C. In contrast to standard methods, the study of heat resistance was carried out under thermal cycling conditions when the sample was placed in a heated furnace to a temperature of 1200 0C and isothermal holding for twenty minutes. The maximum weight gain is observed during the first three cycles of material oxidation. At the fifth and sixth cycles, the increase in the mass of samples is practically equalized amounting approximately 10-5 g/ cm². The film, formed on the alloy with the aluminum of less than 1% consists continuous film of spinel (NiCr₂O₄). Chromium-nickel spinel has higher protective properties than nickel oxide, in which oxidation is controlled by diffusion of oxygen ions through the spinel film. Increasing the aluminum content leads to the formation of a mixture of chromium oxides with a small amount of nickel spinel. However, with an increase in the aluminum content to 6% or more, a continuous alumina film is formed. The material has maximum heat resistance. With an increase in the aluminum content above 6% heat resistance is retained upon alloying nichrome with titanium, niobium, and molybdenum in a wider concentration range. Aluminum is the main component that determines the heat resistance of the alloy.

Melting Phase Diagram of the Cu-Ti-Zr System in the Ti-CuTi₂-CuZr₂-Zr Region

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Interest to the Cu-Ti-Zr system is due to presence of a wide range of bulk metallic glass forming alloys with excellent mechanical properties. Phase equilibria in the system were investigated repeatedly. As a result, isothermal sections at 703, 750 and 800 °C and two isopleth sections were reported. But there is a lack of information on phase equilibria at the melting/crystallization temperatures. The isopleth section CuTi₂-CuZr₂ is quasibinary. So the phase equilibria in the Ti-CuTi₂-CuZr₂-Zr subsystem are independent. In the present work that region was studied at the melting/crystallization temperatures. The alloys for investigation were prepared in an arc furnace in Ar from iodide processed Ti and Zr and electrolytic Cu. Then they were annealed in evacuated quartz tubes at 750 °C for 536 h. As-cast and annealed alloys were studied by differential thermal analysis (DTA), x-ray diffraction phase analysis (XRD), scanning electron microscopy (SEM) and electron probe microanalysis (EPMA). Ternary as-cast and annealed alloys contain only two phases, γ -Cu(Ti_xZr_{1-x})₂ (tI6, MoSi₂-type) and α -(Ti, Zr) (hP2, Mg-type, transformed bcc β -(Ti, Zr)). So the liquidus surface in the subsystem consists of two fields of primary crystallization, solid solutions based on γ - and β -phases, which intersect along a curve, connecting the respective binary eutectics in the Cu-Ti and Cu-Zr systems. The liquidus temperature decreases from the boundary binary systems to the ternary one up to the minimum at 847°C at the point Cu_{29,5}Ti_{27,5}Zr₃₄ of the two-phase ternary eutectic $Le \leftrightarrow \beta + \gamma$. As expected, the solidus surface in the subsystem consists of two fields of β - and γ -solid solutions and a wide ruled surface of the $\beta + \gamma$ region.

Use of mathematical modelling to optimize the external influence on the processes in the dislocation structure during underwater welding

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The peculiarity of obtaining welds underwater is the influence of the aquatic environment on the processes of melting and crystallization of the metal. To intensify the processes of metal degassing, grinding of the structure, increasing the values of strength and ductility of the joints, it is proposed to use external electromagnetic influence (EEI) on the melt of the welding bath. A mathematical model and software package for calculating the density of welding and eddy currents in massive conductors, the density of magnetization currents on the surface of ferromagnetic bodies have been developed. They were used to analyze the distribution of electrodynamic forces in arc welding and EEI, evaluated the developed mathematical models for the adequacy and reliability of the results. The influence of the external electromagnetic field on the parameters and defects of the crystal lattice (dislocation) in the metal of welded joints made of low-alloy steel made underwater has been studied. It is established that the EEI improves the quality of the welded metal, which is very important when welding critical structures operating in the aquatic environment. It is shown that when welding joints underwater and applying EEI, a finer-grained substructure is formed in the metal of the thermal zone with a general decrease in the density of dislocations and its uniform distribution. Considering the peculiarities of the distribution and density of dislocations in the structural components, it is shown that the use of EEI leads to a decrease in the level of local internal stresses. This is facilitated by the general reduction of the density of dislocations and their uniform distribution in the structural components of the lower bainite, which should provide resistance to cracks of welded joints. The structural conditions for obtaining high-quality welded joints during welding of low-alloy steels underwater ensure their resistance to cracks.

Laser spot welding in different spatial positions

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In modern structures of thin-sheet shells, the multilayer shells became widespread, in which a high load-bearing capacity is achieved with a minimum loss of metal due to a rational distribution of it in the separate elements of a structure. Such structures with a relatively small mass have high strength and rigidity characteristics, good sound and thermal insulation properties. A honeycomb panel with cellular filler represents a composite welded three-layer structure of thin-sheet metal, consisting of two load-bearing layers, cellular filler located between them, and frame elements. The manufacture of a panel requires producing a large quantity of welded spot joints. As compared to continuous welding, spot provides minimal deformations of structures and allows their manufacturing with a high accuracy. The use of spot welding provides high efficiency and quality of performed works and saving of time and material resources due to reduction in works on straightening of products, required because of their buckling after welding, and decrease in electric power consumption. The aim of the work is a comparative analysis of structural features and mechanical characteristics of spot welded joints of thin-sheet stainless steels 03Kh11N10M2T and 12Kh18N10T, produced by laser welding in different welding positions. The change in the welding position from vertical to flat allowed extending the ranges of variation of welding modes from about $\pm 5\%$ to $\pm 10\%$, at which it is possible to produce welded joint with satisfactory shape and mechanical characteristics. Higher stress values are typical for welded joints obtained in the flat position. It also concerns to the maximum value of the shear stress, which for the flat position is higher by approximately 10%, and the average value, which is higher by approximately 24%.

Thermodynamic properties of Bi-Tm melts

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Thermodynamic properties of melts Bi-Tm system were firstly studied by the calorimetry method at $0 < x_{Tm} < 0.2$ and $T = 1100$ K. The partial enthalpies of the thulium after $x_{Tm} > 0.15$ became more exothermic than they are in the initial region of compositions, because it points out the transition in a heterogeneous region. This indicates that $T_{liq} = 1100$ K at $x_{Tm} = 0,15$. The approximation of the experimental datas allowed to calculate integral mixing enthalpies and the partial enthalpies of the components in the whole range of concentrations (minimum of integral mixing enthalpies is equal to -75 at $x_{Tm} = 0.65$; the first the partial enthalpies of the bismuth and thulium is equal to -230 and -150 kJ/mol respectively at 1100K). To expand the information on thermodynamic properties of Bi-Tm phases we calculated and optimized these parameters according to the ideal associated solutions (IAR) model, and obtained their temperature dependences. It is turned out that the the partial enthalpies of the bismuth curves show a large steepness in contrast to the gradual decrease of the exothermic similar parameter for thulium. This indicates on large changes in the structure of melts with increasing temperature. The activities of the components and molar fractions of three associates $TmBi_2$, $TmBi$ and Tm_2Bi simulated on IAR model. The activities of the components demonstrates very large negative deviations from ideal solutions, the value of which for the equiatomic composition is close to zero. The maximal molar fractions of $TmBi$ and Tm_2Bi associates are 0.92 and 0.7 respectively. This confirms the high energy of interaction between dissimilar atoms at these concentrations and the predominant role of associates in them. IAR model allows us to estimate the enthalpies of formation of intermediate phases and associates. The value of enthalpies of formation of the associates Tm_2Bi and $TmBi$ are the exothermic (-80 and -90 kJ/mol), which agrees with minimum of integral mixing enthalpies -75 kJ/mol. Comparison of enthalpy and Gibbs energy of mixing of melts in the Bi-Tm system has shown that ΔH is higher in absolute values, just as it is characteristic of melts with a strong energy of interaction between different particles.

Thermodynamic Properties of the alloys of In - Lu system

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Indium and indium alloys with liquid metals are used as fusible, heat-conducting, semiconductor materials, as well as lead-free solders. Data of the thermodynamic properties of the various phases and, in particular, the liquid, are necessary for the scientifically sound development of the methods of obtaining said materials and alloys. Therefore, the purpose of the study is to investigate the enthalpy of mixing melts of the In - Lu system in the range of compositions $0 < x_{Lu} < 0.3$ and a temperature of 1645 ± 1 K. Partial lutetium and integral enthalpy of mixing of alloys of the In - Lu system were approximated by polynomials of the form by which the thermochemical properties at rounded concentrations were evaluated. The first partial for terbium and minimal integral enthalpy of mixing of the In-Lu system are -155 ± 7 and $-45,1 \pm 0,2$ kJ/mol in accordance. These parameters are similar to those previously established for liquid alloys of binary In - La (Ce) systems and difference slightly from In - Eu (Yb). On this basis it is possible to predict the thermochemical properties of the melts of In - REM systems, which have not yet been fully investigated. This dependence is almost monotonous, due to the close values of the differences between the mole volumes and the electronegativities. We have come to the conclusion that activities of the components and entropy of the mixing will be similar to those characteristic of the melts In-La (Ce) of the systems.]. This significantly expands the information on the nature of the interatomic interaction in the melt under consideration. Thermodynamic properties of the alloys of the binary Sn (Sb) -RZM melts were compared It was found that the interaction energy between the data p-elements and REM grows in the following order: In - REM \rightarrow Sn - REM \rightarrow Sb - REM. This is due to the fact that stybium is the best electron acceptor.

CERAMICS

KEYNOTE: Design of deformation resistant ceramics with superior flexural strength for next-generation structural systems with specific features under extreme conditions

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The request in ceramic, able to act as plasma-facing parts in fusion reactors, as a special engine & vehicle protection for aerospace cause the demand in new ultra-high temperature ceramics with sufficient balance between high strength, toughness and hardness, and high-modulus. We analyze the mechanical behavior of a bulk polycrystalline boron prepared by SPS of β -boron powder. Bulk boron showed a steady increase in strength up to 1200 °C, which is 0.66 of the absolute melting point for boron. It was determined that fracture at elevated temperatures follows a quasi-transgranular mechanism, where the sub-grains of the boron fracture as plate-like structures. Despite showing clear signs of plastic deformation on the strain-stress curves, the yield strength of the monolithic boron ceramic exceeds 1.2 GPa at 1200 °C which surpasses the data currently available for boron carbide bulks. Similar to its direct prototype β -boron boron carbide possesses high hardness, high anisotropy in elastic moduli, as well as a moderately low fracture toughness. In boron carbide, similar to diamond, the dislocation activity and hence plasticity is not expected at room temperature due to a high lattice resistance. This yields an ability to possess high flexural strength at room temperature, and allows boron carbide bulk to serve a structural material for harsh conditions. Ultra-high temperature flexure driven amorphization in polycrystalline boron-rich boron carbide was accompanied with strength of up to 8.8 GPa at 2000 °C. Finally, we explored the formation of deformation-resistant Ta_{0.2}Hf_{0.8}C solid-solution ceramic with flexural strength of 600 MPa at room temperature and superior flexural strength at 2000°C. Furthermore, a strength exceeding 500 MPa for Ta_{0.2}Hf_{0.8}C been observed through all testing temperatures up to 2000 °C. This incredible deformation resistance is beneficial for design of novel aerospace vehicles with operation under extreme reentry conditions.

KEYNOTE: Effect of pressure, synthesis and sintering technology on the structure and properties of composite ceramic materials

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The effect synthesis and sintering technologies in a wide range of pressures (from vacuum to 2 GPa) on the structure and properties of composite ceramic materials will be considered by the example of obtaining such ceramic composite materials as ultrahigh-temperature ceramics based on hafnium and zirconium borides, shock-resistant materials based on aluminum dodecaborides and boron carbide, superconducting materials based on magnesium diboride and melt textured ceramics based on yttrium cuprates, as well as MAX phases of Ti (Nb)-Al-C systems (in the form of bulk materials and vacuum-arc deposited coatings). The appropriate functional characteristics of the materials obtained using pressure less sintering, hot pressing, spark plasma sintering, and quasi hydrostatic high pressure -high temperature technique will be compared. The results of the materials structural studies using X-ray diffraction with Rietveld refinement, TEM, SEM and polarized light microscopy, Auger and Raman spectroscopy will be discussed. The investigations were performed in the frames of the project NATO SPS G5773 "Advanced Material Engineering to Address Emerging Security Challenges" for 2020-2023, the project 03-03-20 of Ukrainian-Belorussian cooperation for 2020-2021, and the projects III-3-20 (0779), III-5-19 (0778), and II-5-19 (IHM-29/20) supported by the National Academy of Sciences of Ukraine

The morphology of directionally crystallized eutectic NbB₂+SiC+B₄C colonies

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The micro- and macro-morphology of eutectic colonies in the alloys of the NbB₂+SiC+B₄C system formed during directional crystallization have been investigated. The microstructure of the samples was studied on SEM SELMI PEM 106И and TESCAN VEGA 3. Local chemical composition was analyzed on micro-analyzers Jeol JXA-8530F and SELMI PEM 106И (WDS and EDS). The phase composition was determined on X-ray diffractometer Rigaku Ultima IV. It is shown that at the beginning, the dendrites of primary crystals of proeutctic phases are nucleate and grow. Only one of them SiC nucleates to others crystals and serves the base for the eutectic colony. Therefore, the formation of primary NbB₂ and B₄C crystals in alloys of appropriate compositions only promotes the nucleation and growth of primary SiC crystals. The micro- and macro-morphology of the three-phase eutectics in alloys of all concentrations are of the same type and consists of a two-phase structural constituent (SiC+NbB₂) solidified during cooperative crystallization and third eutectic B₄C phase growing synchronously by the mechanism of autonomous growth. Due to the stepped relief of the primary base SiC crystal formed in the process of dendrite branching, the two-phase eutectics (SiC+NbB₂) is based and grows on the branches of this dendrite in the form of eutectic cells consisting of a main lamellar two-phase (SiC+NbB₂) package and second part of honeycomb or/and skeletal morphology. The obtained patterns are embodied in a 3D structural model. Re-nucleation of eutectic phases was not found, which indicates their continuous growth from the nucleation to the end of the solidification. Thus, the common accepted model of the eutectic as a "mechanical mixture" is not adequate. Acknowledgements This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0108).

EPR spectroscopy characteristics by mathematical lorentz theoretical model of Sm₂O₃ doped with CeO₂ after high temperature treatment

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The spectral characteristics demonstrate the dominance of the samarium ion line Sm³⁺ with the configuration (6H_{5/2}) and the form of the electronic configuration (4f⁶5s²5p⁶) in the EPR spectrum of samarium oxide Sm₂O₃-CeO₂ after thermal treatment of these samples at temperatures of 120°C, 1100°C and 1500°C. The changes in the intensity of the spectral lines of the EPR for the corresponding ion state are almost linear, which corresponds to the law of conservation of the integral number of spins in the corresponding state in the samples. The electron configuration for (REE) ion suggests Electronic Configuration in the Sm⁰ form of electron configuration 4f⁶5s²5p⁶6s². The modification of the electron configuration differs with the form of the crystal lattice, lattice constant and number of the ions per unit cell. The modification of the crystal lattice includes the forms of the cubic phase, octahedral phase, orthogonal phase, tetragonal phase, hexagonal phase lattices. According to modification of the certain phase the mods of the ion electron configuration changes to the form of the certain ion electron configuration. For REE oxide ceramics containing 90 mol.% Sm₂O₃ - 10 mol.% CeO₂ electron characteristic and ion characteristics of the ion included in the oxides (REE) can be a cerium ion Ce⁰ with atomic number 58, with appropriate form of ion configuration 3H₄ and the form of the electronic configuration 4f²5s²5p⁶6s². The oxide also includes cerium ion Ce¹⁺ with ion configuration 4H_{7/2} and the form of electronic configuration 4f²5s²5p⁶6s, for the cerium ion in Ce²⁺ corresponding oxide with ion configuration 3H₄ and the electronic configuration form of 4f²5s²5p⁶ and cerium ion Ce³⁺ in electron configuration with corresponding configuration 4f¹5s²5p⁶ and the form of ionic term in 2F_{5/2}.

High-temperature properties of high-entropy ceramics MeB₂

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The high, middle, and low-entropy borides based on diborides (TiB₂, ZrB₂, HfB₂, NbB₂, TaB₂) were obtained by hot pressing. It is shown that hot pressing temperatures from 1900 °C are required to obtain single-phase materials. The average grain size of as-sintered ceramics in optimal conditions does not exceed 5 μm. The HfB₂ is present in all materials in an amount of up to 3 vol.%. To reduce the content of hafnium diboride, a two-step process was developed. This process consists in vacuum annealing of pre-compressed materials followed by hot pressing. The flexural strength of as-sintered ceramics at room temperature was in the range from 350 to 500 MPa. The hardness of the obtained composites was ranged from 20 to 22 GPa at a load of 2H and 19-18 at a load of 200 N. The flexural strength at 1600 °C was 543 MPa for hot-pressed ceramics, and 900 MPa for two-step process. The increase in strength is most likely due to plastic deformation in the material. The flexural strength at 1800 °C sharply decreases to 197 MPa. However, the strength is at the level of high-temperature ceramics ZrB₂-15 vol. % SiC. Resistance to oxidation in air of high-entropy ceramics was determined at a temperature of 1500 °C. It is shown that the high-entropy alloy (Ti, Zr, Hf, Nb, Ta)B₂ melted due to the oxidation of TiB₂ to the low-melting phase Ti_xByO_z. Removal of titanium diboride from (Ti, Zr, Hf, Nb, Ta)B₂ leads to increased resistance to oxidation. However, the maximum oxidation resistance at 1500 °C is achieved on a triple alloy (Zr, Hf, Ta)B₂. For creating high oxidation resistance high-entropy ceramics, it is necessary to replace TiB₂ and NbB₂. Thus, high-entropy ceramics have high strength at temperatures of 1600-1800 °C in vacuum, which will allow its use in a protective environment. However, it has low high temperature oxidation resistance, which requires the creation of composites based on them.

Modification of atomic chains in boron carbide with silicon

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In our previous works, modification of atomic chains between icosahedra in B₄C with Al was shown to be effective against the amorphization of material upon dynamic load. The objective of this work was to explore the possibility of atomic chains modification in boron carbide with silicon atoms and their possible influence on the structure of the material. Powder samples were prepared by interaction between boron carbide with gaseous silicon in vacuum at 1400 C. X-ray diffraction was used to establish the resulting phase composition and changes in lattice constants and wet chemical analysis to determine the elemental composition. Density functional theory (DFT) was employed to assess the relative stabilities of various chains, possibility of Si substitution into -C-C-C- and -C-B-C- chains, probable geometry of the resulting -C-Si-C- chains. The experiments on boron carbide with maximum amount of carbon show that B₄C(s) and Si(g) intensively interact at 1400 C, when Si vapor pressure exceeds 1.3 Pa, producing 15.41 wt.% SiC and 83.88 wt.% of a phase with hypothetical formula B₁₂(CSiC); the rest is 0.71 wt.% of Si. The formation of B₁₂(CSiC) is suggested by the change in lattice parameters of boron carbide from initial a=0.56022 nm, c=1.20883 nm to a=0.56455 nm and c=1.23266 nm and proved by wet chemistry elemental analysis. Specimens produced in further experiments with industrial boron carbide containing 19 wt. % of carbon also contained 18-20 wt. % of B₁₃C₂ suggesting that Si atoms can substitute a carbon in the middle of the chain but can not do the same for a boron. DFT studies provide further evidence for this suggestion as both linear -C-B-C- and angled -C-Si-C- chains have similar formation energies which are significantly lower than that of the -C-C-C- chain. Angled Si-containing chains indicate that the material should be less prone to amorphization as they are expected to compress under dynamic load and then relax without permanent structural changes. This work is supported by the NATO SPS Programme, Project G5773.

Preparation and materials involving cast tungsten carbides

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It has now been shown that solid refractory compounds (SRC) - carbides, borides, nitrides and their alloys are promising materials, primarily for the creation of tool, wear-resistant materials, products and coatings. It has also been shown that fused refractory compounds are promising for the production of such materials, which have almost 100% density, do not contain impurities and have higher properties characteristic of tool materials, especially those used for abrasive processing of materials. Among hard refractory compounds, tungsten carbide has a special place, which has found wide application as a base for tungsten-containing hard alloys, wear-resistant surfacing materials, materials for spraying wear-resistant coatings by thermal methods, and abrasive materials. Taking into account the above, it seems to us urgent to obtain fused solid refractory compounds, in particular, tungsten carbide. A feature of obtaining fused refractory materials is that in most cases they dissociate upon melting, followed by congruent or incongruent evaporation. To suppress the evaporation processes, melting is carried out at the pressure of a protective or active gas in the working chamber. In the case of obtaining fused tungsten carbide at a gas (argon) pressure in the working chamber of 6–8 MPa, the product consists of WC, W₂C, C phases. With an increase in the WC content in fused tungsten carbide, the strength of the grains and their abrasive ability increase. Extrapolation of the abrasive ability and strength of the abrasive grain to zero free C content shows that the attainable abrasive ability of fused WC can be 2.6 relative units, and the strength of the abrasive grain is 10.8 N / grain, which exceeds the strength of ACB diamond grains of similar grain size. As our studies have shown, the use of cast tungsten carbide in the composition of composite materials with a binder of self-fluxing alloys, which operate under conditions of intense abrasive action, is promising.

DFT band-structure calculations and X-ray spectroscopy measurements of two different phases of Tl₃PbBr₅

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As the demands and increasing challenges of electronics, optoelectronics, nonlinear optics, dosimetry, and other fields of technology increase, there is a shortage of new materials that can successfully solve these problems. Numerous studies have emerged due to these requirements, they have influenced the development of new complex nonhygroscopic and nonlinear optical lead halides with the general formula APb₂X₅ and Tl₃PbX₅ (where A = K, Rb; X = Cl, Br or I). A number of experimental and theoretical studies to elucidate the electronic structure of the single crystal Tl₃PbBr₅ have been carried out [1-2]. X-ray diffraction structure data for the compound Tl₃PbBr₅ in two phases, low- and high-temperature ones, gave the following results: at room temperature, the compound crystallizes in an orthorhombic lattice (space group P212121) with unit cell parameters $a = 15.396 \text{ \AA}$, $b = 9.061$. When heating to 300 ° C, the transition of the orthorhombic LT - Tl₃PbBr₅ phase to the tetragonal modification HT-Tl₃PbBr₅ (space group P41) with lattice parameters $a = b = 8,892 \text{ \AA}$, $c = 15,791 \text{ \AA}$ is observed. Due to the theoretical data obtained by the FP-LAPW method, it can be stated that the compound Tl₃PbBr₅ is an indirect band semiconductor with a band gap $E_g = 2.26 \text{ eV}$ and 1.76 eV for NSOC and SOC calculations, respectively. After processing XPS data obtained at a temperature of 20 and 300 C, it was found that the charge states of the atoms constituting lead tritribromide do not change during the orthorhombic to tetragonal transition. However, a small shift (approximately 0.3 eV) of the XPS valence band spectrum to the Fermi level was detected during the transition from LT-Tl₃PbBr₅ to HT-Tl₃PbBr₅. 1. NM Denisyuk, VL Bekenev, MV Karpets, OV Parasyuk. Journal of alloys and compounds, 2013, V 35, I 5, P. 1081-1089. 2. OY Khyzhun, VL Bekenev, OV Parasyuk, SP Danylchuk. Optical Materials, 2013, V 576, P. 271-278.

Effects of Si-doping on mechanical properties of boron carbide. A first-principle study.

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Due to low density and high hardness, the icosahedral boron carbide is widely used in industry, in particular, for manufacture of armored materials. At the same time, its area of application is limited due to high brittleness and the phenomenon of amorphization, i.e. the localized structure degradation observed under the non-hydrostatic stress. According to a number of studies, the amorphization resistance of boron carbide and its ductility can be significantly improved by Si-doping [1, 2]. However, the mechanisms of this effect, including even possible localization of the embedded silicon atoms, still remain poorly known. The purpose of this work is to address these issues by examining the behavior of Si-doped icosahedral boron carbide under non-hydrostatic loads on the basis of ab initio computer simulations. The calculations were carried out in a unified manner, on the basis of density functional theory with the use of PAW pseudo-potentials with exchange-correlation energy given in Perdew–Burke–Ernzerhof GGA form. We considered several different stoichiometries based on the conventional and polar boron carbide with embedded silicon atoms, including (B₁₂)-CSiC and (B₁₁SiP)-CBC configurations. In simulations, the stability of the compounds and their strain-stress behavior, in particular, the structural transformations and the associated strain failure under the uniaxial (along carbon-silicon chains) and shear stress were examined. The results of calculations indicate that the Si-enriched icosahedral boron carbide can exhibit significantly modified strain failure and ductility index as compared to conventional boron carbide, which suggests that Si-doping of boron carbide may be a potentially promising processing in the context of improving its mechanical properties. 1. J E Proctor, V Bhakhri, R Hao, et al., J. Phys.: Condens. Matter 27 (2015) 015401 (8pp) 2. Atta U. Khan, Anthony M. Etzold, Xiaokun Yang et al., Acta Materialia 157 (2018) 106-113

High temperature enthalpy of Yb₄Hf₃O₁₂ in the temperature range 471-1930 K

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Oxide materials crystallizing with the fluorite structure exhibit a variety of materials properties that make fluorites suitable for a wide range of technological applications including thermal barrier coatings, electrolytes in solid oxide fuel cells, and crystalline nuclear waste forms. To evaluate the stability and reactivity of the materials under different conditions of their synthesis, processing and operation the information about thermodynamic properties of substances in a wide temperature range is needed. The experimental data for the high temperature thermodynamic properties of Yb₄Hf₃O₁₂ was not found in literature. The objective of this research is to study the enthalpy increment of Yb₄Hf₃O₁₂ in the range 471-1930 K and calculate the temperature dependences of the main thermodynamic functions in the range 298.15-1930 K. Ytterbium hafnate Yb₄Hf₃O₁₂ was produced chemically by inverse precipitation from ammonia solution and a mixture of Hf and Yb nitrates followed by hydroxide decomposition at 900 °C in air and melting of the oxide mixture at 1500 and 1600 °C. The formation of Yb₄Hf₃O₁₂ was ascertained by X-ray diffraction. The lattice constants of Yb₄Hf₃O₁₂ are $a = 9,60182$, $c = 17,97293$ nm that are in good agreement with literature data. The Yb₄Hf₃O₁₂ enthalpy increment was measured for the first time in interval 471-1930 K by drop calorimetry using a Setaram HT-1500 high-temperature differential calorimeter (471-1055 K) and a high-temperature calorimetric device (1150-1930 K). The data obtained with two calorimeters in the temperature of overlapping region agree within the error of measurements (1,5 %). There are no phase transitions on the curve of Yb₄Hf₃O₁₂ enthalpy temperature dependence. A fitted equation for the enthalpy increment was used to calculate the temperature dependences of heat capacity, entropy, and Gibbs energy in the interval 298.15-1930 K.

Aging of materials in the ZrO₂-Y₂O₃-CeO₂ system

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The main reasons for the using of ZrO₂ in orthopedic surgery are increased mechanical properties, which are the result of the transformational toughness and high chemical resistance to the aggressive environment of a living organism. Aging occurs by the phase transformation T-ZrO₂ → M-ZrO₂ on the surface caused by the presence of moisture, which leads to surface roughness and microcracking. This inevitably affects the wear of the heads of the hip arthroplasty, as the appearance of roughness increases the rate of abrasion on the surface of the prosthesis. The purpose of the study: to investigate the “aging” of the materials in the system ZrO₂-Y₂O₃-CeO₂ of compositions (mol.%) 97ZrO₂-3Y₂O₃ (Zr(3Y)), 95ZrO₂-3Y₂O₃-2CeO₂ (Zr(3Y2Ce)), 92.5ZrO₂-2.5Y₂O₃-5CeO₂ (Zr(2.5Y5Ce)), 90ZrO₂-2Y₂O₃-8CeO₂ (Zr(2Y8Ce)) and 88ZrO₂-12CeO₂ (Zr(12Ce)). To determine the phase stability of ceramics, the method of accelerated aging of materials in hydrothermal conditions was used. Testing of samples in hydrothermal conditions (137 °C, 7h) is equivalent to 20 years of finding a bioimplant in the human body [1]. The test was performed in an autoclave, which was used to produce the starting powder. The phase stability of materials was determined by the results of X-ray phase analysis. Evaluation criterion - the absence or presence of a small amount (up to 5%) of M-ZrO₂ on radiographs of samples after accelerated aging. The preservation of 100% T-ZrO₂ in the composites Zr(2Y8Ce) and Zr(12Ce) indicates their increased phase stability in a humid environment. It is determined that the powders of Zr(2Y8Ce) and Zr(12Ce) are promising for the creation of bioimplants for various purposes and ceramic layer on metal implants in order to increase their wear resistance. [1] Deville S. Influence of surface finish and residual stresses on the aging sensitivity of biomedical grade zirconia / S. Deville, J. Chevalier, L. Gremillard // *Biomaterials*. - 2006. - V. 27. - P. 2186-2192.

Interaction of phases in the TiB₂-TaB₂ system at high pressure and temperatures and mechanical properties of obtained composites

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Sintering of powders of Group IVa, Va transition metal diborides at high pressures makes it possible to obtain highly-dense ceramics without the use of activating additives and to most fully realize the potentially high properties of these compounds in finished products. Such ceramics have a combination of increased hardness and reduced brittleness due to the fine-grained structure of the material. Of these, TiB₂ has the highest hardness, and NbB₂, ZrB₂ and especially TaB₂ have the highest plasticity, of which tantalum diboride has a higher hardness. Therefore, of interest are composites in the TiB₂-TaB₂ system, which will have a higher hardness than tantalum diboride and lower brittleness than titanium diboride. At present, the interaction of phases in the TiB₂-TaB₂ system at high pressures and temperatures and the physico-mechanical properties of such composites have not been practically studied. The aim of this work was to study the interaction of phases in the TiB₂-TaB₂ system, and the microstructure by XRD, EDX, SEM, as well as the hardness and fracture toughness of the obtained composites, depending on the modes of thermobaric treatment at pressures of 2.5 and 4 GPa in the temperature range 1500-1900 °C with exposure from 1 to 15 min. It was found a new boron-depleted Ta₃B₄ phase with an orthorhombic structure along with the initial TiB₂ and TaB₂ phases in compact samples sintered at high pressures and temperatures. The P-T-conditions for the appearance of the Ta₃B₄ phase are determined and the mechanism of its formation is proposed. The achieved values of hardness HV₁ and fracture toughness K_{1C} (22.9 ± 0.7 GPa and 7.7 ± 0.6 MPa.m^{1/2}) of the composite with Ta₃B₄ phase indicate the possibility of its use as a cutting material for processing non-ferrous Metals and Alloys.

LOW-DIMENSIONAL AND NANO MATERIALS

KEYNOTE: 2D Carbides and Nitrides (MXenes) Open New Horizons in Electronic and Communication Technology

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Discovery of new materials provides moments of inspiration and shifts in understanding, shaping the dynamic field of materials science. Following the graphene breakthrough, many other 2D materials emerged. Although many of them remain subjects of purely academic interest, others have jumped into the limelight due to their attractive properties, which have led to practical applications. Among the latter are 2D carbides and nitrides of transition metals known as MXenes [A. Vahid Mohammadi, J. Rosen, Y. Gogotsi, *The World of Two-Dimensional Carbides and Nitrides (MXenes)*, **Science**, **372**, eabf1581 (2021)]. The family of MXenes has been expanding rapidly since the discovery of Ti_3C_2 in 2011. More than 30 different stoichiometric MXenes have been reported, and the structure and properties of numerous other MXenes have been predicted. Moreover, the availability of solid solutions on M and X sites, multi-element high-entropy MXenes, control of surface terminations, and the discovery of out-of-plane ordered double-M *o*-MXenes (e.g., Mo_2TiC_2), as well as in-plane ordered *i*-MAX phases and their *i*-MXenes offer a potential for producing dozens of new distinct structures. This presentation will describe the state of the art in the manufacturing of MXenes, their delamination into single-layer 2D flakes and assembly into films, fibers and 3D structures. Synthesis-structure-properties relations of MXenes will be addressed on the example of Ti_3C_2 . The versatile chemistry of the MXene family renders their properties tunable for a large variety of applications. In particular, the interaction of MXenes with electromagnetic waves can be controlled via their composition and structure. Many MXenes offer high electronic conductivity and outstanding electromagnetic interference shielding. They can also be used in telecommunication, energy, medical and electronic device applications.

KEYNOTE: Topological Functionalities of Ferroelectric Nanomaterials

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Formation of unusual textures of polarization is imminent for nano-scale ferroelectric samples, films, rods, and granules, where the depolarization surface effects play the crucial role. The topologically protected stability of such textures and security of information storage is coming from polarization vorticity, provided by condition of absence of the energetically-unfavorable depolarization charge. The endurance of ferroelectric formations with respect to high-energy irradiation makes them ideal for the aerospace industry, and the periodic domain walls structures can be used as a platform for terahertz radiation generators and detection devices. Polarization domains that alternate the surface charge distribution can be formed in ferroelectric thin films as an effective mechanism to confine the depolarization field to the near-surface layer and diminish the depolarization energy. However their existence have long been considered as barely possible until the direct theoretical predictions and experimental evidences in thin oxide-based superlattices. Very recently, we have demonstrated that the effective capacitance of ferroelectric layers and capacitor nanodots with domains is negative. This effect is explained by the opposite orientation of the depolarizing field with respect to the field-induced averaged polarization. This phenomenon is currently considered as the platform for realization of the dissipation-free high performance nano-circuits. Moreover, in sub-THz region the resonance plasmonic effect can be induced by oscillating domain walls and can be suitable for design of the ultra-small low-energy THz chips. Multi-vortex, skyrmion and Hopfion states with tunable chirality can be formed inside ferroelectric cylindrical nano-dots and nanorods and nanoparticles to reduce the depolarization energy. We study the stability of such states and demonstrate that the topological class of the most stable topological excitations can be driven by the geometrical and electrical parameters of the system, external field and temperature. We target the multi-domain and topological excitations in FE nanodots as a platform for IT-secured multivalued logic units, breaking ground for neuromorphic computing.

D.c. Charge Carrier Transport in Layered InSe Intercalated with RbNO₃

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Layered InSe crystals are an excellent material for innovative technologies. In particular, insertion of ferroelectric molecules into them enables to achieve new mechanisms of charge accumulation, which is promising for solid-state supercapacitors. Their electrical properties have been studied so far only by means of a.c. impedance spectroscopy. Here, we report on the influence of ferroelectric RbNO₃ intercalation on electrical parameters of n-InSe crystals and their anisotropy probed with d.c. techniques. Single crystals of n-InSe were grown by the Bridgman method from a melt In_{1.03}Se_{0.97}. Measurements of the dependences of the conductivity along the layers and Hall coefficient RH were carried out in the range 80 to 400 K. Intercalation was carried out by exposing InSe in a melt of RbNO₃ at T = 370 C for 10 min. To measure the conductivity across the layers we used a four-probe method. For the intercalated crystals we revealed the increase of RH values, extrema in the RH(T) dependences as well as lower values and non-monotonous changes of the in-plane Hall mobility. The results are interpreted within a model that considers the contributions of 3D and 2D electrons to the transport of charge carriers along the layers. It is assumed that 2D carriers largely determine the transport properties at low temperatures. With increasing T they thermally activate into the c-band of n-InSe and the dimensionality of electron transport changes. The values of $n_2(T)$ and $n_3(T)$ were numerically calculated. For the pristine samples there are only slight variations of out-of-plane conductivity and conductivity anisotropy with T. The insertion of RbNO₃ leads to a decrease (by a factor of 80 to 800) of the transversal conductivity, and the anisotropy ratio considerably increases by a factor of 10 to 40 at 80 K. For the pristine n-InSe samples the value of the interlayer energy barrier is small (7.6 meV) but it essentially increases (to 15–23 meV) after intercalation.

A porous carbon material from agricultural production waste

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Activated carbon materials (ACM) are promising materials for supercapacitors (SCs) due to their amazing microstructure properties. Synthesis of porous carbon from biowaste, in particular of agriculture production, takes a great importance because of their natural existence and low cost. Since electrodes are an important component of SCs, researches of materials suitable for applying as electrode components are given priority. Corn is a widespread farm crop. Corn processing waste due to their properties (structure and high lignin content) are suitable for receiving carbon. In our study we used several types of corn waste: corn husk (CH), corn silk (CS), corn smut (CSm). Each of them has a fibrous structure, which is kept at the micro-level after carbonization. Differences in their original structure enable to compare the quality of the obtained electrode materials. To obtain ACM samples we used two-stage processing - carbonization and chemical activation. At the both stages we applied a technique of "free" carbonization (activation), i.e. a material under processing was placed into a closed reactor with a free flow of the reaction's gaseous products. After carbonization the obtained materials differ in conductivity. It follows from our estimations that the conductivity increases in the next sequence: $CS < CSm < CH$. The specific capacitance of the activated materials was determined for experimental samples of SCs with an aqueous electrolyte. Their disk-like electrodes were done from the pure materials without binding and conductive agents. The SCs samples were tested by using a "Series 2000 Battery Test System" setup. The obtained average values of the specific capacitance are as follows: for the materials activated in water vapors - 60-80 F/g and for those activated in alkaline conditions - 200-250 F/g (CS), 210-270 F/g (CH) and 90-100 F/g (CSm). Based on the above, the waste of corn production are forward-looking materials to produce electrodes for high-power SCs.

Low-dimensional Intercalated, High-Entropy, Synergized van der Waals Nanoheterostructures of Transition Metal Dichalcogenides (2D) and Trichalcogenides (1D): New Approaches to Expanded Applications

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The review is devoted to last results of nanotechnologies and new low-dimensional nanomaterials science of van der Waals (vdW) nanoheterostructures on the basis of 2D semiconducting (MCh_2 , $M = Mo, W, Re$; $Ch = S, Se, Te$), 2D metallic ($M = Nb, Ta$), 1D metallic or semiconducting (MCh_3 , $M = Nb, Ta, Ti, Zr, Hf$) Transition Metal Chalcogenides. Key problems of vdW nanoheterostructures design are analyzing on the basis of new literature data and own results. Various design strategies of vdW nanoheterostructures as new 2D nanomaterials are reviewed: design of new vdW nanoheterostructures: 2D/2D, including graphene; 2D/1D, 2D/3D); dimensionality properties tuning; heterointerface and band-gap engineering; defect control and pore texture tailoring; surface sensitization and functionalization; functional architecture 2D assembly; structure-, surface-sensitive semiconducting 2D properties tuning (intercalation); p-n-nanoheterojunction construction. We summarize and highlight recent advances and state-of-the-art investigations on low-dimensional intercalated, high-entropy, synergized van der Waals nanoheterostructures of Transition Metal Dichalcogenides (2D) and Trichalcogenides (1D). These approaches are analyzed as new paradigms of expanded low-dimensional van der Waals nanomaterials applications: radar absorbing materials, electromagnetic radiation screens; electro(photo)catalysts for Hydrogen production; sensors (humidity, gases, biosensing); sorbents, photocatalysts for water treatment (organics, heavy metals); optoelectronics; biomedical materials; biosensors, disinfection (COVID-19); etc.

Sensor Properties of 2D Disulfide Molybdenum Nanosheets: Humidity - Dielectric Characteristics

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Recently engineering of 2D Transition Metal Dichalcogenides nanosheets has gained significant development for environmental applications: computerized monitoring of air and soil humidity in agriculture, climate control in closed volumes of space stations, aircraft, special production facilities, etc. We present results of systematic studies on intercalation/deintercalation of water vapor from ambient air (30–100 % relative humidity, room temperature) by graphene-like 2D MoS₂ nanosheets, as well as the corresponding changes of dielectric properties (impedance spectroscopy, 1 Hz – 20 MHz, Novocontrol ALPHA broadband dielectric impedance analyzer). It was established that intercalation / deintercalation processes of water vapor significantly change dynamic dielectric characteristics of 2D MoS₂ nanosheets (total, active, reactive (capacitive) resistances, capacitance, real component of the relative dielectric constant and tangent of the loss angle) at all frequency band (1 Hz – 20 MHz). It was assumed that 2D MoS₂ nanosheets as a result of their interaction with oxygen and humid air formed 2D intercalated MoO_{3-x} - MoO₃ - H⁺_x(H₂O)_yMoS₂ van der Waals nanoheterostructures. Obtained data will be used for mechanism establishing and optimization of 2D MoS₂ nanosheets nanotechnology as well as in the development of new 2D humidity nanosensors, nanosorbents and nanophotocatalysts for water purification, nanoelectrocatalysts for hydrogen production by water electrolysis, design of new intercalated 2D van der Waals nanomaterials, etc.

Anisotropic Semiconducting 2D Rhenium Diselenide Nanosheets: Electrochemical Characteristics for NaCl/H₂O Solution

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It is known that ReSe₂ nanosheets are investigated very intensive as perspective 2D anisotropic semiconducting for new van der Waals nanomaterials design in many prospective applications (electronics, optoelectronics, sensors, catalysts, etc.). The results of electrochemical studies of ReSe₂ nanosheets films in aqueous solutions (3 % NaCl/H₂O) are presented. Aim of this study: prospects of anticorrosion coatings with ReSe₂ nanosheets participation, as well as ReSe₂ nanoelectro (photo, piezo) catalysts for hydrogen production in water electrolysis. According to X-ray studies, X-ray photoelectron spectroscopy and Raman spectroscopy ReSe₂ nanosheets are homogeneous (sizes about 20 nm). The samples of ReSe₂ nanosheets films were prepared on glass / quartz substrates after preliminary ultrasonic treatment in aqueous alcohol solutions. Electrochemical corrosion measurements were performed by potentiodynamic polarization curves method (potentiostat PI-50-1, rate of potential supply was 0.5 mV/s). Platinum was used as the auxiliary electrode; potentials (anode or cathode) applied to the work surface which were determined by AgCl reference electrode. The temperature was 24°C in all experiments, electrolyte was 3 % NaCl/H₂O solution. It was shown that ReSe₂ nanosheets films (after ultrasonic treatment of the starting powder in aqueous solutions of ethyl alcohol) during subsequent contact with air (for 2-4 days) interact of surface nanosheets with oxygen (air) which probably leads to the formation of nanoheterostructures ReO₃ - ReSe₂. These factors change the corresponding polarization anode and cathode curves and enhancing of water wetting. Nanocrystalline ReSe₂ films, as well as possible nanoheterostructures ReO₃ - ReSe₂ are chemically stable in electrochemical processing. Films of ReSe₂ nanosheets and nanoheterostructure ReO₃ - ReSe₂ are promising for future studying of anticorrosive characteristics of coatings with their participation.

The obtaining of nanosized BaO/ZrO₂ compositions by mechanochemical and ultrasonic activation methods

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In the past two decades nanomaterials based on zirconium and barium oxides are widely used since they applied as photocatalysts for environmental control technology, have high strength, toughness, chemical stability, excellent corrosion, and chemical and microbial resistance. Mechanochemical and ultrasonic treatment methods as environmentally friendly ones are alternative to traditional techniques of BaO and ZrO₂-containing material synthesis in nanodimensional state without adding of excipients and purification. The purpose of this work is to study the influence of mechanochemical and ultrasonic treatment on the structural, crystal and photocatalytic properties of the stoichiometric mixture BaO/ZrO₂=1:1. BaO/ZrO₂= 1:1 composites were activated mechanically (MChT) for 4 hours in air at 550 rpm and by ultrasonic treatment (UST) of baria-zirconia aqueous solution for 1 and 2 hours using at 80°C. After sonication obtained precipitates were dried in an oven at 120°C in an air atmosphere for 2 hours. Obtained results by XRD method showed that the isotropic destruction of ZrO₂ and decrease of particle size from 31 nm up to 15 nm after MChT and UST for 1h is carried out. It was found the increase of UST duration leads to increase of size crystallites (up to 32nm). These results are in good agreement with TEM data. According to obtained data using N₂-sorption method the increase of specific surface area from 9 to 12 m²/g and formation of mesoporous structure in the sample after mechanical milling was observed. The studies of Ba/Zr powders by DTA-TG methods showed the two-stage water loss process in temperature region 70-270°C and zirconia crystallization at maximum 480°C with total weight loss 5%. The photocatalytic degradation rate of prometrine under UV-irradiation increases from 0.06 to 0.24 s⁻¹. It can be concluded, mechano- and sonochemical activation of BaO/ZrO₂=1:1 samples leads to formation of nanosized mesoporous composites with improved photocatalytic properties.

Formation of L1₀ phase in FePd(5 nm) films during vacuum and hydrogen annealing

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Magnetic materials on the base of FePd with large perpendicular magnetic anisotropy are perspective for use as ultrahigh density recording media in HAMR and development of magnetic tunnel junctions for future spintronic memory and logic devices. The aim was the investigation of environment (vacuum, hydrogen), temperature and duration of annealing on the phase composition, structural and magnetic properties of FePd(5 nm) films. FePd films of equiatomic composition were deposited at room temperature by magnetron sputtering on SiO₂(100 nm)/Si(001) substrates. Heat treatment was carried out in a vacuum and hydrogen atmosphere in the temperature range of (600-700) °C for 0.5-2 h. The films were investigated by X-ray analysis, RHEED, AFM, SQUID and EPR methods. A disordered A1 FePd phase was observed in the as-deposited films. Ordering processes occur during thermally activated A1 → L1₀ solid-state reaction. Annealing in hydrogen significantly activates this process. During annealing at 650 °C for 1 h in hydrogen the L1₀ FePd phase is formed with a coercivity of 5 kOe while in vacuum the ordering processes proceed much more slowly and the coercivity reaches ~ 1 kE. This is explained that Pd absorbs the hydrogen as much as possible. The acceleration of the ordering process is due to penetration of hydrogen atoms into the film and their location in octahedral and tetrahedral voids that expands the elementary crystal lattice. The atomic bonds of Fe-Pd are weakened which promotes diffusion processes and increases the degree of ordering. In addition, the hydrogen atoms affect the electronic structure of the film. A further increase in the temperature or duration of annealing promotes the disordering process and the transition of FePd films to the superparamagnetic state. Thus, during the formation of the L1₀ phase in hydrogen there is a change in magnetic states: soft magnetic → a paramagnetic or superparamagnetic → hard magnetic → a superparamagnetic.

The study of physical-chemical properties and biological activity of nanocomposites based on cerium and lanthanum oxides doped with silver

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Nanocomposites based on oxides doped with rare earth and noble metals are increasingly used in engineering and biomedicine. Because of the expansion of practical application of this kind of composite materials, it becomes necessary to assess their toxicity and safety for the environment and human health. The aim of the work is to study the effect of Ag-doped La₂O₃ and CeO₂ nanoparticles on the survival of bacteria belonging to different physiological and taxonomic groups, and also having a different structure of cell walls. The synthesis of nanocomposites was carried out by co-precipitation of La and Ce salts with AgNO₃ under conditions of controlled hydrolysis. The precipitates were washed, dried, and calcined at T = 400°C. For comparison, a sample of a Fe₃O₄&Ag obtained by rotational corrosion dispersion was taken. When studying the effect of the obtained nanoparticles on the microorganism's survival, cultures of bacteria of different groups were used: Escherichia coli (G-) and Bacillus sp. (G+). The cell suspension was standardized and the bacterial survival rate was determined by the turbidimetric method. The effect of Ag-doped La- and Ce-containing composites on the microorganism's survival and their ability to withstand osmotic stress, depending on the concentration of nanoparticles in solution from 20 to 2000 mg/dm³, was studied. There were no examples of our nanoparticle's acute toxicity in studied concentration range. In contrast to Fe₃O₄&Ag, for particles containing Ce and La, a process of cellular activity's stimulation was observed, which manifested itself in an increase in the bacterial cells' survival under starvation conditions, as well as in an increased survival of the latter under the influence of osmotic stress. The observed stimulation was dose-dependent. The described effects have significant fundamental and applied interest and require in-depth study to elucidate the mechanisms of such interaction.

Magnetic, electric and thermoelectric properties of Co/Al₂O₃, Co/SiO₂ and Co/TiO₂ ferromagnetic nanocomposites

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Ferromagnetic nanocomposites (FMNC) with Co nanoparticles (NPs) in dielectric matrices Al₂O₃, SiO₂ and TiO₂ were grown by the EB-PVD method in the form of film with thickness from 0.8 to 10 μm on Al₂O₃ substrates (polycor). Electrical, magnetic and thermoelectric properties were investigated in the temperature range of 5 ÷ 290 K and in magnetic fields up to 5 kOe. Scanning electron microscopy studies have shown that for all nanocomposites Co NPs have dimensions 10-50 nm. With increasing of Co concentration size of the NPs increases. The temperature dependences of the resistance for Al₂O₃, SiO₂ and TiO₂ matrices were investigated. In coordinates $\ln(\rho/\rho_{77}) \propto (1/T)^{1/4}$ and temperature range 95 - 290 K resistivity is linear and explained by a hopping conductivity of electrons via the localized states (Mott law). We proposed a mechanism of a thermoelectric power for Co/Al₂O₃ FMNC in a strong magnetic field in conditions of a hopping type of electron conductivity over nonmagnetic localization centers. For Co/SiO₂ FMNC decrease of the thermoelectric power in a magnetic field is explained as a result of the chemical interaction of Co and SiO₂ which is associated with mixture of nanoscale ferromagnetic silicides of cobalt and antiferromagnetic CoO. Co/TiO₂ FMNC had shown similar to Co/Al₂O₃ FMNC thermoelectric properties but with a slight increasing magneto-thermoelectric power. Magnetic behavior of the samples with a concentration of Co below the percolation threshold is typical for a superparamagnetic system with blocking magnetic moments of NPs with decreasing temperature. For the samples with concentration higher percolation threshold superparamagnetic behavior was not detected up to 300 K. Non-zero coercivity observed at room temperature and temperature dependences of the ZFC-FC curves (obtained after cooling from nonequilibrium thermal state), indicates that FMNC consists of much larger particles.

Graphenes and nanotubes in deposits of electric arc synthesis

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Purpose: to study the morphology and structure of the deposit as a composite product of electric arc synthesis, as well as the area of their application. In this work, for the synthesis of the composite (deposit), the electric arc method in a gas medium was used, and the treatment of the synthesis product was carried out using ultrasound. The composite consists of carbon nanotubes and packs of graphene sheets. The obtained carbon nanostructures samples were analyzed by derivatographic method, Raman spectroscopy, transmission and scanning electron microscopy. Key words: carbon nanostructures, nanotubes, graphenes, deposit, plasma, Electric arc synthesis. As the experiments have shown, in the plasma of the arc synthesis in addition to the fullerene soot, in which the endfullerenes are formed, a growth, called deposit. It is established, that at evaporation of pure graphite the formed deposit consists of two parts: core and shell (deposit bark). Core consists of carbon nanotubes (CNT), and shell consists of the graphite mass (packs of graphenes). The researches with the help of electron microscopy have shown, the shell is formed by layered structures (graphenes), the planes of which are located perpendicular to the axis of the deposit and densely stacked in a single structure. Also, in electric arc synthesis, it is possible to create conditions for graphite sputtering rather than evaporation. That allows to obtain graphenes and their highly dispersed packs. However, when a graphite electrode sputtered, fullerenes are not synthesized, since graphite does not have time to pass into the atomic state Preliminary results show that it is possible to obtain graphenes and packs graphene in near-wall soot and from the deposit crust. Such graphenes and packs of graphenes contain a given catalyst, what's important for the technology of creating promising new-generation electrical circuits and batteries.

The influence of uniformity in the size of diamond grinding powders on the performance characteristics of the grinding tool

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One of the most important ways to achieve a higher class of the processed surface of products and increase the wear resistance of diamond tools is the use of diamond grinding powders with a higher content of the main fraction and high uniformity in grain composition. Studies were carried out on AC6 grade diamond grinding powders with a grain size of 100/80. To obtain narrow-grain diamond powders, an additional sieve classification was performed with a set of sieves with the size of the holes of the sieves cells, which decrease exponentially. Diamonds of grain sizes 100/90, 90/80 and 80/72 with a form factor less ($K_f=1.20$), for grain ovalization, were subjected to thermochemical treatment using strong oxidizing agents. In the diamond powders obtained after sorting was determined the content of the main fraction by the sieve method, the form factor (K_f), uniformity in linear dimensions (Cun.l.d.) and defectiveness of the surface by surface activity coefficient (K_a). The performance characteristics of diamond wheels using these diamonds were estimated by the relative consumption of diamonds (q_p) and the roughness of the treated surface R_a . Analysis of the obtained data shows that additional sorting of diamonds with a grain size of 100/80 allowed to increase the content of the main fraction and increase the uniformity of diamond powders along linear grain sizes by at least 15%, which reduced the relative consumption of diamonds by about 20% and somewhat reduced the roughness of the treated surface. In turn, ovalization of diamond grains with a grain size of 100/90 made it possible to increase the defectiveness (development) of the surface of diamond grains with a grain size of 100/90 by at least 40%, and this reduced the relative consumption of diamonds by 40% and the roughness of the treated surface by 30%.

Structural aspects of hydrogenation properties of Ni-based materials

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In this report we will analyze the history of studies of hydrogen interaction with nickel bulk, film and powder materials. Extended and systematic studies of the interaction of Nickel with hydrogen were started from the discovery of nickel hydride by Baranowski in 1958. The existence of two phases was shown: a-NiH with a low H/Ni ratio (up to 0.03) and b-NiH_x, where $0.6 \leq x \leq 0.7$. It was established that the latter has a cubic fcc structure with an increased cell parameter by 6% and is unstable and decomposes rapidly in air. The creation of high-pressure equipment allowed to synthesize b-NiH_x hydride from the gas phase at a hydrogen pressure of 6 kbar and to determine the thermodynamic parameters of phase formation/decomposition. A lot of obtained results demonstrated that the formation of the hydride is influenced by the structure of the source metal. In our systematic studies the different types of Ni and Ni-based nano-powders were synthesized and tested. It was demonstrated that hydrogenation properties critically depend on the structure of the particles. The crystal structure of Ni-based nano-powders has been studied precisely by SEM, XRD and SAXS methods. According to the XRD and SEM analysis the size of the obtained nickel nanoparticles covered the range from 20 to 200 nm. The particles consist from crystallites with size of 5-100 nm. The complicated structure of the particles was confirmed by SAXS method. The gas hydrogenation has been studied using Sievert's type apparatus. Electrochemical charge-discharge characteristics were studied using PGStat-8 equipment. It was revealed that the nano-crystallite structure substantially enhances gas and electrochemical hydrogenation of Ni and Ni-based powders. Hydrogenation and/or catalytic properties of the Ni and Ni-based nano-powders as the additives to hydrogen storage or electrode materials will be demonstrated. The analysis of the structural aspects of the hydrogenation properties will be done.

New size effects in the luminescence of ZnS particles obtained by self-propagating high-temperature synthesis

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This work is devoted to the study of Mn-doped highly dispersed ZnS powders obtained by self-propagating high-temperature synthesis using different Zn/S ratios. Powders were obtained from the gas phase inside the reaction chamber but outside the combustion zone. It is shown that the Zn/S ratio significantly affects the phase composition of crystallites and their size. It was found that the largest crystallite sizes, as well as the concentration of Mn incorporated into the lattice, are observed in the material synthesized at Zn = S in the charge, and the minimum particle sizes are observed with an excess of sulfur (ZnS(S):Mn). The absolute sizes of Mn-doped ZnS particles are in the range of 7-200 nm (note, that the Debye screening length for these materials $L \sim 30$ nm). For all Mn-doped ZnS particles obtained, either the entire volume of a particle or its main part (96%) is in the depletion zone, which determines their properties. It is shown that the concentration of Mn in the powders obtained from gas phase is significantly lower than in the powders synthesized within combustion zone. Another distinctive characteristic is the absence of band-to-band excitation bands in ZnS(S):Mn powders in the excitation spectra of the luminescence band of Mn. This is due to the fact that ZnS(S):Mn material mainly consists of the particles with sizes $d \leq 2L$, and the carriers in the conduction band mainly recombine nonradiatively. According to TEM data, the particle size of ZnS(S):Mn corresponds to $d \approx L$. With such a strong overlap of the space charge region (SCR) in ZnS(S):Mn, the surface barrier decreases, and in the case when its values are about several kT , it can be neglected. Due to an overlap of the SCR the recombination via surface states dominates, and the particles can be approximately considered as "barrier-free" particles.

Characterization of nanocomposite Ti-Nb-C films

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The niobium carbide and titanium carbide have attracted considerable attention as protective coating materials. On account of outstanding properties of TiC and NbC, it is of interest to study the material Ti-Nb-C that would combine the properties of constituents. However, there are only few works in which the films/coatings in the Ti-Nb-C system were investigated. The aim of present work is to make up for deficiency of information about the structure and properties of Ti-Nb-C films. The films were deposited by DC magnetron co-sputtering of elemental Ti, Nb, composite Ti/Nb, and graphite targets. The structure and phase composition were examined by XRD. The chemical states were studied by XPS, and the chemical composition was determined by SEM equipped with an EDS detector. The Knoop hardness and friction coefficient were also measured. For comparison purpose the Ti-C, Nb-C and Ti-Nb-C films were deposited. The Ti-C and Nb-C films consisted of TiC and NbC crystallites, respectively. It was suggested that the Ti-Nb-C films were nanocomposite and represent an aggregate of the crystallites of TiC, NbC and their solid solutions embedded into amorphous carbon-based matrix. XPS results confirmed that suggestion. The hardness of Ti-Nb-C film is higher compared to that of Ti-C and Nb-C films. The observed strength enhancement can be associated with formation of TiC-NbC solid solution. The friction coefficient is lowest for the Ti-Nb-C film. The results showed that TiC and NbC films have nanocomposite structure, nc-TiC/a-C and nc-NbC/a-C, in which crystallites of TiC and NbC are embedded into the amorphous carbon-based matrix. The TiNbC films were found also to be Ti-Nb-C/a-C nanocomposites, and the crystallites are TiC, NbC and TiC-NbC solid solution. It was suggested that an increase of hardness of solid solution can be due to strengthening of metal-metal bonds because of formation new Ti-Nb bonds.

Kinetic characteristics of adsorption moisture processes of two-dimensional molybden disulphide nanosheets

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In present time, 2D materials have shown great promises for humidity sensing due to their high surface to volume ratio and sensitivity of electronic properties with variation in surroundings. The purpose of research is to investigate the influence of relative humidity on the processes of moisture adsorption by 2H-MoS₂ nanosheets and micron powders for comparison. The kinetic dependences of moisture adsorption processes of 2H-MoS₂ nanosheets and micron powders were studied by gravimetry (accuracy: $\sim 1 \cdot 10^{-5}$ g) at room temperature (20 ± 2)°C in the range of relative humidity 30–95 % in an enclosed space and in the open air. The supersaturated aqueous solutions of salts were used to obtain the required values of relative humidity in an enclosed space. A hygrometer (TFA 441004, absolute error: ± 1 %) was also used for control of relative humidity. Under the experimental conditions, the test samples were pre-heat treated at 110°C. The time dependences of the change in the mass values of the adsorbate “ α ” were used to analyze the kinetic processes of moisture adsorption of 2H-MoS₂ powders: $\alpha = \Delta m / m_0$, where $\Delta m = m_i - m_0$ – weight gain of the investigated material; m_0 is the initial mass of the adsorbent after thermal desorption treatment; m_i is the current variable mass at the adsorption process. Thus it was found that α increases with an increasing of the relative humidity: $\alpha = 2\text{--}10$ % for 2H-MoS₂ nanosheets, in contrast to 2HMoS₂ micron powders for which $\alpha = 0.08\text{--}1$ %. The study of moisture adsorption processes and possible water intercalation of 2D MoS₂ nanosheets and micron powders makes it possible to determine the influence degree of the size factor on the intensity of such interactions. The processes of water adsorption and possible intercalation can significantly change the functional properties of both MoS₂ nanosheets and micron powders as a result of the formation of MoS₂ intercalation phases (nanophases), which can be effectively used to expand their applications.

Innovative carbon nanostructured material for reusable protective masks

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The creation of modern face protective masks during the global pandemic and environmental disasters is extremely important. Today, scientists all around the world are actively working for the development of protective masks to combat from coronavirus SARS-CoV-2. However, there are studies that have found that high level of air pollution are the factor of increasing the death risk from COVID-19. The complex of properties of activated carbon fiber nanostructured material (AVVNM) developed by the authors as a filter layer of multiple protective face masks has been investigated . It is shown that AVVNM has a high ability to absorb the main environmental pollutants (phenol; metals Pb ²⁺ , Sr ²⁺ , Cu ²⁺ , Ni ¹⁺ , Co ²⁺ , Al ³⁺ , Cs ²⁺ ; chlorine derivatives; radioactive volatile decay products, etc.) and substances of protein nature. It has been established that AVVNM exhibits the bacteriostatic properties which can be transformed into bactericidal by applying the biologically active substances on the surface of material. It is proved that AVVNM meets the requirements for medical materials and can be recommended for the protective masks manufacture.

SURFACE ENGINEERING AND PROTECTIVE COATINGS

KEYNOTE: Design of self-lubricating metallic alloys for operating in extreme environments

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Self-lubricating materials are a broad class of compounds featuring the incorporation of one or more solid lubricants leading to decreased friction and wear during sliding contact. The main driving force behind their development was initially the need of reducing and controlling friction in applications for which conventional oils and greases were ineffective such as under high temperatures ($>300\text{ }^{\circ}\text{C}$) or in vacuum. More recently, the research focus has shifted towards the complete elimination of additional lubrication in forming and machining processes. This work illustrates the challenges of designing self-lubricating metallic alloys using self-lubricating iron and nickel-base alloys as example. The self-lubricating metallic alloys are deposited using laser cladding. The developed self-lubricating laser claddings incorporate solid lubricants such as metal sulfides and soft metals (silver). Their microstructure and phase composition are characterized using X-ray diffraction, scanning and transmission electron microscopy. The friction and wear performance are evaluated using high temperature tribological tests in air and vacuum. The microstructure of the deposited claddings contains homogeneously scattered silver pockets encapsulated within metal sulfides, determined to be chromium sulfides. This resulting microstructure is able to control friction from room temperature to $600\text{ }^{\circ}\text{C}$ in ambient air and at least until $300\text{ }^{\circ}\text{C}$ in vacuum. In ambient air, the friction reduction mechanism is determined by the silver and chromium sulfide pockets. Atomic force microscope investigations show that chromium sulfides have a high hardness and a low intrinsic friction. At higher temperatures, the contribution of silver diminishes due to oxidation so that the role of chromium sulphides to self-lubrication is dominant. In case of high temperature vacuum, the presented self-lubricating claddings are able to effectively control and reduce friction down to a value of 0.25 against 440C martensitic stainless steel at room temperature and $300\text{ }^{\circ}\text{C}$ by the smearing of silver over the chromium sulfides. This friction reduction mechanism is enhanced by the thermal softening of the pure silver phase at elevated temperatures, contrary to air atmosphere, where smearing is hampered by oxidation. This overall tribological performance makes the presented claddings potential candidates for high temperature forming and space applications.

KEYNOTE: Tribology for European Green Deal

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The European Commission is aiming to significantly reduce net greenhouse gas emissions and to make the Europe climate-neutral by 2050. The actions are directed to reduce energy consumption, improve nature, life of people, while also to create longer-lasting products enabling repair, recycling and re-use. In general, tribology covers interaction of surfaces in relative motion. So, everything that is moving around us and even inside our body is experiencing friction and wear, that can be varied by lubrication. Efficient products with increased lifetime can be created with the help of green tribology. Unfortunately, you can hardly find the term tribology in the documents of the European Green Deal, although it was demonstrated, that more than 20 % of today's global total energy consumption is a result of inefficient performance of the tribological contacts and significant improvements could be achieved. Longer-lasting reliable products can save our planet from pollution, since they reduce the need for production of new products and utilization of failed ones. It is the aim of the current work to emphasize the role of tribology for the European Green Deal and to encourage cooperation.

Anomalous hall effect in the Ni/Gd₂O₃ nanostructure

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In our previous studies, it was established that the galvanomagnetic, magneto-optical and current-voltage characteristics of nanoscale layers of iron group Fe, Co, Ni are enhanced due to their contact with layers of rare earth metal oxides (REM). The enhancement was substantiated by the possibility of an increase in the magnetization of these ferromagnetic metals upon ordering of their magnetic structure by the exchange f - d interaction arising at the contact interface between atoms with unfilled f and d electron shells included in the composition of these layers. The aim of this work is to confirm the possibility of increasing the magnetization of the d-metal layers upon their contact with the layers of REM oxides. The Ni (70 nm)/Gd₂O₃ (40 nm) nanostructure was used as an example. The films were formed on a siall substrate by electron-beam deposition of Ni and after Gd. The latter with oxygen admission into the working chamber at low pressure to form Gd₂O₃. It is known that the value of the voltage V in the anomalous Hall effect is very sensitive to changes in the magnetization. Using this, we compared V₁ in a layer of pure d-metal and V₂ in the same layer after deposition of an REM oxide film. Comparison of the dependence V₁ attained for a pure Ni film showed an increase in V₂ for Ni/Gd₂O₃ nanostructure by 25%. A detailed analysis of the reasons that can lead to such an increase in V₂ shows, the most probable of them is an intensification in the magnetization of the Ni layer associated with the action of the exchange f - d interaction between the Ni and Gd₂O₃ layers.

AlCoNiFeCrTiVx high-entropy coatings resulted from electron-beam cladding

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One of the effective methods for improving the physical-mechanical and operational properties of traditional materials is the application of protective reinforcement coatings from new materials. In the last years, as a branch of high-entropy alloy (HEA) materials, HEA coatings have exhibited the attractive and unique properties, relative to the conventional coating materials. Fabricating HEA coatings by electron beam cladding process is of great significance and potential for extensive use. The effect of V content on structure and mechanical properties of HEA AlCoNiFeCrTiVx coatings prepared by the electron-beam cladding on a steel substrate was studied by XRD analysis, scanning electron microscopy and indentation technique. The analysis of the microstructure by SEM shows that the coatings are metallurgical bonded to the steel substrate. The addition of V element to the V-free AlCoNiFeCrTi HEA coating changes the initial phase composition from two solid solutions with bcc1 and bcc2 crystal structure to single bcc solid solution. Also increase in the volume fraction of intermetallic sigma-phases of different type (Co3Ti, NiTi, NiTiAl, and FeV) was occurred while increasing V content from $x = 0.5$ to $x = 1.5$. Moreover, the lattice parameter of bcc solid solutions is a constant and varies only within the measurement error which indicates a monotonic trend of increasing strength characteristics. With the increase of V content due to increase in the sigma-phase volume fraction the values of Vickers hardness and yield strength increased from 8.4 GPa to 11.0 GPa and from 1650 to 2110 MPa, respectively. The AlCoNiFeCrTiVx HEA coatings exhibit good adhesion to the substrate and high strength characteristics. High hardness and strength of HEA coatings are assumed to originate from severe elastic distortions of the crystal lattice caused by the presence of elements with different atomic sizes and hardening by inclusions of the intermetallic sigma-phases. Acknowledgements This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0108)..

The influence of microstructure on thermal properties of columnar ceramic layer produced by PS-PVD method.

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Problem/objective: Plasma spray physical vapour deposition (PS-PVD) is one of the promising method considered as an alternative to Electron Beam Physical Vapour Deposition process used for production of ceramic columnar layer for turbine blades protection against high temperature. The PS-PVD method enables to control the coating structure. Methodology/results: In presented article the dense to columnar structure was formed during single-step PS-PVD process using yttria stabilized zirconia oxide (YSZ). The ceramic coating was deposited using LPPS-Hybrid (Oerlikon-Metco) system at Rzeszow University of Technology. The IN 713 alloy with aluminide coating produced by CVD method was used as a base material. The inner zone of the ceramic coating was characterized by dense structure and the outer was characterized by columnar structure. The influence of power current, gas composition flow, powder feed rate and coating time on thickness of both zones was investigated using Scanning Electron Microscopy method. The relationship between process parameters and thermal conductivity was also investigated using Laser Flash Method (LFA) Conclusions: Conducted experimental process showed that using of 1800A power current higher Ar flow (80 NLPM) as well as powder feed rate (30 g/min) enables to obtain dense structure of coating. When higher energy of plasma (power current 2200, plasma gasses flow (Ar-35 NLPM, He- 60 NLPM) and lower powder feed rate was used the columnar zone was formed. The thickness of obtained coating was in range 140-200 microns. The formation of thick dense layer increased the overall thermal conductivity of coating in comparison with conventional columnar ceramic layer. The combination of thin 20 microns dense-zone with thick (120 microns) columnar zone reduces thermal conductivity of whole coating.

Thermal spraying of MCrAlY overlay coating using new ethanol-fueled HVOF gun

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The MCrAlY overlay coatings are widely used for high-temperature protection of hot section part of gas turbines and jet engines. This type of coatings are usually thermally sprayed using APS (Atmospheric Plasma Spraying), LPPS (Low Pressure Plasma Spraying) as well as HVOF (High Velocity Oxygen Fuel) methods. In present article the newly developed ethanol based HVOF gun was used for production of this type of coatings. The stainless steel 18-8 type was used as a base material. The AMDRY 386 (Oerlikon-Metco) NiCrAlY powder was used for coatings production. In the research different oxygen (400, 500, 600 NLPM) and ethanol (16.5, 18.3, 21.3, 23.6 and 26.6 dm³/min) flow ratio were selected for experimental processes. The powder feed ratio was also changed during process. After deposition the microstructural assessment using Scanning Electron Microscopy and chemical composition analysis using EDS method were conducted. The obtained results showed that coating was above 100 microns thick dependly of process parameters. The low concentration of pores and oxides was also observed on coatings cross-section. Using of ethanol HVOF gun enables to form good quality MCrAlY coatings with 50% reduction of oxygen consumption in comparison with conventional HP/HVOF torch using kerosene such as JP 5000. The other benefit of its using is lower CO₂ emission and lower concentration of carbon in coating in comparison with classic JP 5000 HVOF gun. The ethanol HVOF is a promising technology and might be considered as an replacement of LPPS and HVOF process for production of MCrAlY type of coatings.

Experimental and theoretical study of the electronic band structure of ternary thallium lead iodide Tl₄PbI₆

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The XPS studies yield high quality of the Tl₄PbI₆ crystal, its low hygroscopicity, high stability regarding Ar⁺-ion-irradiation and comparatively strong degrees of covalency of the chemical Tl-I and Pb-I bonds. The latter peculiarity of the crystal under study is confirmed by first-principles calculations that are made within density functional theory (DFT). In the present DFT calculations we consider different models for exchange-correlation potential, and found that the best agreement between experiment and theory is observed when we use modified Becke-Johnson potential as elaborated by Tran-Blaha and involve also the Hubbard correcting parameter U and spin-orbit coupling (SOC) effect. Employing the TB-mBJ+ U +SOC calculations, we examine in detail partial and projected densities of states as well as band dispersions. The TB-mBJ+ U +SOC calculations indicate that Tl₄PbI₆ is a direct gap semiconductor with the energy band gap value of 2.347 eV. This theoretical value is in excellent agreement with that evidenced from experimental measurements of spectral allocation of the absorption coefficient in the range of the fundamental absorption edge yielding $E_g = 2.35$ eV at room temperature. The present measurements of the second harmonic generation intensity of the Tl₄PbI₆ crystal feature high prospective of its application in NLO devices for the studied range of the fundamental beam, approximately 1 μm . We have established that the ignoring of the SOC effect in the calculations predicts a nondirect semiconductor nature in Tl₄PbI₆ being in conflict with the experiment. Based on the TB-mBJ+ U +SOC model, we have calculated in detail the main optical constants of Tl₄PbI₆ allowing to draw a conclusion that it is a good semiconductor for application in optoelectronic devices.

EPR study of germanium doped diamond-like carbon thin films

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Diamond-like carbon (DLC) films doped by germanium (DLC:Ge) possess high hardness and strength, low absorption, refractive index from 1.7 to 4, and good adhesion comparing to undoped DLC films, making DLC:Ge films a promising material for application in optics and biomedicine. However, for their successful application, a detailed study of the effect of Ge content on the physical properties of DLC films is needed. In this work, we have investigated the properties of carbon-related paramagnetic centers in DLC:Ge films by electron paramagnetic resonance (EPR) method. The DLC:Ge films (~200 nm thickness) were deposited by dual-beam pulsed laser deposition technique on SiO₂ substrate with different Ge content (1 at.% and 2.5 at.%). The EPR spectra were measured on Bruker ELEXSYS E580 spectrometer at X-band (~9.4 GHz) at T=296 K. From the analysis and modeling of experimental EPR spectra in Easypin 5.2.28 package, we have revealed that in DLC and DLC:Ge films the single Lorentzian line with $g=2.0026(3)$ is observed corresponding to paramagnetic center with $S=1/2$. The linewidth (dBpp) of the observed single EPR line increases with the Ge content (in DLC film dBpp=0.38 mT, in DLC:2.5%Ge dBpp=2.31 mT). The obtained g -factor and EPR linewidth value is typical for clusterized pi-bonded carbon-related paramagnetic centers that are lead to the appearance of exchange or motional narrowed Lorentzian EPR line. In addition, it was found that the concentration of paramagnetic centers in DLC:Ge films declines significantly with Ge incorporation. According to literature data [1, 2], it was concluded that the observed broadening of EPR line and the decrease of its intensity with increase of Ge content in DLC:Ge thin films is connected with deformed sp²-carbon nanoclusters.

Influence of deformation on mass transfer and phase formation under nitriding of iron-based alloys

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To increase strength, hardness, corrosion resistance of metal products from alloys and steels, the nitriding is used. In modern technologies, to accelerate saturation, improve the quality of surface layers and reduce costs, various physical and mechanical effects on surface of processed products are used. Such influences affect the structure of surface layers and can lead to a change in mass transfer. Promising possibilities of nitriding open up when it is used in combination with deformation. An urgent task in this direction is to study of mechanisms of mass transfer and regularities of phase formation in nonequilibrium conditions, the influence of defects of crystal structure on diffusion. Solution of this problem will allow to create new resource-saving technologies for hardening Metals and Alloys. The influence of preliminary plastic deformation on microstructure, phase composition, and microhardness of diffusion layers formed in iron upon saturation with nitrogen in a gaseous atmosphere at 853 K for 15 minutes has been studied using the metallography, electron microscopy, X-ray diffraction, and microhardness testing. It has been shown that nitrated layers consist of nitride phases and a solid solution of nitrogen in Fe. The relative amount of nitrides in the diffusion zone depends on degree of deformation. The narrow regions of deformations (3-8% and 20-30%) were revealed, in which the nitriding of Fe results in the formation of layers of nitride phases of maximum thickness and a significant increase in microhardness of surface diffusion layers. The microhardness of the layers of nitride phases also correlates with their thickness and phase composition. Thus, an increase in mass transfer of interstitials in deformed Fe is associated with the formation of Cottrells' atmospheres of nitrogen on dislocations and its additional transfer by mobile dislocations according to the dislocation-dynamic mechanism.

The cytotoxicity of ZnO nanostructures doped by Mg and Co

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Zinc oxide, due to its unique physicochemical properties, biocompatibility, and synthesis methods availability, has found a wide range of developments from the production of semiconductor and optoelectronic devices to applications in biomedical devices. Recently, ZnO has also attracted attention as an effective photocatalytic material. However, the main disadvantage of zinc oxide is unable to effectively absorb light in a wide range of the optical spectrum, which significantly narrows its use for photocatalysis. Therefore, we supposed that the incorporation of metals into the lattice of ZnO could improve not only photocatalytic activity but cytotoxicity as well. The report considers results of cytotoxicity of pure ZnO nanostructures (NS) and ZnO NS doped by Mg and Co, which were grown on silicon substrates by Atmospheric pressure metal-organic chemical vapor deposition (APMOCVD) method using mixtures (1÷10wt.%) Zinc Acetylacetonate (AA) with Magnesium (AA) and Cobalt (AA). In addition, the result of the X-ray diffraction and photoluminescence study will be presented. The cytotoxicity of ZnO NS doped by Mg and Co and undoped ZnO films for the comparison were studied in two epithelial cell lines: Hep-2 susceptible to human adenovirus and MDCK susceptible to an influenza virus, at 24h, 48h, and 72h using the MTT method. The Hep-2 cell line is more sensitive than MDCK cultures to test pure and doped ZnO NS. The dose-dependent effect was observed for the Hep-2 cell line since, with increased dilution, the cytotoxicity decreased. The highest cytotoxic effect was about 97-100% inhibition of cell viability at undiluted samples of pure ZnO NS and ZnO NS doped by Mg, Co after all time of incubation at Hep-2 cell line. For a dilution of 1:10 and 1:100, the percentage inhibition of cell viability ranged from 3 to 40%. The largest cytotoxicity for the MDCK cell line was observed for ZnO: Co NS about 50-70 % for as undiluted and as diluted samples after 48 h.

Surface hardening of 40X steel by the sequent electric-spark alloying with niobium and chromium

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One of the most important problems of science and technology is to ensure the durability and reliability of the machine parts and tools that works in difficult conditions. The direction of solving this problem is hardening of the surface layer of products. A promising method of creating of coatings, which operated in extreme conditions, is electric-spark alloying (ESA). In this method by means of concentrated flows of electric energy, surface layer chemical composition, structure-phase state and properties is being modified. The aim of this work is to investigate the influence of sequence of electric-spark alloying by niobium and chromium on the kinetics of formation, structure, phase composition, microhardness of surface layers of the steel 40X. The "ELITRON-26A" unit was used at ESA. Niobium and chromium anodes were chosen due to the formation with the base iron of solid solutions or intermetallics to increase the surface microhardness. Discovered, that with changing the sequence of alloying with niobium and chromium leads to surface microhardness and thickness changes. The possibility of creating reinforced coatings on 40X steel by electrospark alloying with chromium and niobium both separately and in different sequences has been established. The influence of ESA Cr and Nb sequences on the microstructure, microhardness and phase composition of 40X steel surface layers was established. In ESA in the Cr - Nb sequence, high values of microhardness 13 GPa are combined with a relatively thick layer thickness of 35 μm , which is due to the formation of a solid solution of Cr-Fe and the formation of the intermetallic $\text{Fe}_{6.8}\text{Nb}_{6.2}$. When ESA in the sequence Nb - Cr microhardness is 13.5 GPa, and the layer thickness is 25 μm .

Vacuum studies of wetting and adhesion in the semiconducting tin and indium oxides - metal melts systems

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Due to the unique combination of electric and optical properties such semiconductor oxides as tin and indium oxides are very perspective multifunctional materials for the wide range of industrial sectors and variety of microelectronic devices production. Experimental studies of these materials are of apparent interest from the point of view of physics, solid state chemistry, material science as far as they allow to define, for example energetic characteristics and physical parameters of the devices created and also to improve existing technologies of films formation, joining of electrocontacts to tin and indium oxides based materials by way of e.g. brazing which require additional wetting studies. It should be noted that data on wetting of mentioned oxides by metals are practically absent in literature. A detailed study of the interfacial interaction, adhesion and wetting of ceramic SnO₂ and In₂O₃ materials with some pure metal melts in vacuum was performed. Wetting experiments were performed by the sessile drop method using foto- and videocamera for processes fixing. Concentration, temporal and temperature dependences of contact angles were obtained. The microstructure of the ceramic-metal contact zone was also investigated. It was found that majority of the pure metals don't wet SnO₂ ceramics. However the quite intense chemical interaction taken place in vacuum at high temperatures in contact of some metals (Sn, Ge, In) with the surface of tin dioxide. The kinetics of wetting and interfacial interaction of Sn and Cu in contact with SnO₂-ceramics was studied. It was shown, that wetting angles for powdery specimens in the temperature range studied don't change noticeably and vary in a narrow range. For example, for Ga wetting angles vary from about 138 to 128 deg. and for Sn - 125-119 deg., demonstrating as a whole low degree of wetting of powdery pressed substrates of In₂O₃ by metal melts studied.

AlB12-Al electric spark coatings on steel 45

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Up to 70% of machine parts and technological equipment are known to fail as a result of natural wear and tear. To increase the wear resistance, protective electric spark (ES) coatings applied to the working surfaces of parts are quite effective. Investigated in the work is the study of the structure and properties of ES-coatings of AlB12-50 wt.% Al aluminum-matrix composite electrode material on the Steel 45. Fundamental possibility of such coatings obtaining is estimated by theoretical calculation of Palatnik's criterion ($P = 0.11$). Mass transfer kinetics at ES alloying is studied. Microhardness of the coatings H_{μ} was measured on a PMT-3 microhardness tester at a load of $P = 0.5$ N. Tribotechnical studies of the coatings were carried out on a MT-68 friction machine according to the pin-on-disk scheme in the mode: $P = 0.2$ MPa, $V = 4$ m/s, friction path $S = 3$ km. The hardened U8 steel (HRC 61-63) was used as a counterbody. Phase composition of the coating was studied with Rigaku MiniFlex 300/600 diffractometer ($\lambda = 1,5418$ Å) and elemental X-ray spectrum analysis of the surface and cross-section was carried out using a JEOL JSM-6490 LV scanning electron microscope. Considering a rather high values of the cathode mass gain, the coating applied in 4 mode ($E = 0.61$ J, $\tau = 170$ μs, ALIER-52 setup) was selected for further research. The thickness ($h \sim 53$ μm), microhardness ($H_{\mu} \sim 10$ GPa) and wear at dry friction (5.01 mg/(km•cm²)) were determined for the coating. The following phases namely Al₁₃Fe₄, AlFeO₃, AlB₂ и Al₂O₃, and small quantity of Al, B, B₂O₃, AlBO₃, AlFe, AlFe₃ и AlB₁₀ were revealed by X-ray analysis in the coating. The wear of the ES-coated specimens is shown to be 2.7 times less than that of the uncoated one, which is attributed to the formation of intermetallic and boride phases in the coating structure. A conclusion is made about the possibility of using this electrode material for ES alloying of structural steels.

Hardfacing with flux-cored electrodes containing a reaction mixture of Me / B-C

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The aim of the study was to develop the flux-cored electrodes with increased wear resistance for hardfacing of working surfaces of tools that works under conditions of intensive abrasion wear and with cyclic loads. Such equipment are machines for woodworking and production of building ceramics. Researched flux-cored electrodes containing a reaction mixtures of pure metal powders of Ti and Mo, fine powders of B and C. Methods of research are scanning electron microscopy (SEM), optical microscopy, X-ray spectroscopy, abrasion resistance measurement ASTM G65. It was established that offered materials are characterized with fine structure, containing hard Mo₂FeB₂ phase with high microhardness (~ 30 GPa) that forms around the fine grains of TiC that work as a modifier for the main hard phase formation. Was investigated, that proposed flux-cored electrodes can increase the abrasion wear resistance in 2.0 - 2.5 times comparing with serial flux-cored electrodes based on Cr.

Influence of the initial structure on superficial characteristics of the metastable β titanium alloy after ball burnishing

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The correlation dependencies between ball burnishing parameters and roughness, surface topography and hardness of the metastable titanium alloy (Ti-5Al-5Mo-5V-1.5Cu-Fe) with the single β -phase, two $\alpha+\beta$ -phase lamellar and equiaxed initial structures were investigated. It was shown that burnished load increment up to 300 N, the surface topography improves regardless of the initial structural state of the alloy. At burnished load with more than 400 N the surface quality deteriorates due to spalling of the surface layers. Also, with a load increasing during burnishing from 100 to 400 N, the surface microhardness of the alloy with initial two-phase structure increase due to a decrease of grain α -phase size in the subsurface layer. On the other hand, the alloy with the original single β -phase structure is not sensitive to such treatment. This indicates that in the process of surface deformation, the main strengthening effect was occurred due to the twinning of small lamellar or globules of the α -phase. Moreover, for large grains of the β -phase, the implementation of the process of grain refinement by fragmentation requires higher loads. Regarding the influence of the number of passes, then with their increase, regardless of the initial structural state, the surface topography of the alloy was improved due to the smoothing of the grooves, which contributes to improving roughness. However, an increase in the number of passes has little effect on the surface hardening of the alloy of various initial structural states.

Electrodeposition of protective tungsten coatings obtained from ionic melts

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Melts containing tungstates, which are typically ion liquids, are thermally stable, have comparatively high melting temperatures and viscosity, and rather high conductance and high disintegration stress. A collection of electrochemical and physicochemical methods was used in investigating the deposition of coatings, including potentiostatic and galvanostatic electrolysis, X-ray phase analysis, profilometry, and wear and abrasion tests. Tungsten coatings in a $KCl-NaCl-Na_2WO_4-NaPO_3$ melt were produced within the 973-1073 K range at cathodic current densities up to 25 A/dm², once the previously determined relation $0.02 < [PO_3^-]/[WO_4^{2-}] < 0.18$ was satisfied. Tungsten coatings in a $Na_2WO_4-NaPO_3$ melt were obtained within the range 1023-1123 K at current densities up to 40 A/dm² and a metaphosphate concentration from 0.5 up to 15 mol.%. Adhesive, uniform tungsten coatings on nickel, copper, graphite, tungsten, and molybdenum were obtained from oxyhalide electrolyte. Steels, solid alloys tungsten-cobalt, as well as copper- and nickel-plated titanium were added to these substrates in the oxide melts. The microhardness is in the range 4.5-4.8 GPa. A diffusion zone extending for 5-20 μm , which is revealed by microscopic X-ray spectrum analysis of a transverse micro-section of a sample, attest to interdiffusion of the elements of the coating and the base and maintains excellent adhesion of the coating. The continuity of the transition of the coating into the base is confirmed by stereoscopic scanning patterns of coated samples cross-sections on which the columnar structure of the deposit is also clearly visible. As a result of deposition of the coating the abrasion resistance increased by from 4.5-fold to 5.7-fold. Abrasion resistance tests of samples of steel with tungsten coatings were conducted by subjecting a 100 μm fraction of electrocarborundum to a load of 52 ± 0.25 N. Thanks to the coating, the abrasion resistance grew by from 2.5-fold to 4.3-fold.

Morphology and properties of cobalt deposits obtained by electrocrystallization in a magnetic field of low induction

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Problem statement and objective. Cobalt deposits are used in industry as functional coatings. In terms of properties, they are worse with nickel deposits, but their corrosion resistance is higher. It is known that low induction magnetic field (MF) influence on electrocrystallization and the properties of copper and tin deposits. We carried out a study of the relationship between the surface morphology electrocrystallized in low induction MF of cobalt deposits with their properties. The aim of the work is cobalt deposits with improved physical and mechanical characteristics. Methods. The electrocrystallization of cobalt deposits was carried out from a solution containing, M: CoSO₄ - 1.6, H₂SO₄ - 0.4, H₃BO₃ - 0.65. The current density was 5–15 A/dm². The cell was a glass container, around which a uniform magnetic field was created with an induction of about 1 mT. The morphology of was studied by scanning electron microscopy (SEM-106I). Main results and Conclusions. It was proved in the work that the electrocrystallization of cobalt in low induction MF affects the morphology and properties of the deposit. An increase in the current density leads to a decrease in the size of the granular aggregates. The same effect is observed with increasing MF induction. The deposits obtained at the highest current density and magnetic induction have grain aggregate sizes up to 500 nm, which affects the reflectivity and microhardness of the deposit. The reflectivity of deposits obtained by deposition in MF is significantly higher compared to deposits obtained without MF and is equal to the reflectivity of the reference sample (with a specular reflectance of 65%). The microhardness of cobalt deposits obtained by electrocrystallization in MF is 3000 MPa, which is comparable to the microhardness of nickel deposits. The study determined the optimal parameters of electrolysis to obtain deposits with high hardness and reflectivity, as well as low surface roughness.

Deposition and characterization of multilayer Ti-B/C coatings

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Present-day industry needs coatings which would combine high hardness with low friction coefficient. In recent years the efforts were directed to development and study of multilayer coatings that consist of sequential layers properties of two different materials. An attention of researches has attracted the nanocomposite coatings in the Ti-B-C system. However, the works on multilayer Ti-B/C coatings are practically absent. The present work is aimed to meeting a lack in that field of materials science. The nanolayered TiBC/C coatings were deposited from the target of 90 at. % TiB₂+10 at. % C and graphite target using a commutator that sequentially activated magnetrons. Crystalline structures and the chemical bonds of coatings were studied by XRD and XPS methods, respectively. Coating morphology and roughness were studied by SEM method. The Knoop hardness and tribological properties of coatings were also investigated. Four coatings with varying thickness of carbon layers were deposited. XRD revealed three peaks corresponding to crystalline phases in deposited coatings. Experimental data and the results of first-principles calculations have made it possible to conclude that layered TiBC/C coatings are a sequence of nanocrystalline Ti(B,C)₂ solid solution with grain size about 8-10 nm and amorphous carbon layers. This suggestion is also supported by the XPS results which showed presence of Ti-B, Ti-C, B-B, C-C, and B-C bonds in coatings structure. An increase in the thickness of carbon layers resulted in decrease in friction coefficient from 0.73 to 0.38. The Knoop hardness showed that there is an optimum Ti-B to C layers thicknesses ratio at which the coating hardness is maximal (37.5 GPa).

Structure and wear behavior of (Ti,Cr)C-Ni detonation-sprayed coatings

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This study reports the influence of Ni content on the structure and wear resistance of (Ti, Cr)C-based coatings. The (Ti,Cr)C-based composite powders, clad with 18, 25 and 33 wt% Ni, were used to deposit coatings on stainless steel substrate by detonation spraying technique. The thickness of the coatings reaches 350-500 μm , the porosity is less than 2%. The (Ti,Cr)C-Ni coatings have a dense lamellar microstructure with uniform distribution of refractory particles and metal binder. The wear behavior of the (Ti,Cr)C-Ni coatings against steel ring were investigated by dry sliding wear tests. The results show that the (Ti,Cr)C-Ni coatings exhibit good wear-resistance with wear rates of 2.5-5 $\mu\text{m}/\text{km}$. Depending on the Ni content and wear test mode the wear mechanism of the (Ti,Cr)C-based coatings changes from delamination and abrasive wear to oxidative wear.