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SYNTHESIS, STRUCTURE, AND PROPERTIES OF HIGH-ENTROPY MATERIALS

Abstracts of the III International Conference and School of Young Scientists

Institute of Metallurgy, Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia, October 11-15, 2021

FEDERAL STATE AUTONOMOUS EDUCATIONAL INSTITUTION OF HIGHER EDUCATION
"BELGOROD STATE UNIVERSITY"

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Salishchev G.A*. – Doctor of Technical Sciences, Professor, Head of the laboratory of the Belgorod State University;*

Tikhonova M.S. *– Ph.D., senior researcher of the laboratory of the Belgorod State University;*

Povolyaeva E.A. *– Laboratory engineer at of the Belgorod State University.*

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The collection contains the abstracts of III International Conference and School of Young Scientists "Synthesis, structure, and properties of high-entropy materials". It presents reports by leading scientists, young scientists, graduate students, students, industry representatives and highlights current trends in the development of high-entropy alloys and coatings, new materials, modern methods of their study and technologies for the manufacture of promising products. The School of Young Scientists is held within the framework of the implementation of the RSF agreement No. 19-79-30066.

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ФЕДЕРАЛЬНОЕ ГОСУДАРСТВЕННОЕ АВТОНОМНОЕ ОБРАЗОВАТЕЛЬНОЕ УЧРЕЖДЕНИЕ ВЫСШЕГО ОБРАЗОВАНИЯ
«БЕЛГОРОДСКИЙ ГОСУДАРСТВЕННЫЙ НАЦИОНАЛЬНЫЙ
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(НИУ «БЕЛГУ»)

ПОЛУЧЕНИЕ, СТРУКТУРА И СВОЙСТВА ВЫСОКОЭНТРОПИЙНЫХ МАТЕРИАЛОВ

Тезисы III Международной школы-конференции молодых ученых

Институт металлургии Уральского отделения Российской Академии Наук,

г. Екатеринбург, Россия, 11-15 октября 2021 г.

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Составители:

Салищев Г.А. *– д.т.н., профессор, заведующий лабораторией НИУ «БелГУ»;*

Тихонова М.С. *– к.ф.м.н., старший научный сотрудник лаборатории НИУ «БелГУ»;*

Поволяева Е.А. *– инженер лаборатории НИУ «БелГУ».*

П 92 **ПОЛУЧЕНИЕ, СТРУКТУРА И СВОЙСТВА ВЫСОКОЭНТРОПИЙНЫХ МАТЕРИАЛОВ:** Тезисы III Международной школы – конференции молодых ученых (г. Екатеринбург, 11-15 октября 2021 г.) / под ред. Г.А. Салищева, М.С. Тихоновой, Е.А. Поволяевой. – Белгород : ООО «Эпицентр», 2021. – 100 с.

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Сборник содержит тезисы международной школы – конференции молодых ученых «Получение, структура и свойства высокоэнтропийных материалов». В нем представлены доклады ведущих ученых, молодых ученых, аспирантов, студентов, представителей промышленности и освещены актуальные направления в области разработки высокоэнтропийных сплавов и покрытий, новых материалов, современных методов их изучения и технологий изготовления перспективных изделий. Школа молодых ученых проводится в рамках реализации соглашения РНФ№19-79-30066.

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A.K. Stepchenkov, Junior Researcher, Laboratory of Mechanical Properties, Institute of Metal Physics, RAS Ural Branch;

E.A. Povolyaeva, Engineer, Laboratory of Bulk Nanostructured Materials, Belgorod State National Research University.

TOPICS

Main directions of work:

- High- and medium-entropy alloys, compositionally complex alloys: fabrication and processing methods, structure, mechanical, and functional properties, phase stability and phase transformations, deformation mechanisms, diffusion and ordering;
- High-entropy and compositionally complex coatings, methods of their production, structure, and properties;
- High-entropy ceramics, methods of their preparation, structure, and properties;
- New compositionally complex materials for technology and medicine, including nanostructured materials, microstructure design of multicomponent materials, practical applications;
- Advanced methods of fabrication and processing of metallic and non-metallic materials for structural and functional applications, including additive technologies, new methods of casting, powder metallurgy, welding, surface treatment;
- Other promising developments of new metallic and non-metallic materials;
- Computer modeling of the behavior of compositionally complex alloys, coatings and ceramics in different conditions.

The school will be supported under RSF grant No. 19-79-30066 "Advanced alloys and technologies for the aerospace industry."

Lecturer of the Young Scientists School

THE EFFECT OF NITROGEN AND CARBON ALLOYING ON TEMPERATURE DEPENDENCE OF DEFORMATION BEHAVIOR, STRAIN HARDENING AND DEFORMATION MECHANISMS OF CANTOR ALLOY

Astafurova E. G.*, Reunova K. A., Astafurov S. V., Melnikov E. V., Panchenko M. Yu., Moskvina V. A.

Institute of Strength Physics and Materials Science SB RAS, 2/4 Akademicheskii ave., 634055, Tomsk, Russia
*elena.g.astafurova@ispms.ru

The deformation behavior and hardening mechanisms of the nitrogen- and carbon-alloyed multicomponent alloys (FeMnNiCoCr – 1 at.% N, C) in comparison with interstitial-free Cantor alloy (FeMnNiCoCr) were explored in a wide temperature range (77-673 K). For single-phase interstitial-containing alloys, the temperature dependences of the yield strength, tensile strength, elongation-to-failure were analyzed in the correlation with deformation mechanism and microstructure. Additionally, the effect of hydrogen-charging on deformation mechanisms, dislocation arrangement, tensile properties and fracture was studied for carbon- and nitrogen-alloyed alloys.

Both nitrogen and carbon alloying cause sufficient hardening and influence dislocation arrangement, deformation and fracture mechanism of the Cantor alloy. Interstitial-hardening forces the temperature dependence of the yield strength of Cantor alloy. At room temperature deformation, interstitial alloying assists planar dislocation slip and suppresses deformation twinning due to increase in stacking fault energy of the alloys relative to interstitial-free alloy. Planar dislocation arrangement in interstitially strengthened alloys forces the formation of high dense dislocation walls and planar dislocation arrays, which cause strain hardening higher than wavy slip and cellular dislocation arrangement (with mechanical twinning at high strain) in interstitial-free alloy. All alloys possess high elongation-to-failure in high-temperature deformation regime and fracture in ductile transgranular mode. The decrease in deformation temperature facilitates planar slip and twinning in all alloys, causes high strain hardening of all alloys. Plasticity of the Cantor alloy at 77K is visibly higher than at higher temperatures, which is the result of high planarity of dislocation slip and activation of deformation twinning. Despite the similar deformation mechanisms, the elongation-to-failure in interstitial-bearing alloys decreases in low-temperature deformation regime relative to the values characteristic for the interstitial-free Cantor alloy. Nevertheless, it is still as high as in high-temperature deformation regime, and specimens fracture in ductile manner (dimple transgranular fracture) at 77K. To conclude, interstitial-hardening assists the formation of multicomponent alloys with excellent mechanical properties in temperature range 77-673 K.

Interstitial-alloyed alloys possess higher stability against hydrogen embrittlement (in electrolytical hydrogen-charging) in comparison with Cantor alloy. Relative to the deformation mechanisms, hydrogen effects similar to other interstitials – assists planar dislocation glide.

The research was supported by the Russian Science Foundation (project No. 20-19-00261).

EFFECT OF HEAT TREATMENT ON THE STRUCTURE, MECHANICAL AND ELECTRICAL PROPERTIES OF WIRE ALLOY Al–3.3Cu–2.5Mn–0.5Zr (wt%) MANUFACTURED BY ELECTROMAGNETIC CASTING

Belov N.A.[1*], T.K. Akopyan T.K.[1], Cherkasov S.O.[1], Timofeev V.N.[2]

[1]National University of Science and Technology MISiS, Moscow, Russia
[2]Siberian Federal University, Krasnoyarsk, Russia
[*]nikolay–belov@yandex.ru

The experimental heat resistant Al-3.3Cu-2.5Mn-0.5Zr (wt.%) alloy has been manufactured using the electromagnetic casting (EMC) technique providing casting at an ultra-high solidification rate. The obtained long-length cast rods (~20 m) with diameters of 8 mm and 10 mm have been subjected to combined processing including cold rolling, drawing and intermediate annealing. The effect of processing parameters on the structural evolution, mechanical and electrical properties has been analyzed using thermodynamic calculations and experimental studies including transmission electron microscopy (TEM), atom probe tomography (APT), microhardness and specific electrical conductivity measurements, and uniaxial tensile tests.

In the as-cast state, the EMC rod shows a very fine homogenous microstructure with extremely thin eutectic veins of 0.5 μm. All Zr and Mn are dissolved in the aluminum solid solution (Al). This type of structure provides for sufficient plasticity of the alloy. Successful cold rolling of the 10 mm EMC rod down to 2 mm strip has confirmed this assumption. Cold rolling has led to a remarkable increase in hardness (from 60 to 130 HV). Annealing of the cold-rolled strip at 350 ^{0}C for 48 h insignificantly reduces the hardness, but the electrical resistivity (ER) decreases by almost 3 times (from 115 to 40 nΩm). Electron backscatter diffraction (EBSD) analysis has revealed complete recrystallization after annealing at 450 ^{0}C, while at 350 and 400 ^{0}C the non-recrystallized structure is retained.

The experimental alloy has shown excellent processability in wire manufacturing from the as-cast EMC rod both for rolling and drawing. The large deformation during rolling (reduction 98.4%) and high fraction of the Zr- and Mn-bearing nano dispersoids ($Al_{20}Cu_2Mn_3$ and Al_3Zr-$L1_2$) have stipulated the high set of mechanical properties and electrical conductivity after annealing at 400 ^{0}C (UTS~330 MPa, YS~250 MPa, EL~7%, 42.5IACS). Alloying of pure metals is known to increase their electrical resistivity. A calculated model of ER dependence on the phase composition has been proposed. We show that at high annealing temperatures starting from ~ 400 °C there is a good agreement between the calculated and experimental values. With a decrease in temperature the difference between the calculated and experimental values increases that can be attributed to exposure times insufficient for achieving the equilibrium (Al) composition. Since the ER is primarily dependent on the (Al) composition, precision evaluation of the Cu, Mn and Zr concentrations in (Al) at different temperatures (350-450 ^{0}C) has been carried out by atom probe tomography analysis (APT). Root-mean-square (RMS) diffusion distances have also been calculated for estimating the time required for reducing the Cu, Mn, Zr concentrations in (Al) to equilibrium at a specific temperature.

According to the experimental data, annealing at between 350 and 400 ^{0}C allows achieving (Al) compositions close to the equilibrium state in reasonable time while with decreasing temperature the diffusion rate of zirconium in (Al) decreases and thus it requires extremely long exposures, e.g. at 300^{0}C it is about 23,000 h. From this viewpoint wire annealing at below 350 °C appears to be unreasonable des potential for achieving lower ER.

The study was carried out with the financial support of the grant of the Russian Science Foundation № 20-19-00249.

THERMAL STABILITY OF Ti-O-N FILMS

Boytsova E.L.

Tomsk Polytechnic University, Lenin av. 30, Tomsk, 634050, Russia
boi5@list.ru

Thin oxynitride films of Ti-O-N titanium, used in various industries and medicine, are subjected by high-temperature treatment. The perfection of the film structure is de-termined by the method of deposition of the films, the annealing regime, the type of substrate and adhesive sublayers [1]. Crystalline modifications of titanium compounds, such as anatase and rutile, have various chemical, thermodynamic, and mechanical prop-erties. Therefore, the control of the crystalline perfection of a thin film and its relation on physical parameters are the most important stage of the study of the formed multi-layer thin-film compositions. The purpose of this work is to investigate possible phase transformations of Ti-O-N films under exposition of high temperatures.

Films of 30-50 nm thick, formed by magnetron sputtering on a silicon substrate [2], were annealed at the temperature range 600-1300 ℃, which was controlled by DTA analysis (SDT Q600). SEM analysis (Vega3 SBU) does not reveal visible integrity prob-lems of the films at the temperature 1300 ℃. Films have good adhesion to the substrate, which is also confirmed by DTA and EMF analysis [3]. The structure of coatings before and after annealing was investigated by Raman spectroscopy (Centaur U HR) [4]. The Raman spectra of the initial samples of the film showed a two-phase structure, after an-nealing, the intense peaks in the spectra correspond to the rutile phase (310 cm-1 and 430 cm-1).

Thus, the obtained data indicate the thermal and mechanical stability of the oxynitride film of titanium, and also indicate the uniformity of the nanocrystalline structure. The predominance of the rutile phase in the films confirms the photocatalytic activity of the oxynitride coatings.

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DEVELOPMENT OF THE THEORY OF GROWTH OF PRODUCTS OF CHEMICAL REACTIONS IN SOLUTIONS BASED ON VARIATION PRINCIPLES OF THERMODYNAMICS

Dudorov M.V.

South Ural State University (national research university),
Department of Pyrometallurgical and Foundry Technologies, Chelyabinsk, Russia
dudorovmv@susu.ru

An important task in the study of high-entropy alloys is to investigate the regularities of the growth of crystals of a new phase from the initial multicomponent melt under various cooling conditions [1]. In this work, on the basis of the variational principles of thermodynamics, a theory

of the growth of nucleus of the new phase of the products of chemical reactions in solutions was developed. This theory can be extended to various systems, including metastable ones.

The processes of growth of the nucleus of the new phase from the initial multicomponent solution were described by methods of non-equilibrium thermodynamics, taking into account the influence of thermal and diffusion processes in both phases. The processes at the phase interface were presented in the form of chemical reactions of the formation of products from the initial components of the solution. Taking into account that chemical reactions can proceed non-linearly, a new approach to describing the regularities of the processes at the phase interface has been developed on the basis of the variational principles of thermodynamics. The method allows to describe the growth of the nucleus taking into account the mutual influence of thermal, diffusion, and vacancy processes in the growing nucleus and the initial phase of the solution, taking into account the influence of "metastable" effects. Thus, the description of the growth of nucleus under the condition of local equilibrium at the surface of the nucleus is a special case of the developed theory [2].

Different directions of development of the theory for the description of various physico-chemical processes in multicomponent melts were considered. To study solid solutions, the developed software package made it possible to calculate the growth of α-Fe (Si) nanocrystals upon annealing the $Fe_{73.5}Cu_1Nb_3Si_{13.5}B_9$ amorphous alloy in order to obtain a nanocrystalline state [3]. The regularities of crystal growth were studied, and the influence of metastable effects on the deviation of the component concentrations at the crystal surface from equilibrium values was estimated. For the study of eutectic systems, investigations of the supercooled melt of the composition $Fe_{83}B_{17}$ were carried out. An analogue of the equilibrium phase diagram of the Fe-B system was constructed, taking into account the growth of equilibrium and metastable phases. The regularities of the growth of Fe and Fe_2B crystals, as well as of metastable Fe_3B crystals, have been studied under various rates of melt supercooling.

The physico-chemical processes of the solid-phase reduction of iron in multicomponent systems were described, in which, along with thermal and diffusion processes, the influence of vacancy movement was observed. Thus, the possibility of applying the developed approach to the description of various problems of the growth of nucleus of the new phase in multicomponent solutions, including high-entropy alloys, has been demonstrated.

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Lecturer of the Young Scientists School

SIMULATION STRACTURE OF HIGH-ENTROPY MATERIALS USING MACHINE LEARNING INTERATOMIC POTENTIALS

Mirzoev A.A.1, Balyakin I.A. 2, Gelchinski B.R.2*, Rempel A.A.2

[1]South Ural State University, Chelyabinsk, Russia,
[2]Institute of Metallurgy, Ural Branch of the RAS, Ekaterinburg, Russia
[*]b.gelchinski@gmail.com

Computer simulation plays an important role in the design of promising High-Entropy Materials and the prediction of their properties. Ab initio methods based on the theory of density

functional theory (DFT) provide high accuracy of calculations, but their high computational costs limit application scales to hundreds of atoms and picoseconds. Atomistic simulations by Monte Carlo (MC) and molecular dynamics (MD) methods open the way to large scales of size and time. However, MD and MC simulation requires an interatomic interaction model that would predict the forces acting on atoms, depending on the location of their surrounding neighbors. This requires knowledge of the potential energy surface (PES) of the material under study. Several approaches can be used to construct the PES. The most accurate approach is based on the calculation of potential energy within the framework of the density functional theory (DFT), but, as we have already noted, it is very computationally demanding and not suitable for simulation High-Entropy Materials. The second approach is empirical or semi-empirical PES models, which allow fast calculations of large atomistic systems (up to millions of atoms) for a long time (up to microseconds), but their accuracy is often insufficient for quantitative analysis. This is what stimulated the emergence of a new class of models of interatomic interaction - machine learning interatomic potentials (MLIP). If semiempirical potentials are used to represent the energy surface, then it is decomposed into functions of a certain type, adapted to describe a specific type of chemical bond. On the contrary, when developing MLIP potentials, very general functional forms (for example, splines or Gaussians) along which the PES is decomposed are used. In this case, the number of adjustable parameters increases sharply; therefore, ab initio calculation data are used to construct reliable potentials, and detailed checks of the obtained PES are required to make sure that it has the correct shape. However, if successful, the constructed potentials can be very numerically accurate, and they describe any type of interaction equally well, whether metallic or covalent or ionic. Over the past decade, machine learning interatomic potentials have reached a certain maturity and have become a worthy alternative to conventional interatomic potentials. This success was largely facilitated by the American Materials Genome Initiative, as well as the support of the European Council for Materials Modeling, within the framework of which the open Internet platform NanoHUB, Quantum Material Properties Database (OQMD), the integrated software infrastructure for automated materials design (AFLOW) and many others were founded. Compared to the traditional approach, the process of designing potentials using machine learning methods has several features. In this paper, we present data on the possibilities of using MLIP for simulation High-Entropy Materials.

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CARBOSILICOTHERMIC SYNTHESIS OF HIGH-ENTROPY MX CARBIDES

Istomina E. I.*, Istomin P. V., Nadutkin A. V., Grass V. E.

Institute of Chemistry of Komi SC UB RAS, Syktyvkar, Russian Federation
*Istomina-ei@yandex.ru

The group IV and V transition metal binary carbides with the rock salt type structure (B1), including TiC, ZrC, HfC, NbC, and TaC, are well known as the most refractory compounds having melting temperatures above 3000 °C. At the same time they exhibit extremely high hardness and elastic moduli, providing a rationale for their use in high and ultra-high temperature structural applications. Along with the growing interest in the binary carbides listed above, the group IV and V transition metal high-entropy carbides (HECs) have recently attracted great attention. These multi-principal element carbides are found to crystallize in the B1 structure in which the atoms of metals in near-equimolar ratios share a cation position, giving increase in thermodynamic stability due to mixing entropy factor. They have much lower thermal conductivity and diffusivity and better mechanical properties in comparison to those of the binary carbides. This makes HEC ceramics a very promising candidate for various industrial applications, e.g., for the components

of high temperature nuclear reactors, jet engines and hypersonic vehicles operating under the most extreme environments, etc. Several approaches to fabricating HEC ceramics and ceramic powders are currently known, including pressure-assisted reactive sintering of binary carbides mixtures, carbothermal reduction of metal oxides mixtures with either graphite or carbon black, mechanosynthesis through reaction between metallic powders and graphite.

In the present study we have proposed a two-step technique for preparation of fully dense HEC ceramic from a mixture of the group IV and V transition metal oxides. In the first step, a composite powder containing approximately 75 vol.% HEC, 20 vol.% (Nb1-xMex)Si2 (where Me = Ti, Zr, Hf, Ta), and 5 vol.% SiC was prepared through the VCSTR synthesis at 1600 °C for 1 h. In the second step, the as-synthesized product was hot pressed under 40 MPa at 1750 °C for 1 h into a nearly single-phase HEC ceramic with a relative density of 99.4 %. It was found that the reaction between (Nb1-xMex)Si_2 and HEC took place during hot pressing, thereby allowing effective sintering to occur. Flexural strength and Vickers indentation fracture toughness of the obtained HEC ceramic were measured to be 438 MPa and 4.0 MPa m1/2, respectively. Its microhardness, which was measured at a load of 1.98 N, was as high as 32.1 GPa. These values were comparable to or even slightly better than those of HEC ceramics prepared by other methods under more extreme sintering conditions. Thus, it can be concluded that the use of VCSTR synthesis as a key step in the preparation of fully dense HEC ceramic was somewhat effective both in lowering the sintering temperature and in improving the mechanical properties.

This work was financially supported by the Russian Foundation for Basic Research (grant № 19-08-00131).

Lecturer of the Young Scientists School

PRECIPITATION OF SECONDARY PHASES AT ANNEALING OF NANOCRYSTALLINE CO1CR0.25FE1MN1NI1 ALLOY WITH 2 AT. % OF CARBON

Lu Y.[1], Zherebtzov S.[2], Stepanov N.[2], Salishchev G[2], Ivanisenko Yu.1[*]

[1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany
[2]Laboratory of Bulk Nanostructured Materials, Belgorod State University,
308015 Belgorod, Russia
[*]julia.ivanisenko@kit.edu

CoCrFeMnNi type alloy with reduced Cr content and addition of 2 at. % C was processed by high pressure torsion (HPT). Uniform nanocrystalline single fcc phase microstructure was present in as-deformed alloy [1]. Subsequent post deformation annealings were conducted in temperature range 200-600 °C for 1 h. A sequence of precipitation – dissolution of secondary phases reactions was observed starting at 500 °C. At that temperature minor grain growth was accompanied by the precipitation of CoFe and NiMn phases, whereas Cr segregated at grain boundaries. Significant increase of the precipitates volume fraction and notable grain growth were observed after annealing at 530 °C for 1 h. Cr-rich carbides with amorphous structure confirmed by TEM diffraction formed at grain boundaries. CoFe and NiMn phases were identified using HR-STEM combining micro probe diffraction characterization. CoFe phase shows a chemically ordered structure with a few substitutions known as B2 phase, while NiMn phase has a tetragonal structure with chemical disordering. After annealing at 600 °C for 1 h, CoFe phase and NiMn phases re-dissolved in the fcc matrix and amorphous Cr-rich carbides evolved to M_7C_3 type carbide.

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www.knmf.kit.edu), a Helmholtz Research Infrastructure at Karlsruhe Institute of Technology (KIT, www.kit.edu).

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LASER SHOCK PEENING AS RESIDUAL STRESS ENGINEERING TECHNIQUE FOR IMPROVING THE FATIGUE PERFORMANCE OF SAFETY CRITICAL COMPONENTS

Kashaev N.1*, Keller S.[1], Ventzke V.[1], Klusemann B. [1,2]

[1]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon,
Max-Planck-str. 1, D-21502 Geesthacht, Germany
[2]Institute of Product and Process Innovation, Leuphana University of Lüneburg,
Universitätsallee 1, D-21335 Lüneburg, Germany
[*]Nikolai.Kashaev@hereon.de

Aircraft structures are subjected to a cyclic load and therefore can fail due to fatigue. To extend their fatigue life compressive residual stresses can be introduced in critical regions to reduce crack driving tensile stresses and to retard the fatigue crack growth or even to suppress the fatigue crack initiation. Laser shock peening (LSP) as a very promising technique for introducing of deep compressive residual stresses is investigated in this study. A multi-step simulation approach is proposed to connect LSP process simulation regarding the generation of tailored residual stresses with a fracture mechanical analysis of a specimen with fatigue crack to predict the fatigue crack growth taking into account LSP-induced residual stresses [1]. The experimentally validated approach can be used to design LSP process and the areas where the process can be applied on a component to improve its fatigue resistance. A positive application scenario of LSP to recover the fatigue life of laser beam welded AA6056-T6 butt joints with surface fatigue cracks is discussed [2]. Ultrasonic testing was utilized for in-situ measurement of fatigue crack growth during the fatigue test. This procedure allowed preparation of welded specimens with fatigue cracks of approximately 1.2 mm in depth. The pre-cracked specimens showed a 20% reduction of fatigue limit in comparison to specimens without cracks in as-welded condition. Through the application of laser shock peening treatment on surfaces of the pre-cracked specimens, it was possible to recover the fatigue life to the level of specimens tested in as-welded condition. The results of the study showed that laser shock peening is a very promising technique to recover the fatigue life of welded joints, where the cracks can be detected by non-destructive testing.

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THE ROLE OF CE PACKING STATE IN GLASS-FORMING ABILITY FOR CE-BASED BULK METALLIC GLASSES

Yong Z., Kiminori S.*

Department of Environmental Sciences, Tokyo Gakugei University, 4-1-1 Koganei, Tokyo, 184-8501, Japan

*sato-k@u-gakugei.ac.jp

Formation mechanism of bulk metallic glasses (BMGs) with high glass-forming ability (GFA) has been a long-standing subject in the field of solid state physics. To highlight the GFA-associated local atomic structure, Ce-based BMGs were investigated by element-specific positron annihilation spectroscopy coupled with other techniques [1]. The packing state of Ce atoms, concentrated more than Ce crystal, was identified in the glass matrix of Ce-Ga-Cu BMGs under the condition of ambient pressure [2]. First-principles calculations predicted that this anomalous packing state is caused by Ga element chemical pressure induced partial Ce-4*f* electron delocalization, triggering shortness of Ce-Ce distance. Here, we discuss how the above-mentioned Ce agglomeration has influences on BMGs, crystallization [3], and so on, along with open spaces intrinsically available in the glass matrix [4].

Acknowledgments

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FORMATION MECHANISM OF CRYSTALLINE SOLID SOLUTIONS UO_2 - ThO_2 AND UO_2 - ThO_2 - ZrO_2 IN MOLTEN SALTS. INFLUENCE OF CURRENT ON THEIR COMPOSITION

Krotov V.E.

IHTE Ural Branch of RAS, Ekaterinburg, Russia
vekro@ihte.uran.ru

It's known that UO_2-ThO_2 and UO_2 - ThO_2 - ZrO_2 solid solutions are a nuclear fuel. These systems have been prepared only in a powder state. It seems possible to synthesize their crystalline forms in a molten salt as a result of the simultaneous occurring out of two processes on the cathode: the reactions of electrochemical reduction of UO_2^{2+} ions to crystalline uranium dioxide UO_2 and a chemical reaction between UO_2 and thorium and zirconium cations present in the molten salt. The process can be represented in a simplified manner using the following equations:

$$UO_{2\,(melt)}^{2+} + 2e^- = UO_2(s) \qquad (1)$$

$$UO_{2(s)} + xMe^{4+}_{(melt)} = xMeO_2(1-x)UO_2 + xU^{4+}_{(melt)} \quad (2)$$

The proposed method is of undoubted scientific interest for another reason. In the literature, electrochemical reactions are known accompanied by previous or subsequent chemical reactions. However, there no information about the electrochemical reactions, when simultaneously with them on the cathode chemical reactions occur.

The solid solutions were synthesized at 750 °C in a molten equimolar NaCl-KCl mixture containing UO_2Cl_2, $ThCl_4$, and $ZrCl_4$. A decrease in the content of ThO_2 and ZrO_2 in cathode deposits with by an increase in the electrolysis current was established, which is explained by an increase in the rate of the electrochemical reaction, while the rate of the chemical reaction remains constant. The three-phase system consisted of two binary cubic solid solutions and contained mol. %: UO_2 (38-71) - ThO_2 (6-16) - ZrO_2 (23-46). The crystal lattice parameter of one phase was (5,476 – 5,492) and the other - (5,460 – 5,484) Å. The maximum content of ThO_2 or ZrO_2 in systems with UO_2 was 50 and 98 mol. % respectively. Cathode deposits of the UO_2 - ThO_2 system was a single-phase cubic solid solution, the crystal lattice parameter of which increases linearly with an increase in the content of thorium dioxide.

Conclusions. For the first time, crystalline solid solutions of uranium dioxide with thorium and zirconium oxides were prepared. The mechanism of their formation is shown. The effect of electrolysis current density on their composition has been revealed.

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ATOMISTIC SIMULATION OF ORDERING AND DIFFUSION ON THE EXAMPLE OF HIGH-ENTROPY REFRACTORY ALLOYS VCRxNBMOTAW

Lipnitskii A.G. *, Maksimenko V.N.

Belgorod National Research University, Belgorod, Russia
*lipnitskii@bsu.edu.ru

Atomistic simulation of ordering and diffusion effects makes a significant contribution to understanding the physical nature of processes in high-entropy alloys for predicting the formation of a structural-phase composition in them depending on the temperature and concentration of components. Experimental research in this direction is limited by the methodological complexity and insufficient resolution of the instrument base. At the same time, the reliability of predictions by the CALPHAD method decreases with an increase in the number of components due to the neglect of the energy of the interface between the phases [1]. CALPHAD also faces the problem of taking into account the near-order for the correct assignment of Gibbs energy models.

The basis of atomistic simulations is made up of interatomic potentials, which are subject to certain requirements for the correct definition of diffusion, taking into account the ordering effects. This report presents interatomic potentials for modeling BCC alloys of d-metals of the V-Cr-Nb-Mo-Ta-W system at any concentrations of components in a wide temperature range, taking into account angular dependencies in interatomic interactions. Taking into account the angular dependencies is fundamentally important because of the significant contribution of the covalent component in the interaction between the BCC atoms of d-metals.

The report presents the results of modeling of VCrxNbMoTaW alloys (x=0,1,2,3) in the framework of the original modification of the Monte Carlo method for modeling the NPT ensemble using parallel calculations based on the effective account of the relaxation of the positions of atoms by the molecular dynamics method (MD+MC) [2]. Unlike the previous analogues, which use a combination of molecular dynamics (MD) and Monte Carlo (MC) methods, the new MD+MC method will allow us to obtain equilibrium states of the system with a minimum value of the Gibbs free energy for given T and P.

The results of MD+MC modeling showed that there is an agreement of MD+MC and CALPHAD data in the temperature and concentration regions containing a single BCC phase according to the known CALPHAD predictions. A more accurate prediction of the existence of a single-phase region of a multicomponent alloy by the MD+MC method follows from a comparison with experimental data in comparison with CALPHAD. The calculated values of the diffusion displacements of the components in the CrxMoNbTaVW alloy obey the rule of smaller displacements for components with a higher melting point. There is a deviation of the temperature dependence of the diffusion coefficients in the considered multicomponent solution from the Arrhenius law.

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Lecturer of the Young Scientists School

ROOM-TEMPERATURE SHEAR-INDUCED CHEMICAL SEGREGATION IN A FE-BASED BULK METALLIC GLASS

D. V. Louzguine-Luzgin

Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Sendai 980-8577, Japan
Mathematics for Advanced Materials-OIL, National Institute of Advanced Industrial Science and Technology (AIST), Sendai 980-8577, Japan
dml@wpi-aimr.tohoku.ac.jp

Shear-induced segregation takes place in the flow of colloids and granular media, but is unexpected at the atomic level in the deformation of solid materials, especially at room temperature. In nanoscale wear tests of an Fe-based bulk metallic glass at room temperature, without significant surface heating, it is found that intense shear localization under an indenter tip induces strong segregation of a dilute large-atom solute (Y) to planar regions that then crystallize as a BCC Y-rich solid solution leading to stiffening of the alloy [1]. The underlying structural changes are characterized by transmission electron microscopy. The key influence of the soft Fe-Y interatomic interaction is investigated by ab-initio calculation. The driving force for the induced segregation, and its mechanisms, are considered in comparison with effects in other sheared media.

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PROSPECTS FOR THE APPLICATION OF LASER SURFACE FOR THE FORMATION OF HEAT-RESISTANT COATINGS FROM HIGH-ENTROPY ALLOYS

Makarov A.V.*, Korobov Yu.S., Stepchenkov A.K.

M.N. Mikheev Institute of Metal Physics of the IMP UB RAS, Ekaterinburg, Russia
*avm@imp.uran.ru

In many industries, a significant group of equipment is subjected to high temperature and mechanical loads which are often accompanied by an aggressive environment. In many cases surface coatings provide a long-term performance of such equipment. In the majority of parts and mechanisms the surface is a place where the failure initiates by wear, corrosion, cavitation destruction and the nucleation of fatigue cracks.

Laser processing is a cost effective method of a formation the high quality coatings in terms of hardness, wear/heat resistance, plasticity. It is used both in the restoration of worn surfaces and in the manufacture of new parts.

One of the most priority areas of modern material science is associated with the development of high-entropy alloys (HEAs). These alloys contain at least 5 elements, and the amount of each of them lays in the range of 5-35 at. %. Equimolar or quasi-equimolar proportions of elements in HEAs contribute to the formation of a single-phase or a fully eutectic microstructure, which leads to the appearance of potentially new material properties. A single-phase solid solution forming in the HEAs is a direct consequence of the high value of their entropy. In these alloys, a strong distortion of the crystal lattice is also observed. These features determine the microstructure and properties of the HEAs. It is established that these alloys are characterized by high values of hardness, strength, wear resistance and corrosion. The pointed properties are close to and sometimes superior to the best high-strength steels and nickel/cobalt superalloys, with significant potential for further improvement and optimization.

Such a combination of properties is extremely demanded in the basic industries of Russia - metallurgy, power engineering, gas-oil, automotive industry, aviation, etc.

Obtaining HEA based coatings by high-energy laser surfacing qualitatively expands a variation of coating compositions. R&D significant directions in relation to HEAs, including laser HEA coatings, are the following: methods and equipment for producing HEAs in the form of spherical powders and flux-cored wires; technologies of additive manufacturing and lased deposition using HEA feedstock materials; methods and equipment for studying the physics-mechanical characteristics of coatings operating under external loads (high-temperature wear, cavitation, high-temperature loading); study of the influence of deformation effect on the HEA properties.

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MACHINE LEARNING METHODS FOR MODELING THE PROPERTIES OF MULTI-ELEMENT MATERIALS

Mirzoev A.A.[1*], Gelchinskii B.R.[2], Rempel A.A.[2]

[1]South Ural State University, Chelyabinsk, Russia,
[2]Institute of Metallurgy, Ural Branch of the RAS, Ekaterinburg, Russia
[*]mirzoevaa@sus.ru

Computer modelling plays an important role in the design of promising multi-element materials and the prediction of their properties. Ab initio methods based on the theory of density functional theory (DFT) provide high accuracy of calculations, but their high computational costs limit application scales to hundreds of atoms and picoseconds. Atomistic simulations by Monte Carlo (MC) and molecular dynamics (MD) methods open the way to large scales of size and time. However, MD and MC simulation requires an interatomic interaction model that would predict the forces acting on atoms, depending on the location of their surrounding neighbors. This requires knowledge of the potential energy surface (PES) of the material under study. Several approaches can be used to construct the PES. The most accurate approach is based on the calculation of potential energy within the framework of the density functional theory (DFT), but, as we have already noted, it is very computationally demanding and not suitable for modelling multi-element systems. The second approach is empirical or semi-empirical PES models, which allow fast calculations of large atomistic systems (up to millions of atoms) for a long time (up to microseconds), but their accuracy is often insufficient for quantitative analysis. This is what stimulated the emergence of a new class of models of interatomic interaction - machine learning interatomic potentials (MLIP). If semiempirical potentials are used to represent the energy surface, then it is decomposed into functions of a certain type, adapted to describe a specific type of chemical bond. On the contrary, when developing MLIP potentials, very general functional forms (for example, splines or Gaussians) along which the PES is decomposed are used. In this case, the number of adjustable parameters increases sharply; therefore, ab initio calculation data are used to construct reliable potentials, and detailed checks of the obtained PES are required to make sure that it has the correct shape. However, if successful, the constructed potentials can be very numerically accurate, and they describe any type of interaction equally well, whether metallic or covalent or ionic. Over the past decade, machine learning interatomic potentials have reached a certain maturity and have become a worthy alternative to conventional interatomic potentials. This success was largely facilitated by the American Materials Genome Initiative, as well as the support of the European Council for Materials Modeling, within the framework of which the open Internet platform NanoHUB, Quantum Material Properties Database (OQMD), the integrated software infrastructure for automated materials design (AFLOW) and many others were founded. Compared to the traditional approach, the process of designing potentials using machine learning methods has several features. In this paper, we present data on the possibilities of using MLIP for modelling multi-element materials.

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HYPEREUTECTIC ALLOYS OF THE AL – CA-MN– (NI) SYSTEM AS AN ALTERNATIVE TO THE FM180 ALLOY

Naumova E.A.*, Belov N.A., Doroshenko V.V., Barykin M.

National Research Technological University "MISiS", Moscow, Russia
*jan73@mail.ru

In the present work, Natural Metal-Matrix Composites (NMMC) based on the multicomponent hypereutectic Al-Ca-(Mn)-(Ni) alloys were studied in as-cast, annealed and rolled conditions. Thermo-Calc software and microstructural observations were utilized for analyzing the equilibrium and actual phase composition of the alloys. The composition and morphology of the primary crystals that appeared in the hypereutectic Al–(3-10)Ca–(0-3)Mn–(0-4)Ni alloys were studied using experimental and computational methods including the construction of the liquidus projections. As a result, the hypothetic Al-Ca-Mn и Al-Ca-Mn-Ni phase diagrams were proposed in an Al-rich angle.

A previously unknown $Al_{10}CaMn_2$ was discovered by both electron microprobe analysis and X-ray studies. It was found that the crystal lattice belongs to the tP52/2 space group and has the parameters a=1.2845 nm and c=0.5134 nm. The new compound was observed with a relatively compact shape and medium size of 20 μm.

The Al–6Ca–3Mn, Al-8Ca-2Mn, Al-8Ca-2Mn-1Ni alloys with representative NMMC structure included ultrafine Ca-rich eutectic and various small-sized primary crystals.The ternary Al–6Ca–3Mn and Al-8Ca-2Mn alloys were found to have high processability at hot and cold rolling. A crack-free hot-rolled sheet was manufactured from the quaternary Al-8Ca-2Mn-1Ni alloy.

Analysis of tensile samples' fracture surfaces revealed that primary intermetallics may act either as stress raisers or malleable particles depending on their stiffness under deformation.

It is shown that several features of the primary crystals must be maintained for achieving the appropriate performance of the Al-Ca hypereutectic alloys. While some primary crystals (Al_8CaNi_2) with equiaxed shape and uniform distribution can not act as a structural component in the new alloys, the $Al_{10}Mn_2Ca$ compound may be considered as most appropriate.

A comparison of the physical and mechanical properties along with processability of the Al-6Ca-3Mn, Al-8Ca-2Mn, Al-8Ca-2Mn-1Ni experimental alloys and the commercial FM180 piston alloy was performed. The Al-8Ca-2Mn-1Ni was found to be an effective basis for the development of new-generation natural metal matrix composites alternative to the Al-Si counterparts. What is more, experimental alloy exhibit microstructure characterized both by small-sized primary crystals and fine eutectic structure. In this respect, no special modification operation during melting and casting is required.

Summing up the results, the Al-6Ca-3Mn, Al-8Ca-2Mn and Al-8Ca-2Mn-1Ni alloys may be reasonably considered as a promising basis for developing novel alloys for special applications as an alternative to the hypereutectic Al-Si alloys (for example FM180).

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SYNTHESIS AND THERMODYNAMICS OF DOUBLE DY-GA AND TRIPLE DY-GA-AL, PR-GA-IN ALLOYS IN MOLTEN SALT/LIQUID METAL SYSTEMS

Novoselova A. V.*, Smolenski V. V.

Institute of High-Temperature Electrochemistry UB RAS, Ekaterinburg, Russia
*alena_novoselova@list.ru

Currently, rare earth metals and their alloys are essential and very important for various branches of industries, primarily in metallurgy, electronics, nuclear power, and in the production of catalysts, magnetic materials, etc. Molten chloride salts are good reaction electrolytes for production alloys with the necessary specified characteristics. The goal of this research was to study the reaction of the cathode formation of the alloys, the conditions for its production and calculation of its thermodynamic characteristics.

The electrochemical experiments were carried out in a standard quartz cell using a three electrodes setup by an AUTOLAB PGSTAT302N potentiostat-galvanostat. Cyclic, square wave voltammetry, and open-circuit potentiometry were used for study.

Cyclic and square wave voltammetry were used to establish the reaction of electrochemical reduction of Ln(III) ions in different molten salts on inert and active electrodes. The shift of the dysprosium or praseodymium potentials deposition peak to the electropositive region on the active electrodes by comparison with inert ones can be associated with the process of alloy formation. It was determined by chronopotentiometric study that the value of depolarization lies in the range of 0.4-0.6 V. To confirm the reaction of alloy formation, a potentiostatic electrolysis was carried out. XRD pattern of the samples obtained on different active electrodes after electrolysis showed the formation of the intermetallic compounds of different composition. So, the reaction of alloy formation can be written by the following scheme:

$$x[LnCl_6]^{3-} + 3\bar{e} + y(Me_1 + Me_2) = Ln_x(Me_1 + Me_2)_y + 6xCl^- \quad (1)$$

where Ln is lanthanide; Me_1 and Me_2 are an individual active metal.

For calculation of the thermodynamic characteristics of the alloy formation processes open-circuit potentiometry were used. The value of the partial excess Gibbs free energy change of Dy or Pr in liquid alloys of different composition was calculated according to equation (2, 3):

$$\log \gamma_{Ln(alloy)} = \frac{3F}{2.303RT}(E^*_{Ln(III)/Ln} - E^{**}_{Ln(Alloy)}) \quad (2)$$

$$\Delta G^{ex.}_{Ln(alloy)} = 2.303RT \log \gamma_{Ln(alloy)} \quad (3)$$

$$\Delta G^{ex}_{Dy(Ga)} = -195.4 + 0.081 \cdot T \pm 2.8\ kJ/mol \quad (LiCl\text{-}KCl)_{eut.} \quad (4)$$

$$\Delta G^{ex}_{Dy(Ga-20wt.\%\ Al)} = -201.5 + 0.078 \cdot T \pm 2.8\ kJ/mol \quad (LiCl\text{-}KCl)_{eut.} \quad (5)$$

$$\Delta G^{ex}_{Pr(Ga-20wt.\%\ In)} = -243.8 + 0.072 \cdot T \pm 3.6\ kJ/mol \quad (LiCl\text{-}KCl\text{-}CsCl)_{eut.} \quad (6)$$

$$\Delta G^{ex}_{Pr(Ga-40wt.\%\ In)} = -232.9 + 0.075 \cdot T \pm 3.1\ kJ/mol \quad (LiCl\text{-}KCl\text{-}CsCl)_{eut} \quad (7)$$

$$\Delta G^{ex}_{Pr(Ga-70wt.\%\ In)} = -215.9 + 0.071 \cdot T \pm 3.9\ kJ/mol \quad (LiCl\text{-}KCl\text{-}CsCl)_{eut.} \quad (8)$$

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NANOPOROUS HIGH-ENTROPY ALLOYS BY LIQUID METAL DEALLOYING

Okulov I.V.

Leibniz Institute for Materials Engineering - IWT, Badgasteiner Str. 3, 28359, Bremen, Germany
i.okulov@iwt.uni-bremen.de

In this lecture, we will talk about one of the most fascinating synthesis methods for assembling several quintillions of nanoscale objects into a macroscopic body in a very efficient way. This synthesis method is called dealloying. There are four main types of dealloying methods, namely, electrochemical, liquid metal, solid-state, and vapor phase dealloying. These dealloying methods are complementary to each other and enable researchers to design porous materials of nearly any chemical composition from reactive materials such as magnesium or titanium to noble ones such as gold and modern one such as high-entropy alloys [1–3].

Among all these dealloying methods, we will particularly focus on liquid metal dealloying invented in the group of Prof. Kato about a decade ago [4]. Liquid metal dealloying can be compared with electrochemical dealloying, but unlike the latter one, this utilizes the difference in enthalpies of mixing between each element of the precursor alloy with the metallic melt and is several orders of magnitude faster. The metallic melt may consist of one or more elements and acts as corrosive medium. The sacrificial element dissolves out from the precursor alloy when this is immersed in the metallic melt due to a positive enthalpy of mixing between the elements. We will talk about the selection of suitable combinations of metallic melts and precursor alloys for liquid metal dealloying as well as touch on the topic of dealloying kinetics.

Since the discovery of liquid metal dealloying, many new functional porous materials have been synthesized by this method, including nanoporous steels, niobium, magnesium, silicon, titanium to list a few. Specifically, liquid metal dealloying enables synthesis of compositionally complex alloys such as high-entropy alloys [1–3]. Since nanoporous high-entropy alloys are attracting growing attention as advanced functional materials, we will focus on this particular class of materials in more details. Generally, liquid metal dealloyed porous metals and composites combine moderate strength with low elastic modulus suggesting their application in biomedical implant devices for bone fixation. Moreover, the outstanding functional properties of these materials due to the high surface area envision many opportunities for their application in capacitors, batteries, and catalysis.

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EFFECT OF GRADIENT STRUCTURE ON MECHANICAL PROPERTIES OF METASTABLE AUSTENITIC STAINLESS STEEL

Panov D.O.*, Chernichenko R.S., Naumov S.V., Stepanov N.D., Zherebtsov S.V., Salishchev G.A.

Belgorod State University, Belgorod, Russia
*panov_d@bsu.edu.ru

Metastable austenitic stainless steels (MASS) possess excellent synergy of ductility, impact toughness, and corrosion resistance, but low yield strength limits their application as a structural

materials. The gradient structure formation is considered as one of the most promising ways to achieve both high yield strength and excellent ductility simultaneously. Cold swaging and subsequent reverse annealing at low temperatures may result in the gradient structure formation and good mechanical properties [1]. The aim of the current study is to explore the effect of annealing at low temperatures on the structure evolution and mechanical properties of a 321-type MASS subjected to cold swaging.

Gradual decrease in the α-phase fraction from edge to center after 90% cold swaging was revealed. In the center, both strain-induced martensite and retained austenite have globular and lamellar morphology. Yet a mainly globular structure consisting of martensite and austenite is detected at the edge. Due to partial recrystallization and martensite-to-austenite reversion, low-temperature annealing at 500 °C results in structure refinement [2]. An increase in ultimate tensile strength and yield strength, associated with nanocarbide precipitation, was revealed. The estimation of Orowan strengthening showed increasing of yield strength to ~150 MPa and ~300 MPa at the centre and edge, respectively [1]. Moreover, notch toughness of the MASS doubled after annealing.

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THE FREQUENCE DISPERSION FEATURES OF THE DIELECTRIC CHARACTERISTICS OF HAFNIUM DISULFIDE INTERCALED WITH SILVER ATOMS

Pleshchev V. G.

Institute of Natural Sciences and Mathematics, Ural Federal University named after B.N.Yeltsin, Ekaterinburg, Russian Federation.
v.g.pleshchev@urfu.ru

The atomic structure of hafnium disulfide, like other dichalcogenides of transition metals, is characterized by a set of structural fragments (layers) interconnected by a weak van der Waals (VdV) interaction [1]. Earlier, polarization phenomena in a constant electric field were discovered in the Ag_xHfSe_2, indicating the redistribution of mobile silver ions [2].

In this work, using the data of impedance spectroscopy, we analyzed for the first time the dielectric properties of Ag_xHfS_2 compounds (x = 0.1; 0.2) in a wide range of linear frequencies and at various temperatures. A significant frequency dispersion of the real and imaginary components of the relative dielectric constant was found in these compounds. Frequency dependences in the investigated frequency region is monotonic and does not exhibit characteristic maxima for the imaginary part. More informative may be the presentation of the results in the form of an electrical modulus, the complex value of which is the reciprocal of the complex dielectric

constant M*= M '+ i M"=1/ ε *. In this case, as noted in the literature, the imaginary part of the electric modulus transforms the low-frequency increase of the dielectric constant into a relaxation peak, from the position of which the relaxation time can be determined [3]. The representation of the components of the electrical module on the complex plane had the form of circular arcs corresponding to the Cole-Cole diagrams. As a result, the modular representation made it possible to determine the characteristic times of dielectric relaxation, as well as to estimate the values of the high-frequency dielectric constant for compounds of different compositions.

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HIGH- AND MEDIUM-ENTROPY ALLOYS: PRINCIPLES OF ALLOYING, THE SYNTHESIS AND STRUCTURE

Pushin V.G., Kuranova N.N., Makarov V.V., Marchenkova E.B., Rasposienko D.Yu., Svirid A.E., Uksusnikov A.N.

Institute of Metal Physics named after M.N. Mikheev, Ural Branch of the Russian Academy of Sciences, Yekaterinburg, Russia
pushin@imp.uran.ru

An overview of the state-of-the-art of the high- and medium-entropy metal alloys (H&MEMAs), principles of their alloying, synthesis conditions, as well as the structure and phase composition is presented. The features of the multicomponent optimum doping and structural-phase transformations, both during the synthesis and subsequent thermal deformation processing of H&MEMAs, – are considered. Special attention is paid to multicomponent metal systems based on the structural aluminum alloys, multifunctional low-modulus copper and titanium alloys, and intermetallides, as well as (on) the nickel-based intermetallic compounds (Heusler phases) capable of experiencing highly reversible thermoelastic martensitic transformations.

MACHINE LEARNING METHODS FOR PREDICTING THE STRUCTURE OF MATERIALS

Ryltsev R. E.

Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia
rrylcev@mail.ru

One of the main tasks in materials science is the prediction of the structures of solid phases for given chemical composition and given values of thermodynamic parameters (temperature, pressure, etc.). Modern methods for solving this problem are based on machine learning algorithms. There are two main groups of such methods, which are discussed below.

The most widely used and effective methods for structure prediction utilize direct *ab initio* calculations of energies and interatomic forces. Among them are the methods based on evolutionary algorithms [1]. The main idea behind such methods is to perform an evolutionary search of the most stable structure by comparing the ground state energies (enthalpies) of the candidate structures. These methods are the most effective at low temperatures where one can consider only the ground state of the system. If the unit cell of the ground state phase is not very large (no more than 50-60 atoms), such algorithms allow exact predicting its structure.

However, evolutionary algorithms fail in many practically important cases, such as disordered or partially disordered systems (glasses, high-entropy solid solutions), complex structures and finite-temperature phases. In such cases, the exact prediction of the structure is hardly possible. However, some general conclusions regarding the tendencies for the formation of some structures can be made. For that purpose, one can investigate the structural heredity relating high-temperature (disordered) and low-temperature (ordered) phases [2, 3, 4]. Here, under the structural heredity, we imply the existence of "genetic" relationships between the structures of disordered and ordered phases. The study of such heredity makes it possible to predict the structure and properties of ordered phases from the experimentally measurable structure-sensitive characteristics of disordered phases, such as X-ray structural data, density, viscosity as well as from the results of atomistic simulations. This approach requires simulating of the disordered phases in a wide range of parameters that is computationally costly, especially in the case of *ab initio* simulations. One of the most promising and widely accepted techniques to solve this problem is using machine learning interatomic potentials [5,6]. Such potentials can provide nearly *ab initio* accuracy with orders of magnitude less computational cost.

Essentially different ideas underlie black-box methods [7], which utilize machine learning models to find general relationships between a target property (structure, diffusion coefficient, etc.) of the material and a set of simple characteristics that can be either easily estimated for a given composition or extracted from experimental data (atomic radii, valence electron concentration, mixing enthalpy, etc.). Such methods are not as accurate as *ab initio*-based ones but they are being actively developed and are very promising in the light of current resolution in machine learning.

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SOLID-SOLUTION STRENGTHENING IN HIGH ENTROPY ALLOYS

Salishchev G.A.

Belgorod State University, Belgorod, Russia
gsalishchev@gmail.com

The strategy of using a large number of multiple principal elements for the formation of a single-phase solid solution instead of one as in conventional alloys should contribute to obtaining a higher strength of metallic materials. This is the basis of the concept of high-entropy alloys [1,2]. Mixing of many components in equiatomic concentrations inevitably leads to the formation of a

solid solution in which practically each of the atoms has foreign atoms as neighbors. In relation to conventional solid solutions based on one element, this should lead to an even greater distortion of the lattice due to the asymmetry of interatomic binding forces, the difference in the radii of atoms and their electronic structure, and, accordingly, to hardening. It is of interest both to analyze the structure and hardening of such solid solutions and their features upon additional alloying.

The presentation examines the structural features of fcc and bcc solid solutions of high-entropy alloys and the development of plastic flow in them. Careful studies of the lattice distortion by the neutron radiation method did not show the expected anomalous line broadening, and local deformations generally correspond to those observed in ordinary metals [3]. However, the lack of periodicity of the composition in the lattice can lead to a randomly distributed local Peierls-Nabarro stress field with different rates of energy changes. Strengthening is associated with the contributions of the Peierls barrier, and to a greater extent with the collective effects of the interaction of dislocations with dissimilar atoms, determined by their size and the mismatch of the elastic moduli in the lattice [4, 5]. Strengthening can be increased by additional alloying with various elements [6,7], calculated by the Labouche method. In highly concentrated solid solutions, the formation of short-range order is quite expected, which significantly contributes to the strengthening of alloys due to an increase in Peierls barriers and a change in the nature of dislocation slip [8, 9]. Examples of solid solution strengthening of high-entropy alloys are given and contributions from various factors are analyzed.

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SHS-METALLURGY OF DISPERSION HARDENED CAST HIGH-ENTROPIC ALLOYS BASED ON TRANSITIONAL AND REFRACTORY METALS

Sanin. V.N.*, Ikornikov D.M., O.A. Golosova, Yukhvid V.I.

Merzhanov Institute of Structural Macrokinetics and Materials Science Russian Academy of Sciences (ISMAN),
Academician Osipyan str., 8, Chernogolovka, Moscow Region, 142432, Russia
*svn@ism.ac.ru

It has already been shown that high-entropy alloys (HEAs) can demonstrate unusual physical and mechanical properties that significantly expand the area of application of modern metallic materials [1].

Initially, the objects of study in field of HEAs were systems based on transition metals of equiatomic compositions. At present, more than 400 HEA compositions have already been studied,

including refractory metals and systems with a significant deviation from the equiatomic composition.

From the point of view of further expanding the practical demanded properties of HEAs based materials, special particular interest are arise for HEAs with a heterogeneous structure, including dispersive precipitates of refractory compounds with the participation of non-metals, such as Si, B, N, etc. The search for metal-ceramic composite materials based on HEAs has begun. In such materials, a powerful effect of structural hardening is observed due to the specifics of the formation of the structure in the composite materials based on HEAs.

Earlier, the authors firstly successfully applied the method of SHS metallurgy to obtain cast HAEs based on transition metals (Co-Cr-Fe-Ni-Mn), including their structural strengthening by dispersion precipitates of borides and silicides of refractory metals (Mo, Nb and Ti) formed in-situ SHS [2-5]. As a continuation of these studies, this work will present experimental data on the synthesis of cast HAEs based on refractory metals (Nb-Mo-Cr-V-Ti) modified by the added additives (Si and B) directly in the synthesis process (combustion process).

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POSITRON ANNIHILATION STUDIES IN CONCENTRATED SOLID SOLUTION ALLOYS WITH FCC STRUCTURE TO REVEAL THE PROPERTIES OF THERMAL VACANCIES

Sprengel W.

Graz University of Technology, Institute of Materials Physics, Graz, Austria
w.sprengel@tugraz.at

A brief introduction into positron-electron annihilation in solids and its application to vacancy studies will be given. Then results on the formation of thermal vacancies will be presented that have been obtained for the new material class of concentrated solid-solution alloys, often referred to as high-entropy alloys by applying the techniques of positron-lifetime spectroscopy.[1] Coarse-grained, single-phase samples were prepared for various face-centered-cubic concentrated solid-solution alloys with varying number of constituents. These homogeneous samples were brought and held at temperatures close to their melting temperature and then rapidly quenched and

kept at liquid nitrogen temperature immediately afterwards. In this state, the concentration of quenched-in vacancies was determined by the acquisition of positron lifetime spectra also at low temperatures.

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DENSITY AND ELECTRICAL RESISTIVITY OF Al-Ni-Co-R GLASS-FORMING ALLOYS

Rusanov B. A.[1*], Sidorov V. E.[1], Moroz A. I.[1], Svec P. Sr.[2], Janickovic D.[2]

[1]Ural State Pedagogical University, Ekaterinburg, Russia
[2]Institute of Physics Slovak Academy of Sciences, Bratislava, Slovakia
[*]rusfive@mail.ru

Aluminum-based amorphous alloys, especially Al-Ni-R and Al-Co-R compositions, have unique mechanical and corrosion properties. These alloys are beginning to be actively used as protective coatings for steel constructions. In this work we investigated density and electrical resistivity of Al-Ni-Co-R alloys in crystalline and liquid states.

The alloys of $Al_{86}Ni_6Co_2R_6$ (R = Nd, Sm, Gd, Tb, Yb) compositions were prepared by remelting of pure initial components in arc-melting furnace in argon atmosphere. Density of the alloys in crystalline and liquid states was measured by the absolute variant of gamma-absorption method on an automated experimental set-up in helium atmosphere. Electrical resistivity of the alloys in crystalline and liquid states was investigated by contactless method in rotating magnetic field on automated experimental set-up in helium atmosphere.

It was found that all the compositions have a wide two-phase zone (transition from solid to liquid state) and specific behavior of properties (density and electrical resistivity) at liquidus temperature (T ~ 950 K). Hysteresis of density at T < 1300 K (i.e. incoincidence of heating and cooling curves) was found for all the alloys. This can indicate the fact that the alloys remain microheterogeneous after melting and come to homogeneous state at T > 1300 K only.

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COMPOSITE MATERIAL ALUMINUM-TITANIUM

Skachkov V. M.

ISSC UB RAS, Ekaterinburg, Russia
skachkov@ihim.uran.ru

The laboratory of chemistry of heterogeneous processes has developed and patented [1] a method for producing high-strength composite materials Al (Al-alloy) - Ti with an increased content of fine titanium (standard powder, crushed titanium sponge, etc.), cemented with an aluminum matrix. Such a material is suitable for use as modified deformable and cast aluminum composite alloys, and is a titanium metal powder distributed in an aluminum matrix or an alloy based on it. The method of obtaining such material includes several sequential operations: 1) melting of aluminum or aluminum alloy at a temperature of 780±20ºC; 2) introduction of titanium metal powder into the melt by injection with an inert gas; 3) temperature recovery within

5-10 minutes to 780±20ºC; 4) centrifugation of the liquid melt at a rotation speed of 1000-3000 rpm for 10-12 minutes before solidification; 5) separation of the bottom sediment along the outer boundary (the sediment is darker) after crystallization and cooling. The results of measuring the microhardness of the obtained materials are presented in the table.

Table – Microhardness of samples

№	Composite alloy	Initial alloy, microhardness, HV, GPa.	After centrifugation, the bottom sediment	
			The content of Ti, wt.%	Microhardness, HV, GPa.
1	01421-Ti	1,33	3,2	1,71
2	01570-Ti	1,03	6,4	2,60
3	Al-Ti	0,39	14,8	2,10

It follows from the table that the method developed in the laboratory produces high-strength composite materials Al (Al-alloy) - Ti based on titanium metal powders in an aluminum matrix or an alloy based on it.

The work was carried out in accordance with the state task and plans of the Research Institute of IHTT of the Ural Branch of the Russian Academy of Sciences.

The author thanks the staff of the laboratory of chemistry of heterogeneous processes for their assistance in carrying out work on the study of aluminum alloys and composite materials.

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NON-HIBBS THERMODYNAMICS OF GLASSY SYSTEMS

Son L.D.

IMET UB RAS, Ekaterinburg, Russia
ldson@yandex.ru

Complex (multi – phase and multi – component) systems very often demonstrate non – ergodic or glassy behavior. That means that ensemble average does not coincide with the temporal one, i.e. the configuration probability is being determined not only by its energy, but by some additional considerations. Simple and effective phenomenological theory based on this anzats was formulated long ago [1,2]. More fundamental theory, such as mode coupling one [3], may be formulated by following scheme. Dynamics of arbitrary system described by set of variables $\mathbf{V}(\mathbf{r},t)$ may be written as

$$\frac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} = \hat{\Gamma}\frac{\delta F}{\delta \mathbf{V}} + \theta \ , \qquad (1)$$

where F is a driving functional (free energy as usual), $\hat{\Gamma}$ - some linear operator, and θ - thermal noise. Dynamics (1) leads to the Fokker-Plank equation on configuration distribution function $P\{\mathbf{V}(\mathbf{r},t)\}$:

$$\frac{\partial P}{\partial t} = \hat{\Gamma}\int \mathrm{d}^3\mathbf{r}\frac{\delta}{\delta \mathbf{V}}\left(T\frac{\delta P}{\delta \mathbf{V}} + \frac{\delta F}{\delta \mathbf{V}}P\right), \quad (2)$$

Standard solution of equation (2) is the Hibbs distribution

$$P\{\mathbf{V}\} = A\exp\left(-\frac{F\{\mathbf{V}\}}{T}\right). \quad (3)$$

For complex systems, equation (2) is strongly nonlinear, so that (3) is not its unique solution. As can be seen from existing statistical thermodynamic theories of complex systems [3,4], the nonlinear corrections are accounted by universal way, namely by an arbitrary dependence of $F\{\mathbf{V}(\mathbf{r},t)\}$ on average $<\mathbf{V}>$ with respect to distribution (3). Thus, the self – consistent scheme arises, which features are being discussed.

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MICROSTRUCTURE AND PROPERTIES OF AN AUSTENITIC STAINLESS STEEL DURING AGING AT 923K

Tikhonova M.*, Belyakov A., Kaibyshev R.

Belgorod State University, Pobeda 85, Belgorod 308015, Russia
*tikhonova@bsu.edu.ru

The changes in phase content and mechanical properties during aging at 923 K were studied in an S304H-type austenitic stainless steel. Numerous Cu-rich, NbC-type and Cr23C6-type dispersed particles with sizes of 1.5 nm, 60 nm and 40 nm, respectively, were observed after aging for 100 hours. The copper particles were homogeneously distributed throughout, while the carbides precipitated mainly at grain boundaries. Further aging was accompanied by a progressive precipitation and growth of the second phase particles. Except for the rather stable NbC carbides, the Cu-rich and Cr23C6 particles exhibited rapid coarsening kinetics with a particle growth exponent of about 2. Thus, their mean sizes increased almost fivefold during aging for 3000 hours, leading to a depletion of solid solution and, therefore, to the ferrite appearance primarily along the austenite grain boundaries. The aging treatment resulted in an increase in the strength and a decrease in the impact toughness at room temperature, whereas the tensile behavior at 923 K did not change remarkably.

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SYNTHESIS OF HIGH-ENTROPY ALLOY COATING BY LASER REMELTING OF COLD SPRAY DEPOSITS

Trofimov E. A. [1], Samodurova M. N. [1], Sova A. A. [2], Doubenskaia M. A. [2], Trofimova S. N. [1], Ulianitsky V. Yu. [3]

[1]South Ural State University, Chelyabinsk, Russian Federation
[2]National Engineering School of Saint-Etienne (ENISE), Saint-Etienne, France
[3]Institute of Hydrodynamics M.A. Lavrent'ev SB RAS, Novosibirsk, Russian Federation
[*]trofimovea@susu.ru

High-entropy metal alloys (HEA) are considered as promising materials with significant application potential in different domains of industry [1, 2]. The unique functional properties of HEA coatings deposited on different substrates were reported recent studies [2]. In general, the HEA coatings are produced by laser cladding [3], thermal spray [4] or cold spray [5] methods using pre-alloyed HEA powders as the feedstock material. The main drawback of these approaches is the low commercial availability of HEA powders. In this work the feasibility study of new two-stage hybrid approach of HEA coating deposition on aluminum substrate was proposed. At the first stage of this process, the precursor composite coatings containing the mixture of several low-entropy metal powders is deposited by cold spray. At the second stage, the formation of HEA phases in the coating is induced during laser melting of near-surface zone of the coating.

At the first stage the Al-Cr-Fe-Mo-Ni-Ti and Al-Cu-Cr-Fe-Mo-Ni composite coatings were successfully deposited on aluminum substrate by cold spray. The coatings had the uniform structure with homogenous distribution of the particles. Followed laser melting performed at the second stage allowed formation of uniform layer with visible gradient between melted and non-melted zones. Applied laser melting parameters allowed formation of uniform structure due to efficient material melting and mixing on molten pool. The final composition of remelted layers of the first and the second composite coatings were $Al_{0.1}Cr_{0.5}FeMo_{0.2}NiTi$ and $Al_{0.1}CuCr_{0.5}FeNi_{0.5}Mo_{0.2}$ correspondingly. The XRD analysis revealed the formation of the single-phase HEA with *fcc* structure in the $Al_{0.1}CuCr_{0.5}FeNi_{0.5}Mo_{0.2}$ coating, whereas the $Al_{0.1}Cr_{0.5}FeMo_{0.2}NiTi$ coating contained several *fcc*, *bcc* and σ phases.

Obtained results showed that the developed two-stage approach could be applied for elaboration of high-entropy alloy coatings with other compositions. However, the main challenge in this approach is proper fabrication of cold spray precursor coating with targeted element composition. To reach this goal, the pure powders of metals could be applied instead of alloy powders used in this study.

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ELECTRONIC STRUCTURE AND ELECTRICAL CONDUCTIVITY OF TIZRHFNB HIGH-ENTROPY ALLOY UNDER PRESSURE

Uporov S. A.[1*], Ryltsev R. E. [1], Sidorov V. A. [2], Estemirova S. Kh. [1], Sterkhov E. V.[1], Balyakin I. A. [1], Chtchelkatchev N. M.[2]

[1]Institute of Metallurgy, Ural Branch of Russian Academy of Sciences, Ekaterinburg, Russia
[2]Vereshchagin Institute for High Pressure Physics, Russian Academy of Sciences, Troitsk, Moscow, Russia
[*]segga@bk.ru

Due to specific highly distorted crystalline structure, high-entropy alloys (HEAs) are expected to demonstrate interesting behavior under high pressures. However, this issue is almost not studied so far. Here we address pressure effects on electronic structure and electrical conductivity of TiZrHfNb alloy. Among the multiplicity of single-phase HEAs explored so far, the TiZrHfNb one is an exemplar of thermally stable metallic material that crystallizes into body-centered cubic (BCC) structure and demonstrates excellent mechanical, corrosion and friction properties compared to conventional alloys. We synthesize this material with BCC structure and analyze its electrical, superconducting and magnetic properties. The alloy is a Curie-Weiss paramagnet and a type-II superconductor with the critical temperature of about 6.3 K. The estimated upper critical field and critical current density in the HEA are rather moderate compared to those observed in the superconductors based on Ti-Nb alloys. In the normal state, the alloy demonstrates high electrical resistance that practically independent on temperature but significantly dependent on pressure; it decreases linearly by 12.5 % as the pressure increases up to 5.5 GPa. By analyzing the experimental data, we suggest that alloy resistance is mainly determined by two contributions: the residual resistance and Mott's s-d scattering. We show that a cooperative effect from changes in both the Debye temperature and electronic band structure near the Fermi level are the main factors responsible for the electrical resistance behavior of the HEA under pressure. Ab initio calculations performed at different pressures support this conclusion. The results show that TiZrHfNb alloy is a promising material for designing resistance pressure gauges.

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RECENT ADVANCES IN SPD PROCESSING OF NANOSTRUCTURED MATERIALS WITH SUPERIOR PROPERTIES

Valiev R. Z.

Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, 12 K. Marx str., Ufa, 450000, Russia
Laboratory for Mechanics of Bulk Nanomaterials, Saint Petersburg State University, 28 Universitetsky prospekt, Peterhof, Saint Petersburg, 198504, Russia
Ruslan.valiev@ugatu.su

The recent decade was marked by significant advances in the development of severe plastic deformation (SPD) techniques to achieve new and superior properties in various materials. This report is focused on the achievements in these areas of study and promising trends in further research and development. SPD processing provides strong grain refinement at the nanoscale,

produces high dislocation and point defect densities as well as unusual phase transformations associated with particle dissolution, precipitation or amorphization. Such SPD-induced nanostructural features strongly influence the deformation and transport mechanisms and can produce a substantial enhancement in the performance of advanced materials. The concept of nanostructural design of metals and alloys for multifunctional properties such as high strength and conductivity, superplasticity, increased radiation and corrosion tolerance and others is discussed. Special emphasis is placed on advanced metallic biomaterials that promote innovative applications in medicine.

SYNTHESIS AND STUDY OF HIGH-ENTROPY OXIDE PHASES WITH THE MAGNETOPLUMBITE STRUCTURE

Vinnik D. A. [*], Zaitseva O. V., Gudkova S. A., Zhivulin V. E., Zherebtsov D. A., Myasnikova A. A., Starikov A. Yu., Trofimov E. A.

South Ural State University, Chelyabinsk, Russian Federation
[*]vinnikda@susu.ru

In the course of the research, the following tasks were solving:

- obtaining samples of a new class of high-entropy oxide phases - high-entropy phases with a magnetoplumbite structure;
- investigation of the composition and structure, as well as the properties of the obtained samples;
- analysis of the obtained experimental data in order to formulate the general laws governing the formation of high-entropy phases with a magnetoplumbite structure.

The main result of the investigation was the discovery (for the first time in the world) of a special class of high-entropy oxide compounds - high-entropy phases with a magnetoplumbite structure. The fact of the possibility of obtaining such compounds has been indisputably proven. A number of elements that can participate in the formation of compounds with such a structure have been determined; for a number of other elements, the impossibility of their inclusion in the composition of high-entropy phases with a magnetoplumbite structure in significant amounts has been shown.

The main results of the research also include the following:

1. Synthesized samples of high-entropy oxide phases with a magnetoplumbite structure. Data on temperature and concentration ranges of stability of phases of this kind.
2. A successfully implemented technique for the synthesis of high-entropy oxide phases with a magnetoplumbite structure by means of solid-phase synthesis. Data on the stable modes of obtaining samples, including the composition of the batch, as well as the temperature conditions of the process, ensuring the production of single-phase samples suitable for studying their physical characteristics.
3. A thermodynamic model has been developed for high-entropy oxide phases with a magnetoplumbite structure with a set of model parameters that make it possible to describe the dependence of the thermodynamic functions of such phases on their composition and temperature. The results of modeling the synthesis of high-entropy oxide phases with a magnetoplumbite structure from precursors have been obtained and compared with experimental data.
4. A lot of data have been obtained on the structure and composition of experimental samples. These data were obtained by methods of X-ray fluorescence spectroscopy, scanning electron microscopy, as well as methods of X-ray phase analysis.
5. Obtained data on the magnetic and microwave characteristics of experimental samples. Results of the analysis of the dependence of the magnetic and microwave characteristics on the crystal structure and composition of the samples. Wide possibilities of fine control of these

characteristics (in particular, the Curie temperature, resonance frequency, etc.) by changing the composition of the phases under study have been found.

6. The analysis of the results obtained made it possible to formulate recommendations on the use of crystal phases obtained in the process of research for the manufacture of electronic components.

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DEFORMATION MECHANISMS IN TI-RICH HIGH-ENTROPY ALLOYS

Zherebtsov S. [*]**, Eleti R., Panina E., Stepanov N., Yurchenko N.**

Belgorod National Research University, Belgorod, Russia
[*]ser_z@mail.ru

High-entropy alloys (HEAs) constitute a new class of metallic materials attracting increased attention due to unusual combination of mechanical and functional characteristics. One of a strategy to improve mechanical properties of high entropy alloys is associated with activation of various modes of deformation mechanisms (such as TRIP, TWIP or dislocation slip). The primary objective of the present study is to investigate deformation mechanisms of new Ti-rich bcc HEAs. Three alloys of Ti-Zr-Hf-Ta-Sn, Ti-Zr-Nb-Al-V and Ti-Zr-Nb-Al-Mo systems were considered. The studied alloys demonstrated very unusual combinations of mechanical properties depending on the operating deformation mechanisms. Specifically, the $Ti_{38}Zr_{25}Hf_{25}Ta_{10}Sn_2$ alloys demonstrated exceptionally high strain - hardening and ductility due to deformation-induced martensite transformation. The $Al_5Nb_{24}Ti_{40}V_5Zr_{26}$ and $Al_4Mo_4Nb_8Ti_{50}Zr_{34}$ high-entropy alloys in recrystallized conditions showed properties typical of gum like metals, i.e. high strength, low work hardening and rather large elongation. The manifestation of such behavior can be ascribed to the formation of dislocation channels due to the local disordering of the bcc matrix in shear planes.

Lecturer of the Young Scientists School

DEVELOPMENT OF CO-CR ALLOYS FOR MEDICAL APPLICATION

Zherebtsov S.V. [*]**, Stepanov N.D.**

Belgorod National Research University, Belgorod, Russia
[*]ser_z@mail.ru

Increased interest in the use of Co-Cr alloys in dentistry is associated with their low cost and attractive physical and mechanical properties. These alloys have almost half the density of Au-based alloys, and thus the weight of the fabricated dental products is significantly lower. Besides, higher corrosion resistance and better toxic properties in comparison with the Ni-Cr composition make the co-Cr alloys much more attractive for use in dentistry. Various Co-Cr alloys and influence of alloying elements on mechanical properties are considered in the present work. Structure and properties of some new alloys of the Co-Cr system are analyzed. Some approaches of mechanical properties improvement are proposed.

Исследование выполнено при финансовой поддержке Министерства науки и высшего образования Российской Федерации в рамках соглашения № 075-11-2021-046 от 24.06.2021 с АО «ОЭЗ «ВладМиВа» по комплексному проекту "Организация

высокотехнологичного производства экспортно ориентируемых медицинских изделий на основе инновационных конструкционных материалов с целью импортозамещения на базе разработанных технологий", при участии НИУ «БелГУ» в части выполнения научно-исследовательских, опытно-конструкторских и технологических работ.

The study was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation under the agreement No. 075-11-2021-046 dated June 24, 2021 with JSC SEZ VladMiVa under the integrated project "Organization of high-tech production of export-oriented medical devices based on innovative construction materials for the purpose of import substitution on the basis of developed technologies ", with the participation of the Belgorod National Research University in terms of the implementation of research, development and technological work.

YOUNG SCIENTISTS

INFLUENCE OF TIN TRACE ADDITION ON THE MICROSTRUCTURE AND MECHANICAL PROPERTIES OF AL-CU(-SI) BASED ALLOYES

Akopyan T.K.*, Belov N.A., Letyagin N.V.

National Research Technological University "MISiS", Moscow, Russia
*aktorgom@gmail.com

It is proposed that trace solutes effect on both the precipitation sequence and interfacial energy resulting in increased strength for Al-Cu based alloys at both ambient and elevated temperatures. It is well known [1] that Mg and Ag traces in 2139 type alloys dramatically enhance the formation of hexagonal-shaped plate-like particles of the so-called Ω-phase, forms uniformly on the {111} matrix planes. The superior properties are attributed to both the formation of fine uniform distributed particles with a large width-thickness aspect ratio and high thermal stability of Ω-phase compared to the more common θ′ - Al_2Cu precipitates. However, alloying with expensive silver is irrational in most cases. Another alloy designated 2021 contains a cadmium Cd trace addition (0.05-0.15 wt.%) which, as reported, has a superior tensile and yield strength compared to the base 2219 alloy with no sacrifice of ductility or toughness at low temperatures. The increase in the strength of the alloy is due to the well-known phenomenon of refining of the θ′-phase precipitation structure. However, owning to the exceptional toxicity of cadmium, this alloy has been banned in most productions. One should note that according to numerus reports, tin (Sn) and indium (In) trace additions can be a promising substitute for cadmium [2]. However, surprisingly, to date there are very few works exploring the influence of Sn on precipitation hardening response for the Al-Cu(-Si)-Sn alloys. In current work, both thermodynamic calculations and experimental studies including high resolution transmission electron microscopy, microhardness and specific electrical conductivity measurements have been used to determine the influence of Sn trace addition on the structure and precipitation hardening response in Al-Cu(-Si) based wrought and casting alloys. The analysis revealed that trace addition in Al-Cu(-Si) based alloys catalyzes the nucleation of the θ′-phase result in the significant refinement of the precipitates structure and at least a twofold increase in the number density and aspect ratio of platelets. The Al-Cu(-Si) alloys showed an increase by about 20-25 % the peak hardness for both cast and wrought products as well as significant reduction in the ageing time to peak hardness. Based on the results, one can conclude that the Al-Cu(-Si) alloys can serve as an excellent base for the development of new wrought and casting high strength aluminum alloys.

The study was carried out with the financial support of the grant of the Russian Science Foundation (Project № 20-79-10373).

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EFFECT OF TECHNOLOGICAL FACTORS OF PREPARATION AND ACTIVATION OF THE PISTON SUBSTRATE SURFACE FOR COATING USING ABRASIVE BLASTING MACHINE

Al-Bdeiri M.S.*, Krasilnikov V.V., Sergeyev S.V.

Belgorod State National Research University, Belgorod, Russia
*1270037@bsu.edu.ru

The process of roughing surfaces by sandblasting before coating using galvanic-plasma modification (GPM) is very important to obtain consistently high tensile strength between coating and substrate, to carbon-deposit elimination, and to attempt to remove some flaws such as piston cracks and chips that formed on the surface of the piston during its operation. This work aimed at studying the effect of sandblasting pressure and the volume of alumina on the roughness of a substrate made of AK12MMgN alloy, as well as the effect on the roughness of GPM coatings applied by jet cleaning, as well as on the adhesion strength of these coatings.

A large number of technological factors, such as material and grain size, pressure and time of blasting, distance to abrasive, angle of blasting and hardness of the part / surface subjected to blasting, determine the magnitude and nature of surface roughness. Thus, to obtain a consistently high quality GPM coating with a consistently high coating-to-substrate adhesion value, the sandblasting process must be properly controlled and, more importantly, the process parameters must be optimized.

The results obtained indicate the importance of the roughness of the base after sandblasting of the AK12MMgN alloy and the roughness of the subsequently applied coatings in determining the value of the bond strength.

SPARK PLASMA SINTERING OF CERAMICS BASED ON Si_3N_4 WITH YAG PRECURSOR

Andreev P.V.[1*], Drozhilkin P.D.[2], Alexeeva L.S.[2], Balabanov C.C.[1], Rostokina E.E.[1], Boldin M.S.[2], Karazanov K.O.[2]

[1]Institute of Chemistry of High-Purity Substances RAS, Nizhny Novgorod
[2]N.I. Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia
*andreev@phys.unn.ru

One of the perspective methods of creating ceramic composites based on Si_3N_4 with improved mechanical and high-temperature properties consists in using of spark plasma sintering technology with a pre-applying of sintering additive precursors as an ultra-thin coatings (with a thickness of about several nanometers) by special precipitation methods on the surface of the initial silicon nitride powders.

Silicon nitride powders of various dispersion were used as an initial: amorphous nanopowder with an average particle size not exceeding 15 nm and α-Si_3N_4 powder with an

average particle size not exceeding 5 μm and containing β-phase not more than 5% wt. The content of precursors was calculated so that the molar ratio of oxides, as a result, was 3:5 (stoichiometry of yttrium-aluminum garnet (YAG) $Y_3Al_5O_{12}$), and the total sintering additive content in the mixtures varied from 3 to 15% wt.

Precipitation of the sintering additive by spray drying method was based on a mixture of $Al_5(NO_3)_3(OH)_{12}$ and $Y(OH)_2(CH_3COO)$ sols with Si_3N_4 powder. The water suspension contained 52.5% wt. Si_3N_4-YAG in terms of solid phase, 1.5% wt. of ammonium polyacrylate was added to stabilize it. After stirring in a planetary mill, the suspension was dried by spray drying method at 150°C.

Another method of precipitation consisted in the formation of citrate gels from solutions of nitrates $Y(NO_3)_3$ and $Al(NO_3)_3$ with the addition of citric acid (CA). To a solution of yttrium and aluminum nitrates was added a solution of CA in such an amount that the molar ratio of CA to the total content of nitrate ions was 1:1. Silicon nitride powder was added to the produced gel under continuous stirring. The resulting mixture was dried under continuous stirring to a thick gel. Obtained gel was annealed for 2 h at 300°C.

Ceramics were compacted by the SPS method on a Dr. Sinter model SPS-625 machine at a pressure of 70 MPa with a heating rate of 50°C/min until the end of shrinkage. The formation of the sintering additive from the precursor proceeded directly in the sintering process. In all experiments, the end of shrinkage was achieved at 1400-1500°C. The hardness of the obtained ceramics samples reached 17.4 GPa with a fracture resistance of 5,09 $MPa \cdot m^{1/2}$.

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NEURAL NETWORK ASSISTED MOLECULAR DYNAMICS CALCULATION OF HIGH-ENTROPY ALLOYS MELTING POINT

Balyakin I.A.*, Rempel A.A.

Institute of Metallurgy UB RAS, Yekaterinburg, Russia
NANOTECH Centre, Ural Federal University, Yekaterinburg, Russia
*i.a.balyakin@gmail.com

One of the difficulties for molecular dynamics simulation of high-entropy alloys is the absence of appropriate interatomic potentials for multicomponent systems. However, it is possible to develop such potentials using machine learning techniques [1]. As a reference database for machine learning *ab initio* molecular dynamics is usually used.

In present work a set of *ab initio* molecular dynamics simulations via VASP [2] package for Cantor alloy (CoCrFeMnNi) at different temperatures starting from 300 K and ending up with 2300 K with 500 K step were performed. As an initial configuration for all the calculations FCC five component special quasi-random structure (SQS) was used. SQS was prepared using stochastic algorithm implemented in ATAT [3] package.

The results of *ab initio* molecular dynamics were used as a training set for ADAM [4] machine learning algorithm implemented in DeePMD [5] package. An objective function which represents potential energy surface (PES) has a form of a set of atomic neural networks.

Using constructed model of PES ten independent two-phase systems with liquid-solid interface were prepared. After this, classical molecular dynamics simulations were performed at different temperatures. Analysis of crystallization was performed using polyhedral template matching procedure [6]. All ten independent initial structures crystallized at 1500 K and melted at 1700 K. New temperatures were chosen using dichotomy method. The melting point was calculated to be around 1688 K which is only about 5 % higher than experimental value 1607 K [7].

Thus, algorithm for *ab initio* calculation of high-entropy alloys melting point is proposed.

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STRUCTURE AND PROPERTIES OF THE TiZrHfVNb HIGH-ENTROPY ALLOY

Beltyukova K. V. *, Balyakin I. A., Sidorov N. I., Petrova S. A., Yuryev A. A., Rempel A. A.

Institute of Metallurgy of the Ural Branch of the RAS, Ekaterinburg, Russia
*ms.great28@mail.ru

One of the most important tasks of "green" energy is the development of a technology for storing hydrogen under normal conditions (0.1 MPa, 300K), which will be possible if hydrogen is stored in a bound form, for example, in the form of metal hydrides.

It was reported in [1] that the TiZrHfVNb high-entropy alloy (HEA) absorbs hydrogen up to 2.5 H/M. This value is significantly higher than that of triple BCC alloys consisting mainly of first-row transition metals with a hydrogen content of about 1.8-2.0 H/M. Currently, most research on HEA is devoted to mechanical properties, only a few works has focused on their interaction with hydrogen.

In this work, using the ab initio MD method, the short-range order parameters and their contribution to the structure and properties prediction of the TiZrHfVNb alloy are considered. It is established that the diffusion coefficients decrease with an increase in the atomic radius.

TiZrHfNbV HEA was synthesized in the form of ingots from high-purity metals (>99.9 %), using multistage arc melting in a high-purity argon atmosphere. The phase composition of the ingots was determined by X-ray diffractometer D8 ADVANCE (Cu-Ka radiation, 30 kV, 40 mA, position-sensitive detector VÅNTEC-1, β-filter).

The sample was saturated with hydrogen from the gas phase at the hydrogen pressure of 70 Torr and the temperature of 350 0C, for 100 minutes. The mechanism of hydrogen release was studied by thermal desorption spectroscopy at various heating rates (2 0C / min, 5 0C/min, 10 0C/min and 15 0C/min) in vacuum in the temperature range from 50 to 820 0C at the IMET-PROTIY apparatus. Analysis of the hydrogen desorption curves shows that hydrogen is released in the temperature range of 700-800 0C. According to the thermal desorption data, the activation energy of hydrogen desorption from the TiZrHfVNb alloy was determined.

The computer simulation was carried out on the Uranus supercomputer of the IMM UB RAS. The work was carried out in accordance with the state assignment of the IMET UB RAS. The authors wish to thank to I. S. Sipatov for his help in preparing samples.

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EFFECT OF TREATMENT ON THERMAL STABILITY OF CU-CR-ZR ALLOY

Bodyakova A.I.[1,2*], Lamzina N.A.[1], Botshanov D.S.[1], Lugovskaya A. S. [1], Pilipenko A. G.[1]

[1]Belgorod State University, Belgorod, Russia
[2]National University of Science & Technology (MISIS), Moscow, Russia
[*]bodyakova-ai@yandex.ru

The Cu-0.3%Cr-0.5%Zr (wt.%) alloy was chosen as started materials. The samples were solution treated (ST) at 920 °C for 0.5 hours and quenched in water. Some of ST samples were additionally aged (AT) at 600 °C for 1 hour. ST and ST+AT samples were subjected by four passes of equal channel angular pressing at 400 °C via route B_C. The ultrafine grained structure was observed after deformation. Then, deformed samples were annealed at 300-700 °C for 1 hour. The electrical conductivity was measured by the eddy current method using Constanta K-6 equipment. Vickers hardness test was carried out on WOLPERT 420 MVD device with a load of 100 g with 15 s dwell time.

The effect of initial state on microhardness and electrical conductivity of ultrafine grained Cu-0.3%Cr-0.5%Zr alloy was presented in Table.

Table. Effect of annealing temperature on Vickers hardness and electrical conductivity of ultrafine grained Cu-0.3%Cr-0.5%Zr alloy

Annealing temperature, °C	ST+ECAP		ST+AT+ECAP	
	Vickers hardness, HV	Electrical conductivity, % IACS	Vickers hardness, HV	Electrical conductivity, % IACS
300	195.3	69.5	152.9	76.8
350	194.4	73.0	152.4	76.8
400	188.3	75.8	149.6	78.0
450	184.3	76.0	146.4	79.5
500	173.6	75.4	155.4	79.1
550	149.0	72.9	148.7	74.9
600	125.0	70.4	122.7	72.4
650	111.3	69.5	81.8	69.4
700	84.6	66.1	72.1	64.2

The ST samples demonstrated higher microhardness and lower electrical conductivities in all annealing regions. This fact can result from different phase compositions, and morphologies of fine particles precipitated before and during ECAP.

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BEHAVIOR OF THE PORTEVEN-LE CHATELIER BANDS IN AUSTENITIC STEEL

Borisova Yu.I.*, Yuzbekova D.Yu. Tkachev E. S., Mogucheva A.A.

Belgorod State University, Belgorod, Russia
*borisovayuliya94@mail.ru

S304H stainless steel was recently developed by adding Cu to Fe - 18Cr - 8Ni. This steel is widely used in supercritical steam boilers due to its excellent creep strength and high resistance to steam corrosion. In addition to the unique combination of technological and functional properties, the S304H austenitic stainless steel has excellent mechanical properties. However, this steel has been found to have a tendency to unstable plastic flow, also known as the Portevin-Le Chatelier (PLC) effect at elevated temperatures. However, at present there are no studies that would investigate the behavior of deformation bands in metallic materials due to the difficulties associated with obtaining images at elevated temperatures.

In present work the solution heat treated austenitic stainless steel Fe – 18Cr – 8Ni – 2.8Cu was investigated. The steel was subjected to solution treatment at 1150°C for one hour followed by quenching into water. Mechanical tests were carried out on flat specimens with a 16 mm gauge length and a cross-section of 1.5×3 mm. The deformation of the samples was carried out on an Instron 5882 universal testing machine at temperatures of 530 - 680°C and a strain rate of 1×10^{-3} s^{-1}. PLC bands were observed using the digital image correlation method. Strain fields were measured continuously on the sample surface using a digital camera at a rate of 10 frames per second. The calculations were carried out using the Vic-2D program.

In the entire range of existence of the PLC effect, a continuous propagation of the PLC bands was found. It was also found that an increase in the frequency of stress drops and a corresponding decrease in the distance continuously propagated by the bands is observed up to a temperature of 590°C. Whereas at temperatures above 620°C, an increase in the distance continuously propagated by the bands was observed, despite the increase in the frequency of stress drops. The velocity of the PLC drops shows a continuous increase with increasing test temperature.

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EFFECT OF SWAGING ON IMPACT TOUGHNESS OF AUSTENITIC STAINLESS STEEL

Chernichenko R. S.*, Panov D. O., Naumov S. V., Stepanov N.D., Zherebtsov S.V., Salishchev G. A.**

Laboratory of Bulk Nanostructured Materials, Belgorod State University, 85 Pobeda Str., Russian Federation, Belgorod
*rus.chernichenko@mail.ru, **panovdmitriy85@gmail.com

Austenitic stainless steels possess attractive mechanical properties, but low yield strength restricts their applications. Cold swaging is a promising method to increase yield strength [1]. However, some issues of the swaging behavior of the material remain poorly understood. In

particular, the effect of the structural gradient formed during swaging on the mechanical properties of the material require further study. Thus, the purpose of this work is to study the effect of swaging on Charpy impact toughness of austenitic stainless steel with a gradient microstructure.

The program material under study is 316-type austenitic stainless steel. Cold swaging was carried out by swaging with different degrees (20-95% of the initial diameter of the bar), which led to the formation of a microstructural gradient along the bar section.

In the initial state, the microstructure is represented in the form of equiaxial defect-free grains. Cold plastic deformation leads to an increase in dislocation density and initiation of twinning, which resulted in the microstructure fragmentation. It is worth noting that the cross-sectional microstructure of the bar from edge to center is different. After 95% cold swaging, thin curved lamellae are observed on the edge of the bar, while a less dispersed block-type microstructure can be observed in the center. The microstructure at the middle of the rod radius is represented by the presence of both blocks and lamellae. The presence of the structural gradient is also confirmed by measuring Vickers hardness, namely changing the hardness profile from edge to center. After 40% cold swaging, Charpy impact toughness values decrease from 140 J/cm^2 to ~ 80 J/cm^2. Further increase of deformation degree is associated with stabilization of Charpy toughness at ~ 60 J/cm^2.

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STUDY OF THE INFLUENCE OF THE INITIAL STATE ON THE MICROSTRUCTURE AND MECHANICAL BEHAVIOR OF THE TI49.0NI51.0 ALLOY UNDER DEFORMATION AND THERMAL EFFECTS

Churakova A.A.[1,2*], Kayumova E.M.[3], Vorobiev E.V.[2]

1 Institute of Molecule and Crystal Physics - Subdivision of the Ufa Federal Research Centre of the Russian Academy of Sciences, Ufa, Russia
2 Ufa State Aviation Technical University, Ufa, Russia
3 Ufa State Petroleum Technological University, Ufa, Russia
*churakovaa_a@mail.ru

The NiTi shape memory alloys exhibit excellent characteristics such as shape memory effect and superelasticity and are materials for practical applications [1-3]. The discrepancy between the volumes of the B2/B19' phases during transformation leads to the generation of dislocations and plastic deformation [4-6]. The Ti49.0Ni51.0 two-component alloy was chosen as the material under study. To obtain an ultrafine-grained structure, ECAP was carried out in two states: state after quenched from 800 °C in water and in a state after aging at a temperature of 450 °C for 1 hour. Additionally, the obtained states were annealed in the temperature range from 400° to 550 °C. The fine structure of the material was examined at room temperature using a JEOL JEM-2100 transmission microscope. Mechanical tensile tests were carried out on small specimens at a tensile rate of 0.24 mm/min. According to the results of mechanical tensile tests in the coarse-grained state, subsequent annealing in the aging temperature range, an increase in the yield stress and ultimate strength parameters is observed by 15% to 500 °C, a further increase in the annealing temperature leads to a decrease in strength parameters, which is associated with an increase in the

grain size and aging particles. A similar character is observed in the ultrafine-grained state obtained after ECAP of the quenched state. In the case of ECAP of the aged state, higher values of the ultimate strength were obtained, but additional annealing led to a significant decrease in the strength characteristics, which is probably associated with the embrittlement of the material as a result of a large number of particles.

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EXPERIMENTAL STUDY OF SINGLE TRACKS OBTAINED FROM A MIXTURE OF TI AND AL POWDERS WITH VARYING SELECTIVE LASER MELTING PARAMETERS

Dolbachev A.P.*, Belov N.A., Akopyan T.K.

National University of Science and Technology (NUST) «MISIS, Moscow, Russia,
*adolbachev1@gmail.com

Intermetallic compounds based on γ-TiAl are considered promising materials, but their manufacture is still difficult due to their low ductility at room temperature and poor hot deformability. Selective laser melting, which has been actively developing in recent years, is a promising additive manufacturing technology for manufacturing parts from γ-TiAl alloys. However, despite a fairly large number of works in this area, the study of binary Ti – Al alloys has not been carried out.

To study the effect of laser scanning speed on the morphology of single tracks, single tracks were obtained from a mixture of Ti and Al powders in a stoichiometric ratio of 1: 1 using an SLM 280 HL machine.

The surface morphology of single tracks was studied in longitudinal and cross sections. Metallographic studies of the obtained single tracks were carried out on a TESCAN VEGA 3 scanning electron microscope (Fig. 1, 2).

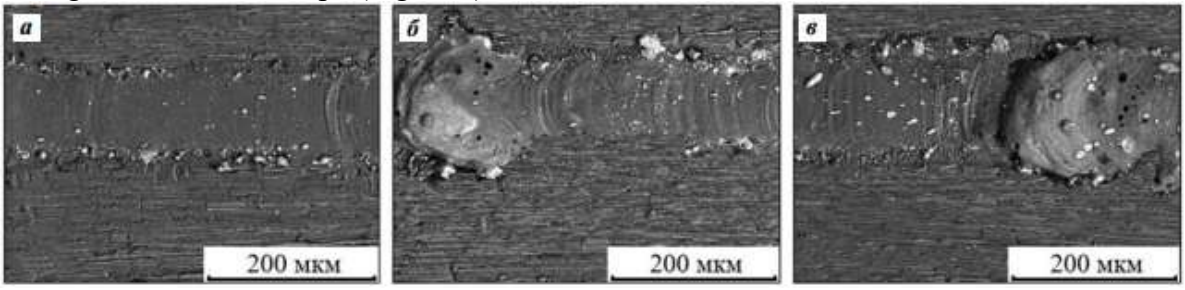

Fig. 1. Surface morphology of single tracks in cross section at different laser scanning speeds, mm/s: 300 (а), 600 (б) and 900 (в) (SEM)

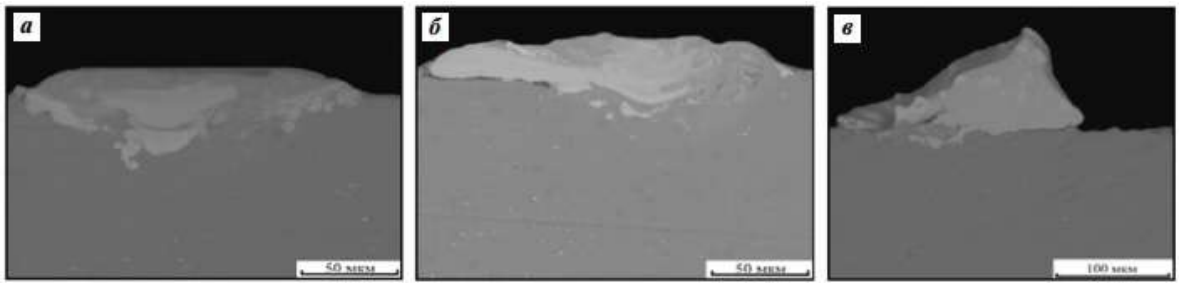

Fig. 2. Structure of single tracks in cross section at different laser scanning speeds, mm/s: 300 (а), 600 (б) and 900 (в) (SEM)

The uniformity of distribution of Ti and Al in the cross section of single tracks was assessed using maps of the distribution of elements. Structural components were determined with using X-ray microanalysis.

Sintering modes determine the morphology of single tracks obtained from a mixture of titanium and aluminum powders, as a result of which their correct selection is necessary to obtain stable tracks.

INFLUENCE OF TEMPFORMING TEMPERATURE ON THE MECHANICAL PROPERTIES OF A LOW-ALLOY CHROMIUM-MOLYBDENUM STEEL

Dolzhenko A.S.*, Lugovskaya A.S., Belyakov A.N.

Belgorod State University, Belgorod, Russia
*dolzhenko_a@bsu.edu.ru

Carbon and low-alloy steels are widely used as structural materials in construction and mechanical engineering. The widespread introduction into industrial production of thermomechanical treatment with controlled cooling has significantly reduced the cost of these steels, which has made it possible to significantly expand the scope of their application. One of the disadvantages of such steels is their relatively high brittle-ductile transition temperature after improvement, which makes these steels brittle and limits their use at low temperatures.

Traditional approach to suppress brittle intercrystalline fracture includes grain refinement and precipitation of dispersed particles along grain boundaries, inhibiting the propagation of an intercrystalline crack. On the other hand, delamination of the material crosswise the direction of crack propagation dulls the crack tip and thus increases the fracture toughness. In this regard, methods for improving the mechanical properties, primarily the impact toughness at low temperatures, of carbon and low-alloy steels are of particular interest.

A low-alloy chromium-molybdenum steel with a chemical composition of Fe - 0.36C - 0.56Cr - 0.57Mn - 0.54Mo - 0.4Si (all in mass%), was subjected to tempforming at 823, 873 and 923 K to a total strain of 1.4. Tensile tests were carried out using an Instron 5882 testing machine at room temperature on flat specimens with a gauge length of 12 mm and a cross section of 3×1.5 mm^2 cut along the rolling direction. Impact tests were carried out on standard specimens with a square cross section of 10×10 mm^2 and a length of 55 mm with a V-notch stress concentrator using an Instron 450 J impact machine with an Instron Dynatup Impulse data acquisition system in the temperature range from 183 to 293 K. Impact test specimens were cut so that the direction of impact was parallel to the normal rolling direction.

Both the yield strength and the ultimate tensile strength decreases while elongation increases with an increase in temperature of tempforming. At tempforming temperature of 823 K, the yield strength is 1540 MPa, and total elongation is 5.3%. With an increase in tempforming temperature to 873 K, the yield strength decreases to 1350 MPa, and total elongation increases to

8.1%. Further increase in tempforming temperature to 923 K results in the yield strength of 1180 MPa and total elongation of 12.1%. The steel samples subjected to tempforming at 823 K exhibit impact toughness of KCV = 265 J/cm^2 at room temperature. A decrease in the test temperature to 233 K leads to a slight decrease in the KCV value to 200 J/cm^2. At a test temperature of 183 K, an increase in the KCV to 276 J/cm^2 is observed. The steel samples subjected to tempforming at 873 K exhibit impact toughness of KCV = 157 J/cm^2 at room temperature. A decrease in the test temperature to 183 K leads to a increase in the KCV value to 400 J/cm^2. The steel samples subjected to tempforming at 923 K exhibit impact toughness of KCV = 190 J/cm^2 at room temperature. A decrease in the test temperature to 273 K leads to a increase in the KCV value to 330 J/cm^2, which practically does not change to a test temperature of 183 K. It should be noted that the impact specimens do not completely destroyed (except for the sample subjected to tempforming at 873 K and tested at room temperature), suggesting underestimation of the impact toughness. The high fracture toughness is attributed to delamination, when the fracture is accompanied by splitting along the rolling plane with high energy absorption.

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A POSSIBILITY OF OBTAINING CORROSION-RESISTANT DEFORMED SEMIFINISHED PRODUCTS FROM AN ALLOY BASED ON THE AL-CA-MG SYSTEM

Doroshenko V.V.*, Naumova E.A., Barykin M.

National Research Technological University "MISiS", Moscow, Russia
*v.doroshenko@mail.ru

The aim of research in this work is to substantiate the possibility of obtaining a corrosion-resistant alloy doped with calcium and magnesium, which has high mechanical properties in comparison with wrought commercial alloys of 5xxx series, such as AMg2 (AA5251). The alloy is additionally alloyed with manganese as one of the strengthening elements of the aluminum matrix, as well as with small additions of zirconium and scandium, which have found wide application in magnals [1]. The final composition is as follows: Al – 2.5Ca – 2.5% Mg – 1% Mn – 0.4% Fe – 0.1% Sc – 0.2% Zr. The presence of iron is due to the ability of calcium to bind it into the ternary compound $Al_{10}CaFe_2$ [2], which is part of the multiphase eutectic.

The structure of the alloy is characterized by the presence of eutectic veins located along the boundaries of dendritic cells (Al). The MPCA data show that the eutectic constituents include 3 phases: (Al), Al_4Ca and $Al_{10}CaFe_2$. At the same time, manganese and magnesium, as well as zirconium and scandium are included in the Al matrix. These data are in good agreement with the calculated data obtained in Thermo-Calc.

In the process of hot rolling (at 400 °C) from an ingot with a thickness of 15 mm, the alloy showed high manufacturability, as evidenced by the absence of transverse cracks and defects on the surface of the hot-rolled semi-finished product (thickness 2 mm, total reduction 87%). In the course of thermal deformation processing, it is possible to change the shape of the structure. Eutectic secretions of compounds with calcium and iron acquired a compact, rounded shape. Also nanoscale precipitates of $Al_3(Zr,Sc)$ and Al_6Mn phases with sizes of 5-10 and 200-300 nm, respectively, are observed in the structure.

The study of mechanical properties showed an increase in hardness by 35% (from 88 to 120 HV). This indicates a high level of strength, which was confirmed. Thus, in the hot-rolled state, the alloy has σw = 391 ± 3 MPa, σ0.2 = 356 ± 3 MPa, δ = 2.6 ± 0.4%. These indicators exceed the values of similar properties of the AMg6 alloy (σ_w = 375 MPa, $\sigma_{0.2}$ = 275 MPa, δ =

6%). At the same time, the experimental alloy with a total proportion of alloying elements <7% showed a similar density AMg6: 2.63 and 2.64 g/cm^3, respectively. And in terms of corrosion resistance during accelerated weight loss tests in an aqueous solution in accordance with GOST 9.021 74, it is slightly inferior to the AMg2 alloy (0.39 versus 0.25% weight loss).

In terms of a set of properties, the experimental alloy can be a replacement for the existing wrought Al-Mg alloys.

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PRODUCTION OF CERAMIC MATERIALS BASED ON Si_3N_4 NANOSIZED POWDER BY SPARK PLASMA SINTERING METHOD

Drozhilkin P.D.*, Andreev P.V, Alekseeva L.S., Boldin M.S., Karazanov K.O.

N.I. Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia
*pddrozhilkin@yandex.ru

In industrial silicon nitride based ceramics the volume fraction of the sintering additive can exceed 10% and more. This significantly limits the possibility of further increases in strength and operating temperature. New precipitation methods for depositing precursors of oxide phases have been tested to obtain fine-grained structure with a minimum content of uniformly distributed sintering additives.

The silicon nitride nanopowder (particle size less than 15 nm) was used as initial material. The Y_2O_3–Al_2O_3 oxide system with various stoichiometric ratios was used as the sintering additive. Molar ratios of yttrium and aluminum oxides were 3:5, 1:2, 1:1, which stoichiometrically corresponds to the complex oxide phases as $Y_3Al_5O_{12}$, $YAlO_3$, $Y_4Al_2O_9$. The content of the additive in the mixtures in each case was 5% wt. The precipitation method consisted in the formation of citrate gels from solutions of $Y(NO_3)_3$ and $Al(NO_3)_3$ nitrates when citric acid (CA) was added. Solution of citric acid was added to solution of yttrium and aluminum nitrates in that amount, which molar ratio of CA to total nitrate ions was 1:1. Silicon nitride powder was added to the resulting gel with continuous stirring. The resulting mixture was dried under continuous stirring to a thick gel. The gel was annealed at 300°C for 2 h.

The ceramic samples were formed from the mixture by spark plasma sintering on Dr. Sinter model SPS-625 at a pressure of 70 MPa and at a heating rate of 50°C/min until the end of the shrinkage. In this case, the formation of the sintering additive from the precursor occurred directly in the sintering process. The end of shrinkage was achieved at 1400-1500°C in all experiments.

The phase composition of the ceramic samples was studied by X-ray diffraction method on a Shimadzu XRD-7000 powder diffractometer (CuKα, λ = 1.5406 Å). The microstructure of the samples was studied by scanning electron microscopy method on a JEOL JSM-6490 microscope with an INCA 350 energy dispersive microanalyzer. Hardness and fracture strength of the ceramics were investigated with using of NanoIndentor G200 (Agilent Technologies) and a QnessA60+ microhardness tester. The fracture distribution was evaluated using a Leica optical microscope.

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Lecturer of the Young Scientists School

ANOMALIES IN TEMPERATURE DEPENDENCE OF MECHANICAL BEHAVIOR OF BODY-CENTERED CUBIC NBTIZR MEDIUM-ENTROPY ALLOY

Eleti R.*, Stepanov N., Maresca F., Yurchenko N., Zherebtsov S.

Laboratory of Bulk Nanostructured Materials, Belgorod State University, 85 Pobeda Str., 308015, Belgorod, Russian Federation
*rajeshwar.eleti@gmail.com

In BCC crystals, due to unusual crystallographic packing of {110}, {112} and {123} planes, screw dislocations motion occurs simultaneously in a 3D space facilitated by the thermally activated kink/kink-pair nucleation. However, kinks are more likely to occupy only two of the three possible slip systems. Under such circumstances, the migration and followed by collision of kinks can lead to the formation of cross-kinks/jogs along the screw dislocations. These cross-kinks may act as strong, local obstacles for the screw dislocations mobility. Maresca and Curtin [Acta Mat., 2019] adopted this aspect of screw dislocations and successfully applied to the concentrated alloys, like medium/high-entropy alloys (MEAs/HEAs). However, the effect of deformation temperature on the kinked screw dislocations and related activation parameters has not been fully explored/understood in the relevance of cross-kink strengthening mechanism. Here, in the present study, we tried to address the above aspect in an equiatomic NbTiZr BCC-MEA.

The as-cast alloy was cold-rolled until 80% height reduction then annealed at 900°C for 30 min, and subsequently water quenched. Tensile tests were performed from 77 K to 1073 K for a constant strain-rate of 10^{-3} s^{-1}.

The yield strength of NbTiZr showed very strong temperature dependence from 1410 MPa at 77 K to 630 MPa at 300 K. The yield strength was relatively independent of the deformation temperature between 473 K and 873 K. The alloy showed serrations and negative strain-rate sensitivity at 473 K indicating dynamic strain-aging phenomena. At 1073 K, the alloy showed a significant drop in the yield strength. Microstructural investigations revealed plastic deformation occurred only by screw dislocations glide at all the above deformation temperatures. Adding to that, the dislocations morphology revealed cross-kinks/jogs along the screw dislocations, except at 1073 K. The drop of yield strength at 1073 K could be due to the annihilation of jogs associated with the possibility of dislocation climb. Later, the dislocations glide related activation parameters were experimentally evaluated and validated with the cross-kink/jog strengthening mechanism. It is shown that the presence of cross-kinks/jogs along screw dislocation does facilitate enhanced strengthening effect of BCC-MEA/HEAs. Also, the effect of deformation temperature on the rate-controlling mechanisms will be discussed.

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EFFECT OF COPPER ON THE SHORT-TERM CREEP PROPERTIES OF THE RE-CONTAINING 10%CR-3%CO-2W STEELS

Fedoseeva A. E.*, Degtyareva S. I.

Belgorod State University, 308015 85 Pobeda, Belgorod, Russia
*fedoseeva@bsu.edu.ru

9-12% Cr martensitic steels are used as materials for fossil power plants with steam temperature more than 600°C [1,2]. Superior creep strength of these steels is attributed to a formation of the tempered martensite lath structure with high density of free dislocations [1]. This

structure is stabilized by a dispersion of nanoscale boundary $M_{23}C_6$ carbides and Laves phase particles as well as MX carbonitrides, which are randomly distributed within the ferritic matrix [1]. The main structural changes during creep at elevated temperature are considered to be the increase in width of the martensitic laths and decrease in the dislocation density that is accompanied with the growth of $M_{23}C_6$ carbides and Laves phase [1,2]. The addition of copper to the 9-12% Cr martensitic steels decreases the nuclei size of Laves phase and slows down their growth [2]. The aim of present work is to report on effect of cupper on short-term creep of the Re-containing 10%Cr-3%Co-2%W steels. Two steels with the different Cu content (10% Cr-0.2Cu and 10% Cr-0.8Cu) were melted and heat treated as normalizing at a temperature of 1050°C during 1 hour, cooling in air, with following tempering at temperature 770°C during 3 hours, air cooling. Flat specimens with a gauge length of 25 mm and a cross section of 7 mm × 3 mm were crept until rupture at 650 °C under the applied stresses of 100 to 200 MPa with a step of 20 MPa. The structural studies were carried out by optical microscopy, transmission and scanning electron microscopies.

Heat treatment of new steels led to the formation of the tempered martensite lath structure in both steels with prior austenite grain size of about 60 μm. The size of the martensite laths was 320-370 nm in both steels, and the dislocation density inside the martensite laths was rather high ($2*10^{14}$ m^{-2}) in both steels. The phase compositions of new 10% Cr-0.8Cu and 10% Cr-0.2Cu steels include ferrite and such secondary phase particles as $M_{23}C_6$ carbides with an average size of about 70 nm, Nb(C,N) carbonitrides with an average size of 30-40 nm and M_6C carbides with an average size of 40-50 nm. The significant differences between the new steels include a reduced volume fraction of $M_{23}C_6$ carbides in 10% Cr-0.8Cu steel and an increased volume fraction of $M_{23}C_6$ carbides in 10% Cr-0.2Cu steel, as well as a reduced fraction of NbX carbonitrides in both new steels as compared to the previously studied 10% Cr steel with Re.

The new 10% Cr-0.8Cu steel at the applied stresses from 200 to 140 MPa demonstrates a significant increase in the creep resistance compared to the previously studied 10% Cr steel: the duration of the primary creep stage increases by a factor of 5, and the minimum creep rate decreases by two orders of magnitude. The increase in rupture time of the new 10% Cr-0.8Cu steel at 200 MPa and 180 MPa was 8 and 4 times in comparison with the previously studied 10% Cr steel. At a stress of 160 MPa, a sample of new 10% Cr-0.8Cu steel that has not fractured yet already has an 8-fold increase in test time compared to the previously studied 10% Cr steel. The new 10% Cr-0.2Cu steel exhibits relatively the low creep resistance at short-term creep tests; the behavior of this steel is similar to the steel-prototype, which does not contain rhenium in its composition. Similar to the steel-prototype, the new 10% Cr-0.2Cu steel can also exhibit high creep resistance at the low applied stresses.

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DEGRADATION KINETICS OF TWO-LAYER TISSUE EQUIVALENTS BASED ON SODIUM ALGINATE IN FLUIDS SIMULATING EXTRACELLULAR BODY FLUIDS

Fetisova V.E.*, Teterina A.U.

Federal State Budgetary Institution of Science Baikov Institute of Metallurgy and Materials Science of the Russian Academy of Sciences, Moscow, Russia
*victoria.phetisova@yandex.ru

Every day many people face skin injuries related to diseases, burns and frostbite. One of the most promising ways to treat such wounds is to replace the damaged areas either with skin or with skin equivalents made of polymers of plant or animal origin. The studies have shown that the most effective of the three options presented is the use of skin equivalents based on polysaccharides of plant origin, such as sodium alginate. [1,2] Sodium alginate has unique properties that allow it to form strong three-dimensional porous matrices of various shapes, which makes it possible to use it for skin regeneration.

For such materials to be suitable for their use in wound care, they need to be double layered. In this case, and the porous layer adjacent directly to the wound will provide rapid vascularization and absorption of excess fluid (lymph) from the wound, which will accelerate the patient's recovery; and the outer layer will maintain the temperature and protect the wound from the environmental influences. To perform these functions, the skin equivalent must be insoluble in water. For this reason, cross-linking, a method of joining individual polymer chains together that leads to insolubility of the materials, is necessary. [3]

Cross-linking of such materials was carried out via bivalent metal cations: sodium cations were replaced by such metal cations, forming a cross-link between the polymer chains. In this work, the complete bilayer structure was subjected to cross-linking with solutions of salts of bivalent metals, in particular: barium ($Ba(CH_3COOH)_2$, $BaCl_2$), calcium ($Ca(NO_3)_2$, $CaCl_2$) and strontium ($SrCl_2$). Thus, due to such a set of salts, we can establish the correlation between the properties of materials cross-linked with different metal cations but in the presence of the same anion (using chlorides as an example) and materials cross-linked with the same cation but with different salt anions (barium chloride and barium acetate, calcium chloride and calcium nitrate pairs).

For the cross-linked materials, their degradation kinetics were studied in SBF buffered solution simulating extracellular body fluid. The samples were left in the buffer solution for 1, 3, 5, 7, 14 and 21 days, and then the trend of property changes was traced. To analyze the phase and microstructural transformations of the materials as a result of cross-linking with different bivalent metal salts, a comprehensive study of physical and chemical properties was carried out using scanning electron microscopy, water and vapor transmission rates, as well as strength characteristics. From the results of the study, the correlation was deduced between the microstructure, degradation kinetics, strength characteristics, and the salts used in crosslinking the materials.

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PHASE COMPOSITION PREDICTION IN HIGH-ENTROPY ALLOYS BY ARTIFICIAL NEURAL NETWORK

Klimenko D. N. *, Stepanov N. D., Zherebtsov S. V.

Laboratory of Bulk Nanostructured Materials, Belgorod State University, Belgorod, Russia
*klimenko@bsu.edu.ru

In contrast to traditional alloys, which are based on one principal element, high-entropy alloys (HEAs) were defined as alloys with five or more principal elements in equal or near-equal atomic percentage (5-35 at.%). HEAs provide a vast compositional space for the design of new alloys. A huge composition space an ampler opportunity to obtain alloys with improved properties (phase composition, strength, etc), but searching without an effective approach can be impractical. In this work, the multi-label (BCC, FCC, B2, BCC1+BCC2, Intermetallic phase) artificial neuron network (ANN) was used for the prediction of phase composition.

Our ANN was trained on 271 HEAs and validated on 69 HEAs. It showed a high level of accuracy of prediction for individual phase (between 84% for BCC and 97% for FCC). The accuracy of predicting the phase composition of alloys is slightly lower and amounts to 70%. The biggest part of incorrect predictions was blinked with the problem of separating of BCC and BCC1+BCC2 phase. The system can predict one of these phases (BCC or BCC1+BCC2) in addition to or instead of another of these phases. In our opinion, in most cases, such an error is not critical.

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STRUCTURE AND PROPERTIES OF ALUMINUM-CALCIUM CONDUCTIVE ALLOYS

Korotkova N.O.*, Cherkasov S.O.

NUST MISiS, Moscow, Russia
*kruglova.natalie@gmail.com

In the present study, the compositions of the Al-Ca-Fe-Si-Zr system promising alloys have been substantiated for obtaining conductive deformed semifinished products in the form of a wire under the conditions of modeling an industrial method of casting and rolling (CCRM). The chemical compositions of the experimental alloys were set to calculate the second phases volume fraction ~ 5 vol. % to provide complex electro-mechanical properties, comparable with the heat-resistant alloy wire Al-7% REM (01417 TU 1-809-1038-96) [1]. Phase composition of two experimental alloys Al-0.75% Ca-0.5% Fe-0.25% Si-0.25% Zr and Al-0.5% Ca-0.5% Fe-0.5% Si -0.25% Zr was investigated by calculation using the Thermo-Calc software and by experimental methods (scanning electron microscopy and X-ray spectral microanalysis). According to the calculated data on the phase composition, the alloys should solidify in the region of the quaternary eutectic, with the formation of phases $Al_{10}CaFe_2$ and Al_4Ca [2]. However, the actual phase analysis of the ingots composition showed that the alloys at a cooling rate of 20 ~ K / s crystallize in the region of the quaternary eutectic (Al) + $Al_{10}CaFe_2$ + Al_3Fe + Al_2CaSi_2. In the structure of alloys, the Al_3Fe phase is presented in the form of finely dispersed plates, and the Al_2CaSi_2 phase - in the form of compact cubic crystals. In this case, the phase diagrams of Al-Ca-Fe-Si in the region of

the aluminum corner [2] indicate the inevitability of the appearance of the Al_2CaSi_2 phase in the structure. This indicates, on the one hand, the minimization of the silicon content in the composition of the solid solution (Al), which can increase the electrical conductivity of the alloy. On the other hand, since the Al_2CaSi_2 phase is formed earlier than the Fe-containing phases, a higher calcium content in the alloy is required to obtain the $Al_{10}CaFe_2$ and Al_4Ca phases in the structure, which can lead to a decrease in electrical conductivity due to the growth fraction of second phases.

In the course of assessing electro-mechanical properties of the wire, it is found that annealing the cold-rolled wire section 1 mm by a two-step regime of 400 °C, 3 h and 450 °C 3 h, allow to achieve electrical resistivity of 32.0 and·31.3 nOhm·m in alloys Al-0.75% Ca-0.5% Fe-0.25% Si-0.25% Zr and Al-0.5% Ca-0.5% Fe-0.5% Si- 0.25% Zr, respectively. Specific electrical conductivity values, as a reciprocal, were 54% IACS and 55% IACS. Further cold wire drawing to a diameter of 0.5 mm allows to obtain the mechanical properties of Al-0,75% Ca-0,5% Fe-0,25% Si-0,25% Zr alloy: tensile strength - 180 MPa, relative extension - 3%. The wire diameter of 0.5 mm of Al-0,5% Ca-0,5% Fe-0,5% Si-0,25% Zr alloy, obtained by an analogous scheme thermomechanical treatment, has a tensile strength of 180 MPa, relative extension of 1%. Short-term annealing of the wire of two alloys at a temperature of 280 ° C for 1 hour reduced the strength by less than 10%, which indicates their heat resistance at this temperature. Thus, the obtained level of electro-mechanical properties makes it possible to consider wire produced from ingots of alloys of the Al-Ca-Fe-Si-Zr system, obtained at cooling rates of ~ 20 K/s, as an alternative to wire produced of alloy 01417, obtained at a cooling rate of ~ 1000 K/s.

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THERMAL STABILITY IN MULTICOMPONENT ALLOYS BASED ON D-METALS

Kurbanova E.D.*, Polukhin V.A.

Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences
Yekaterinburg, Russia
*kurbellya@mail.ru

The processes of amorphization and crystallization of multicomponent melts based on transition metals are considered. A comparative analysis of pre-crystallization structural changes and atomic dynamics under conditions of forced quenching and deep supercooling of metal melts is carried out.

In multicomponent alloys based on transition metals, the presence of surface-active elements, primarily hydrogen, stimulates the dynamics of interatomic interactions and structuring. The degree of influence of hydrogen depends on the composition of the alloy - in the presence of hydride-forming elements in it (for example, metals Zr, Ti; metalloids C, P, B; semiconductors Si, Ge, etc.). A comparative analysis of hydrogen diffusion in amorphous and regular crystal structures was carried out by us on the basis of the results of MD simulation of the hydrogenated binary system Cu-Zr. This model alloy can be considered both as a base for modeling and for

experimental studies of complex amorphous compositions, including highentropy glasses (for example, Zr-Cu-Ti-Ni-Al).

In observations of deep supercooling and glass transition of melts based on palladium, zirconium, iron, etc., the effects of anomalous behavior of their viscosity in certain temperature ranges were recorded, classified as structural crossovers and phonon precursors competing with them dynamic crossovers. Studies of the processes of thermoevolution and glass transition of metal melts carried out with the use of computer simulation revealed that the transformation of short-range order composed of icosahedral clusters (including several hundred atoms and doped with elements (Ni, Ti)) proceeds in an extended range of low temperatures. The onset of the formation of percolating nanoclusters (phase precursors) is preceded by the stage of isomerization with continuous interconversion of short-lived structures with interconversion of different clusters. For more complex and technically important doped glasses based on Cu – Zr and d-metals (Fe, Co, Ni) –Nb – Cu – Si – B alloys, phase separation was observed, which may indicate the existence of chemical inhomogeneity outside the local scale of clusters. short-range ordering already in the glasses themselves immediately after their preparation [1, 2].

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NEW LUMINESCENT CERAMIC MATERIAL BASED ON GLASS WITH CADMIUM SULFIDE NANOPARTICLES

Kuznetsova Yu. V. [*], Popov I. D.

Institute of Solid State Chemistry, Ural Branch of the Russian Academy of Sciences,
Ekaterinburg, Russia
[*]jukuznetsova@mail.ru

In 2020, the global LED market share ranged from 52 to 69% of all light sources according to *Grand View Research*. This demonstrates the huge demand for light sources with energy efficiency in various fields, namely, art workshops, museums, printing, medicine, and light sources for vehicles. These areas have the highest requirements for LED devices: extreme working conditions, high luminous flux, high color rendering index, etc.

However, LED light sources have some drawbacks: 1) a very large luminaire footprint in a high power (> 100,000 lumens) light sources; 2) limited directional illumination; 3) the unbalanced spectrum; 4) overheating of the phosphor and its destruction. Therefore, the direction of designing powerful white light sources overcoming these problems is actively developing at present. The promising concept is laser-based light sources. The use of a laser requires a new design of sources and stability of phosphors to convert large luminous flux. One of the promising phosphor material is a ceramic-based one. It provides less degradation, better control of light scattering and thermal conductivity. However, in the case of creating composite materials, the fundamental problem is how to preserve thier original luminescent properties.

The new ceramic luminescent material was synthesized using a silicate glass with cadmium sulfide quantum dots (CdS QD) and yttrium aluminum garnet (YAG). At once, glass with CdS QDs performs the functions of both a matrix and a phosphor emitting in the yellow and red spectral

regions. This allows compensating the shortcomings of the spectral characteristics of YAG, namely an unbalanced spectral ratio in the luminescence spectrum.

At the first stage, the initial components of ceramics were milled in the mortar. At the second stage, milled glass and YAG were pressed into pills at different ratios, and then sintered at air. The effect of synthesis conditions (ratio of phosphor/matrix and thermal treatment) on functional properties was studied.

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EFFECT OF CARBON ON THE SINTERING BEHAVIOR AND MICROSTRUCTURE OF HARD ALLOYS WITH LOW COBALT CONTENT

Lantsev E. A.*, Nokhrin A. V.

Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia
*elancev@nifti.unn.ru

The purpose of this work is to study the effect of carbon on the kinetics of high-speed sintering of fine-grained hard alloys with small additions of cobalt, as well as to study the effect of carbon additions on the structure and properties of ultralow-cobalt hard alloys obtained by the SPS method.

The research objects of this work were α-WC nanopowders obtained by the plasma-chemical method, in which various concentrations of cobalt (0.3, 0.6, and 1 wt% Co) were deposited by the deposition method. Free carbon in the form of colloidal graphite was mixed into WC-Co nanopowders using a Fritsch-Pulverisette 6 planetary mill in a grinding jar with a hard alloy lining and tungsten carbide balls 1 mm in diameter. The powders were mixed in isopropyl alcohol for 2 h at a speed of 150 rpm.

It is shown that the introduction of graphite leads to the formation of a fine-grained structure (suppression of anomalous grain growth) and a decrease in the intensity of the formation of η-phase particles. It is noted that the formation of particles of the η-phase of the composition Co_3W_3C is observed in the surface layer of the sintered samples, while in the central layers of the samples by XRD, particles of the "low-temperature" η-phase of the composition Co_6W_6C were found. It has been suggested that the formation of particles of the η-phase of composition Co_6W_6C in hard alloys with the addition of graphite is due to a decrease in the characteristic sintering temperatures, as well as a decrease in the total duration of the sintering process as compared to the traditional vacuum annealing of plasma-chemical nanopowders.

Features of the evolution of the structure of ultralow-cobalt hard alloys with the addition of graphite are due to the simultaneous effect of (i) an increased concentration of oxygen adsorbed on the surface of plasma-chemical WC-Co nanoparticles during mixing, and (ii) the effect of graphite, which leads to a decrease in the activation energy of sintering due to a decrease in the intensity of η-phases particle formation in "oxidized" WC-Co nanopowders, as well as the formation of a fairly uniform fine-grained structure.

It is shown that due to the combined use of the technology of plasma-chemical synthesis of tungsten carbide nanoparticles, the chemical-metallurgical method of obtaining nanocomposite WC-Co particles and the technology of spark plasma sintering, samples of ultralow-cobalt hard alloys with the addition of graphite were obtained, which have a homogeneous fine-grained structure (average grain size ~ 1-2 μm), increased density (not less than 98%) and enhanced mechanical properties. For a specimen of hard alloy WC-0.6%Co-0.3%C, the hardness value is H_v = 20.2-20.5 GPa with the value of the minimum crack resistance coefficient K_{IC} = 9.2-10.4 MPa·$m^{1/2}$.

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HYDROFLUORIDE TECHNOLOGY FOR PRODUCING NANOSIZED SILICON DIOXIDE FROM INDUSTRIAL WASTE

Medyankina I.S. [*], Pasechnik L.A.

Institute of Solid State Chemistry UB RAS, Ekaterinburg, Russia
[*]lysira90@mail.ru

Pure amorphous silica can be obtained only by technological means, since its naturally occurring minerals have a number of impurities. Silica can be used as a sorbent, also in the production of electronic components, to increase viscosity, to increase flowability, as a filler in the rubber industry, etc., due to highly developed surface and chemical neutrality [1].

In turn, technogenic waste accumulated in the dumps of the Ural region, such as tailings of wet magnetic separation of titanium magnetite ores and red mud (RM), containing up to 50% SiO_2, are a promising raw material for the production of various purity amorphous silica. The aim of this work is to study the processes of technogenic raw materials interaction with an aqueous solution of NH_4HF_2 to determine the optimal parameters for the extraction of silicon. Hydrochemical fluorination of tailings and RM by NH_4HF_2 solution showed the possibility of separating silicon in the form of a soluble complex $(NH_4)_2SiF_6$. Fluorination was carried out with 1-30% NH_4HF_2 solution with stirring with holding at a temperature of up to 100°C for 1-6h. The process is characterized by low rate constants and high activation energies. Compounds of aluminum, iron, titanium, calcium, magnesium are in the solid residue such the form of fluoro metallates, simple fluorides and / or unreacted initial minerals [2]. The sol-gel method was used to precipitate silica gel from silicon-containing solutions of various concentrations to obtain highly dispersed amorphous silica. At pH 8-9 in the temperature range 25-50°C with constant stirring and slow neutralization with ammonia, a precipitate forms even at a concentration of less than 5 g/l Si by the reaction (1).

$$(NH_4)_2SiF_6 + 4NH_3 + (n+2)H_2O = SiO_2 \times nH_2O \downarrow + 6NH_4F \qquad (1)$$

It was found that the content of SiO2 in the final product is not less than 97% from tailings and 91% from RM. It was shown that the reduction of silicon content in waste less than 20% SiO_2 leads to a significant decrease in the concentration of silicon in solutions and an increase in impurity components. The XRD pattern of silica clearly indicated that no crystalline phases exist, as only a single broad peak between 15° and 30° (2θ) is observed. According to DTA results, the sample is thermally passive. Specific surface area (BET method) reaches 360 m^2/g.

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THE SYNTHESIS OF MEDIUM ENTROPY INTERMETALLIC REINFORCED COMPOSITE COATING BY LASER CLADDING

Mikhailov D. V.[*], Ostovari Moghaddam A., Shaburova N. A., Trofimova S. N., Samodurova M. N., Latfulina Yu. S., Trofimov E. A.

South Ural State University, Chelyabinsk, Russian Federation
[*]tea7510@gmail.com

High-entropy intermetallic compounds have been synthesized by conventional arc melting or mechanical alloying. However, additive manufacturing presents a unique opportunity to

fabricate complicated parts and coatings. Especially, laser cladding is a well-developed additive manufacturing technique to deposit coatings from a wide range of materials. The manufacturing of high-entropy alloys using additive manufacturing was previously demonstrated. However, to the best of our knowledge, the possibility of additive manufacturing of entropy stabilized intermetallic compounds has not been demonstrated. In the absence of any report on the additive manufacturing of entropy stabilized intermetallic compounds, this work demonstrates the possibility of in-situ obtaining medium-entropy intermetallic compounds as a strengthening phase in a multicomponent alloy coating using direct laser cladding [1].

The possibility of stabilizing different amounts of medium-entropy intermetallic compounds with in a multicomponent matrix using laser cladding is demonstrated. The results indicated that medium-entropy intermetallic compound with a B2 structure could be successfully formed within a multicomponent BCC matrix during laser cladding of a proper ratio of Al, Fe, Co, Cu, Mn, and Ni powders. Two coatings with different contents of medium-entropy intermetallic compound were fabricated by changing the feeding rate of the powder mixture. Based on the X-ray diffraction and energy dispersive spectroscopy analyses, the Al-rich intermetallic particles were qualitatively identified as $(Fe_{0.55}Co_{0.18}Cu_{0.22}Ni_{0.03}Mn_{0.02})Al$ medium-entropy intermetallic compound. It was also found that the feeding rate affects the content of medium-entropy intermetallic compound, and consequently, the grain structure and microhardness values. Finally, we propose medium-entropy intermetallic compound reinforced alloys as a more effective alternative system to be used for fabricating high-performance coatings using laser cladding.

The research results showed that additive manufacturing could be successfully employed to fabricate high/medium-entropy intermetallic compound reinforced coatings. However, to stabilize the high/medium-entropy intermetallic compound particles, it is necessary to strictly select the chemical composition of the precursor powders and the processing conditions. In this study, the laser cladding process was carried out at two different feeding rates of 6 g/min and 9 g/min. In both cases, the medium-entropy intermetallic compound particles with a B2 structure were successfully stabilized with in a multicomponent BCC matrix. The lattice parameters of both BCC and B2 phases in the samples are almost identical. The ratio of B2 medium-entropy intermetallic compound particles could be controlled by using the powder feeding rate, and it increased from about 40 wt.% to 60 wt.% when the feeding rate increased from 6 g/min to 9 g/min. By increasing the content of the intermetallic particles, the grain size of the BCC matrix was significantly refined (from 100–800 μm to 25 μm), and the microhardness values of the coating were increased (on average from 425 HV to 475 HV).

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PREPARATION OF FINELY DIVIDED CALCIUM PHOSPHATE COMPOUNDS FROM DICALCIUM PHOSPHATE DIHYDRATE TO HYDROXYAPATITE AT LOW TEMPERATURE CONDITIONS

Mikheeva P. V.*, Teterina A. Yu., Smirnov I. V., Barinov S.M., Komlev V.S.

Baikov Institute of Metallurgy and Materials Science RAS,
Russia, Moscow, Leninskiy prospect, 49, 119334
*mikheevap7@gmail.com

The main direction development of creating biomaterials is a regenerative approach in which the emphasis is not on the displacement of the defect by an implant with suitable mechanical characteristics, but on the rapid biodegradation of the material and its replacement with bone tissue formed by the body itself. Thus, at the first place for such materials comes out their biological and physicochemical properties.

Dense hydroxylapatite ceramics is a low-active material, the processes of resorption of the implant and the kinetics of growth of the contact bone tissue are extremely slowed down. The large specific surface area of calcium phosphates obtained by low-temperature (solution) methods (up to 100 m^2/g) makes them more active in comparison with high-temperature calcium phosphates (~ 1 m^2/g); therefore, that is why it is so important to obtain of finely divided calcium phosphate compounds.

The formation of ceramic structures is realized due to the phase transformation of the initial α-tricalcium phosphate (α-TCP) powder to dicalcium phosphate dihydrate (DCPD), then followed by its hydrolysis to octacalcium phosphate (OCP) and then to hydroxyapatite. Extraction of α-TCP is carried out in a buffer solution of 1.5 M sodium acetate, 0.15 M L-glutamic acid with orthophosphoric acid brought to pH = 5.5, with a sample mass / liquid ratio 1/100, at a temperature of 35 ± 2 °C and constant stirring.

$\alpha Ca_3(PO_4)_2 + 4H^+ \leftrightarrow 3Ca^{2+} + 2H_2PO_4^-$

$\alpha Ca_3(PO_4)_2 + 3CH_3COO^- + 2H^+ = 3Ca(CH_3COO)^+ + 2HPO_4^{2-}$

$Ca^{+2} + HPO_4^{2-} + 2H_2O = CaHPO_4 \cdot 2H_2O$

$Ca(CH_3COO)^+ + HPO_4^{2-} + 2H_2O = CaHPO_4 \cdot 2H_2O + CH_3COO^-$

The OCP composition is obtained by keeping DCPD powder in a buffer solution of sodium acetate. At the first stage, when a sample of DCPD is placed in a buffer solution, the surface layers of the material dissolve and the Ca^{2+} and HPO_4^{2-} ions are released into the solution. The dissolution of the surface is carried out by the dissociation products of sodium acetate. When the maximum concentration of cations and anions in this layer is reached, reverse crystallization of CP occurs in the form of OCP crystals, which begins on the surface of DCPD that has not yet undergone dissolution. With complete recrystallization of the surface, the transformation process becomes diffusional and continues until the moment of complete transformation of DCPD into OCP. In this case, if the transformation process is carried out under conditions conducive to the slow passage of the reaction, then at the macrolevel the shape of the initial DCPD crystals will be preserved, which consist of small, up to 5 μm, OCP crystals. Hydroxyapatite powder was obtained by further transformation of OCP in a buffer solution.

Thus, in this study, was developed a method for the preparation of finely dispersed calcium phosphate compounds at low temperature conditions in different buffer solutions.

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EFFECT OF 1000 H AGING AT 650 °C ON THE IMPACT TOUGHNESS OF ADVANCED 10% CR MARTENSITIC STEEL

Mishnev R. V.*, Dudova N. R.

Belgorod State University, 308015, Pobeda 85, Belgorod, Russia
*mishnev91@mail.ru

Heat-resistant high-Cr martensitic steels are widely used in various critical components of fossil power plants due to their superior creep resistance and low cost. High fracture toughness is an important property to assure the reliability of steam turbine parts produced from these steels. The room temperature impact toughness of 40 J/cm^2 and higher provides sufficiently safe operation of steam turbine parts. The 9% Cr steels exhibit high toughness ≥200 J/cm^2 at room temperature, however the long-term exposition at exploitation temperature leads to a 2–4-fold decrease in the Charpy V-notch impact energy at ambient temperature and to an increase in ductile-brittle transition temperature (DBTT). This is attributed to precipitation of the Laves phase particles. Recently, a new generation of high-boron 9-10% Cr steels with the improved creep properties was developed. It was shown that the new alloying scheme results in a significant increase in the DBTT, for example, the 10%Cr steel demonstrates the DBTT of +10°C that lies within the acceptance limit. It is established that the aging of the 10% Cr steel containing high B and low N contents at 650°C for 100 h leads to the decrease in the impact toughness at 20°C from 240 to 90 J/cm^2 and increase in the DBTT from +10 to +35°C.

In this work, the effect of long-term aging for 1000 h at 650°C on the temperature dependence of impact toughness and fracture behavior of advanced 10% Cr steel with low N and high B contents was studied. Standard V-notch Charpy impact specimens were tested using an Instron 450 J impact machine (Model SI-1 M) with an Instron Dynatup Impulse data acquisition system following the ASTM E-23 standard at temperatures ranging from −40...200°C. It was found that an increase in the aging time at 650°C from 100 to 1000 h has a negative effect on impact toughness. Aging for 1000 h leads to the increase in the DBTT to 50°C as compared with 10°C for tempered state and 35°C for aged for 100 h. Impact toughness after 1000 h aging at room temperature is ~ 40 J/cm^2. It was found that a decrease in the impact toughness with a decrease in the test temperature has a good correlation with a decrease in the size of the zone of stable crack propagation.

EXPERIMENTAL STUDY OF THE INFLUENCE OF HIGH-TEMPERATURE ANNEALING ON THE STRUCTURE, MECHANICAL PROPERTIES AND RESISTANCE OF ULTRAFINE-GRAINED TITANIUM ALLOY PT3V TO CORROSION-FATIGUE FAILURE

Murashov A.A.*, Berendeyev N.N., Nokhrin A.V.

Lobachevsky State University of Nizhny Novgorod, Russia
*aamurashov@nifti.unn.ru

The object of research in this work is the industrial pseudo-α titanium alloy PT3V, which is actively used in nuclear engineering and has a composition of Ti-4.73 wt.% Al-1.88 wt.% V. The ultrafine-grained structure was formed by the rotary swaging method. Rotary swaging was carried out using a R5-4-21 HIP «Heinrich Muller Maschinfabrik» rotary forging machine at room temperature to a degree of deformation of 70%. Fatigue tests were carried out on cylindrical specimens according to the "bending with rotation" scheme in a 3% aqueous solution of NaCl at a

loading frequency of 50 Hz. To anneal titanium samples, an EKPS-10 SNOL type muffle electric furnace was used, annealing was carried out at temperatures of 500, 550, 600, 700 °C for 30 minutes, and also at a temperature of 500 °C for 500 hours.

Studies of the microstructure have shown that after rotary swaging in the PT3V alloy, an ultrafine-grained structure is formed with an average fragment size of ~0.2-0.5 μm, this structure can be characterized as a mixed grain-subgrain structure. After annealing at temperatures of 250, 500, 550 °C, the structure of the alloy does not change. After annealing at 600 °C, recrystallized grains ~1 μm in size are rarely observed. At an annealing temperature T = 700 °C, a completely recrystallized structure with a grain size of 3 to 3.5 μm is observed.

Investigations of the mechanical properties, as well as the resistance of the alloy to corrosion-fatigue fracture before and after annealing have been carried out. It is shown that a significant drop in microhardness is observed at annealing temperatures of 600 °C and 700 °C. A drop in corrosion-fatigue strength is observed in the entire temperature range of short annealing from 500 to 700 °C. However, after prolonged high-temperature annealing at a temperature of 250 °C, no drop is observed.

Fractographic analysis of specimen fractures after corrosion-fatigue tests has been carried out. The main stages of fatigue crack initiation and growth are revealed.

EFFECTS OF DIFFUSION WELDING MODES ON STRUCTURE AND MECHANICAL PROPERTIES OF DIFFUSION BONDING OF ORTHORHOMBIC TITANIUM ALUMINIDE BASED ALLOY

Naumov S.V.[*], Panov D.O.[**], Chernichenko R.S., Stepanov N.D., Zherebtsov S.V., Salishchev G.A.

Laboratory of Bulk Nanostructured Materials, Belgorod State University, 85 Pobeda Str., 308015 Russian Federation, Belgorod
[*]NaumovStanislav@yandex.ru, [**]panovdmitriy85@gmail.com

Alloys based on orthorhombic titanium aluminide (Ti_2AlNb) are one of the most promising heat-resistant alloys for aircraft and aerospace products due to their unique characteristics features like high specific strength, relatively low density and high oxidation resistance. However, technological properties of these alloys, for example, weldability, limits the possibilities of their application. Considering the advantages and disadvantages of various methods of producing permanent joints, diffusion welding (DW) is preferable for obtaining a high-quality welded joint of Ti_2AlNb-based alloys, since there is no need to melt the metal in the welding zone and, therefore, there is no heat-affected zone. Although DW achieves a high-quality welded joint, the process parameters must be thoroughly controlled. Thus, the purpose of this work is to determine the effect of diffusion welding modes of the SPS 10–3 unit on structure and mechanical properties of diffusion bonding of Ti_2AlNb-based alloys.

VTI-4 alloy was used in this work (Ti-23Al-23Nb-1.4V-0.8Zr-0.4Mo-0.4Si at. %). DW was carried out on SPS 10–3 spark plasma sintering unit. The templets were heated by passing pulsed currents through stamping punch and graphite matrix. The blank deformation rate was no more than 10 %. Mechanical behavior of the templets was evaluated using tensile deformation. Enhanced mechanical properties were observed after welding temperature of 940 °C and 960 °C, equalizing time of 2 hours and pressure of 16–18 MPa. With an increase in the welding temperature, O-phase content in blanks increases but α_2-phase content remains almost unchanged. However, with respect to the base material there is a drastic increase in the O-phase. Further work will be aimed at studying the effect of subsequent heat treatment and expanding diffusion welding modes.

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DIFFERENT APPROACHES TO DETERMINATION OF INTERNAL STRESSES BY X-RAY DIFFRACTION METHODS USING TITANIUM ALLOY SAMPLES

Andreev P.V*, Nazarov A.A., Telkov A.P., Smetanina K.E., Drozhilkin P.D., Faddeev M.A.

N.I. Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia
*andreev@phys.unn.ru

X-ray diffraction analysis is a universal non-destructive method of controlling the structure of polycrystalline materials. The position and intensities of diffraction peaks determine the qualitative and quantitative crystal phase composition. Additional information on the structure is given by full-profile analysis of the diffraction patterns. This includes strains, stresses and crystallite sizes of the sample. Full profile analysis requires a careful approach, including knowing the instrumental function of the diffractometer - the dependence of diffraction line broadening on the scattering angle, typical of the equipment configuration used - for high quality results.

Another challenge is to describe the diffraction peak with a suitable approximating function. Third, choosing the right mathematical model of the effect. The study present Williamson-Hall, size-strain plot and Halder-Wagner methods have been used to investigate the particle size and the intrinsic strain from the XRD peak broadening analysis. Further, in Williamson-Hall method, different models have been considered for the determination.

Titanium alloys samples cut from one workpiece, intensively deformed by equal-channel angular pressing, then annealed under different conditions were chosen as an object of investigation. All X-ray diffraction experiments were performed on a Shimadzu XRD-7000 diffractometer. In the first stage, the instrumental function of the diffractometer depending on the slit system used was investigated using reference samples. At this stage the problem of analytical calculation of the diffraction peak broadening according to the parameters of the pseudo-Voigt function approximating it was also considered.

APPLICATION OF PLASMA METALLIZATION TECHNOLOGY FOR RAPID PROTOTYPING OF PRODUCTS

Neulybin S. D.*, Shchitsyn Yu. D., Ovchinnikov I. P.

Perm National Research Polytechnic University, Perm, Russia
*sergeyneulybin@gmail.com

Layer-by-layer plasma deposition of wire spraying products onto a base previously formed from an inexpensive material can be a promising method for forming blanks of large-sized items [1].

Positive experience exists mainly in the creation of coatings of small thicknesses, there is a low utilization rate of materials, a characteristic defectiveness of the materials obtained, a high cost of equipment, and a low environmental friendliness of the process. The production of billets of large cross-sections with layer-by-layer thermal spraying and metallization is constrained by the high cost in the case of using powder materials [2].

Plasma metallization is seen as a promising method for obtaining prototypes of metal products, with wire spraying with a plasma arc of reverse polarity of the current.

Plasma metallization can be performed using one, two or more wires (can be fed simultaneously or layer by layer in series). At the same time, a unique opportunity appears in a wide range to control the chemical composition, structure and properties of the materials obtained.

A distinctive advantage of metallization in additive manufacturing is the minimum heating of the base, because fusion or sintering occurs at temperatures well below the melting point.

During preliminary studies, the optimal power and productivity of the process were selected.

The paper presents the results of spraying bronze of the chrome bronze brand with a productivity of 11 kg/h on a cylindrical steel base. The steel base is used exclusively as a backing material and is removed during subsequent machining.

Based on the results of the technology development, the optimal distances from the nozzle exit to the formed product were established in order to ensure the best sintering and minimize overheating of the product. The results of metallographic processing showed a high continuity of the material, a specific structure characteristic of gas-dynamic spraying. Optimized metallization modes are recommended for testing equipment and technology in the process of rapid prototyping of metal products.

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ELECTRICAL PROPERTIES OF AMORPHOUS $(CD_{0.9}ZN_{0.08}MN_{0.02})_3AS_2$ FILMS

Nezhencev A. V. *, Pilyuk E. A., Nikulicheva T. B., Borisenko A. V.

Belgorod National Research University, Belgorod, Russia
*anton.nezhencev@gmail.com

Studies of topological insulators and films of nanometer thickness occupy a significant place in condensed matter physics [1,2]. The unusual properties of cadmium arsenide such as the anomalously high mobility of charge carriers [3] have long attracted the attention of researchers.

Thin films $(Cd_{1-x-y}Zn_xMn_y)_3As_2$ (x + y = 0.1; y = 0.02) were obtained by high-frequency magnetron sputtering on VN-2000. The substrates were p-type silicon wafer (100) 0.4 mm thick coated with thermally grown SiO_2 oxide. The thickness of the films is 20 nm.

Raman spectrometer LabRam HR Evolution was used to get the spectra of the obtained films $(Cd_{0.9}Zn_{0.08}Mn_{0.02})_3As_2$ shows that they have characteristic peaks at 38, 62, 100, 125, 191, 215, and 247 cm^{-1}. The atomic force microscopy (Ntegra Aura) results show that all films are continuous with a granular surface structure with an average grain size of about 150 nm. The scanning electron microscopy (Nova NanoSem 450) images show that the $(Cd_{0.9}Zn_{0.08}Mn_{0.02})_3As_2$ films are practically homogeneous. According to the distribution of the elements, the films within the measurement range had a homogeneous structure. According to the results of X-ray diffraction using a Rigaku SmartLab diffractometer typical diffraction patterns of films obtained on cold silicon substrates are typical for amorphous materials with broad “halo” peaks.

Measurements of the electrical properties such as conductivity of $(Cd_{0.9}Zn_{0.08}Mn_{0.02})_3As_2$ thin films were taken according to the standard six-point scheme on a Janis CCS-350S helium cryostat in the temperature range 10-300 K and magnetic fields up to 1 T. The results show that

the resistivity of the film is increasing as well as temperature which corresponds to a metal type conductivity.

The concentration and mobility of electrons, calculated using the results of measurements of the Hall constant, were 5.1×10^{20} cm^{-3} and 3.3×10^{2} $cm^2 \cdot V^{-1} \cdot s^{-1}$ at 10 K and 6.6×10^{20} cm^{-3} and 2.1×10^{2} $cm^2 \cdot V^{-1} \cdot s^{-1}$ at 300 K, respectively. The concentration increases with increasing temperature and the mobility decreases with increasing temperature. The magnetoresistance is negative. It is mostly found in ferromagnetics, this can point out to the presence of the variable-range conductivity.

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EFFECT OF AGEING TIME ON THE TENSILE PROPERTIES AND STRUCTURE OF THE HIGH-CHROMIUM MARTENSITIC STEEL

Nikitin I.S., Fedoseeva A. E.*

Belgorod State University, 308015 85 Pobeda, Belgorod, Russia
*fedoseeva@bsu.edu.ru

The structure and tensile properties of the tempered martensite/ferrite lath structure of 12 wt%Cr heat-resistant steel with low N and high B contents after ageing at 650°C for 5 h, 50 h, 200 h, 400 h, 850 h, 8000 h and 12000 h were investigated. Previously, the steel investigated was heat treated consisting normalizing at 1070°C with following tempering at 770°C for 3 h. After heat treatment, tempered martensite/ferrite lath structure of the 12%Cr steel with a mean size of martensitic laths of 290±30 nm and dislocation density in lath interior of 2×1014 m^{-2} was revealed. The boundaries of martensitic laths were stabilized by fine M23C6 carbides with a mean size of 55±10 nm. The tensile tests were carried out at room temperature. The yield strength and ultimate tensile strength were 614±40 MPa and 780±40 MPa, respectively, after heat treatment. Ageing at 650°C for first 50 h insignificantly decreased the yield strength on 20 MPa that was related to two processes: (1) depletion of W from the ferrite matrix and (2) the precipitation of the fine Laves phase particles along lath boundaries. An increase in ageing time up to 400 h led to an increase in the yield strength up to value close to that after tempering. The increment in precipitation strengthening due to the fine Laves phase particles compensated a decrease in the solid solution strenghening due to depletion of W. After 8000 h of ageing, the coarsening of laths and boundary particles took place that led to a decrease in yield strength by 14%, while the tempered martensite lath structure retained without subgrain formation. No significant softening during 12,000 h of ageing at 650°C was observed that indicated high thermal stability of tempered structure of 12%Cr steel at thermal exposure. The relationship between structure and tensile properties of samples aged with different times was evaluated; the effect of ageing time on the strengthening mechanisms was discussed.

AN IMPACT OF B4C IN-SITU ALLOYING ON THE STRUCTURE AND MECHANICAL PROPERTIES OF LASER DEPOSITED MEDIUM-ENTROPY CrFeNi COATINGS

Okulov A. V.[1*], Gokhfeld N. V.[1], Korobov Yu. S.[1,2], Makarov A. V.[1], Kharanzhevskiy E. V.[3], Stepchenkov A. K.[1] and Okulov I. V.[2,4,5]

[1]M.N. Mikheev Institute of Metal Physics, Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia;
[2]Ural Federal University, Ekaterinburg, Russia;
[3]Udmurt State University, Izhevsk, Russia;
[4]University of Bremen, Bremen, Germany;
[5]Leibniz Institute for Materials Engineering - IWT, Bremen, Germany
[*]okulovartem@imp.uran.ru

Metal-ceramic composite (MCC) coatings provide high surface hardness combined with adequate resistance to wear, corrosion and high temperatures. The effective method to synthesize such MCC coatings is the in-situ alloying by laser deposition. The method provides the implementation of the Charpy's principle when the hardest structural components are distributed within the ductile metal matrix in the form of inclusions isolated from each other. Due to their excellent mechanical properties such as high strength, hardness and heat resistance, the following materials were selected to obtain MCC coatings: equiatomic medium-entropy alloy (MEA) CrFeNi and B_4C.

The mechanical mixture CrFeNi-B_4C was prepared by mixing of the multicomponent equiatomic powder CrFeNi with various amounts of B_4C in the range of 2-6 wt.%. The development of the CrFeNi-B_4C coatings on stainless steel 316L substrate was carried out by pulsed laser deposition. The experimental laser setup consisted of an ytterbium fibre laser with a maximum average power of 50 W and a wavelength of 1.065 μm. The laser treatment was performed in a chamber with a controlled Ar atmosphere by pulses of about 40 ns duration. Various research methods were used to study the structure and mechanical properties of the synthesized CrFeNi and CrFeNi-B_4C coatings: high-resolution optics, SEM, XRD analysis, micro- and nanoindentation, tribological tests.

Based on the study results, it was carried out a comparative analysis of the obtained equiatomic CrFeNi coatings before and after in-situ alloying by 2-6 wt.% of B_4C. The effect of varying the amount of B_4C on the mechanical characteristics of the deposited layer was shown. A rational interval of B_4C content was established, in which the deposited layer combines high hardness, strength, and sufficient ductility, expressed in the absence of cracks.

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WIRE-ARC ADDITIVE MANUFACTURING OF 25.1CO-15.1CR-37.8FE-3.4MN-16.3NI NON-EQUIATOMIC HIGH ENTROPY ALLOY

Osintsev K. A.[1,2*], Konovalov S. V.[1,2], Zagulyaev D. V.[1], Gromov V. E.[1], Panchenko I. A.[1], Chen X.[1,2]

[1]Siberian State Industrial University, Novokuznetsk, Russia
[2]Samara National Research University, Samara, Russia
[*]osincev.ka@ssau.ru

Recently, high entropy alloys (HEAs) have attracted attention as a new class of structural materials. Unlike conventional alloy systems, HEAs systems usually contain five main elements at least, at concentrations varying between 5 and 35 at.%. Due to the effect of high mixing entropy,

these newly invented alloys can crystallize as simple phase composition, even form a single solid solution phase rather than complex phases during solidification. It gives them a unique combination of excellent properties, such as good corrosion resistance, good fatigue resistance, high fracture toughness, a wide range of Young's moduli, and high yield strength. The Co-Cr-Fe-Mn-Ni HEA system is known for its good ductility at cryogenic temperature and room temperature. Previously, this alloy was fabricated by conventional methods and additive manufacturing technologies. Traditional methods have limits in the shape and size of the producing components, whereas AM methods have such disadvantages as the high cost of the initial material (powder). Compared with the methods mentioned above, wire-arc additive manufacturing technology (WAAM) has such advantages as a high deposition rate, the possibility of fabricating large-sized components, and cost-effectiveness. Recent studies revealed that WAAM could be successfully applied for manufacturing bulk Al-Co-Cr-Fe-Ni HEA. The obtained alloy has high hardness, and its mechanical properties are comparable with the alloy manufactured by conventional methods.

In this study, as initial material was chosen, combined cable wire composed of three wires with the following chemical compositions: pure Co wire (Co ≈ 99.9 at. %) ≈ 0.47 mm in diameter; Autrod 16.95 welding wire (Fe ≈ 65.3 at. %, Cr ≈ 19.6 at. %, Ni ≈ 7.3 at. %, Si ≈ 1.6 at. %, Mn ≈ 6.2 at. %) preliminary thinned from ≈ 0.80 down to ≈0.74 mm in diameter; Ni80Cr20 wire (Al ≈ 0.8 at. %, Cr ≈ 22.5 at. %, Fe ≈ 1.5 at. %, Ni ≈ 72.1 at. %, Si ≈ 2.9 at. %, Mn ≈ 0.2 at. %) ≈ 0.4 mm in diameter. The HEA was manufactured via layer-by-layer deposition on a 321 stainless steel substrate. X-ray diffraction (XRD) analysis using DRON-2 X-ray diffractometer with Co Ka radiation was used to identify the phases in the alloy. The microstructure and chemical composition were examined using TESCAN Vega SB equipped with an energy dispersive spectrometer INCAx-act. Hardness tests were conducted using Microhardness Vickers Tester HV-1000 under a load of 1 kg for a loading time of 10 s.

The XRD pattern showed that the fabricated alloy was composed of a single FCC phase. The calculated results by SineTheta Software indicate that the lattice constant of the FCC phase is 0.35869 nm. Major diffraction peaks and their inter-planar distance of the alloy are (2Theta = 51.00º; d = 2.077), (2Theta = 53.57º; d = 1.985), (2Theta = 59.70º; d = 1.797), and (2Theta = 89.81º; d = 1.267). There is no distinguishable color difference in any region of the SEM images of the alloy. And no composition difference was detected in any region. According to EDS analysis, the main components of the obtained alloy are Fe (37.8 at. %), Co (25.1 at. %), Ni (16.3 at. %), Cr (15.1 at. %), Mn (3.4 at. %). As impurities introduced in the alloy from the wires were found Al (0.8 at %) and Si (1.4 at. %). All detected chemical elements are homogeneously distributed in the microstructure. The detected microhardness of the alloy is 165.9 ± 5.5 HV. SEM observations also revealed the presence of round in shape pores homogeneously distributed in the alloy's microstructure. The pore diameter is up to 5 μm. The average grain size in the detected structure is ~12.5 μm.

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MICROSTRUCTURE AND MECHANICAL PROPERTIES OF THE MEDIUM-ENTROPY NbTiZr ALLOY-BASED COMPOSITE, REINFORCED WITH BORIDE PARTICLES

Ozerov M. S.*, Stepanov N. D., Zherebtsov S. V.

Belgorod National Research University, Belgorod, Russia
*ozerov@bsu.edu.ru

Titanium alloys of the Nb-Ti-Zr system have a low modulus of elasticity, high specific strength, excellent corrosion resistance and biocompatibility, which determines their widespread use in implantology, traumatology and orthopedics. However, the use of these

alloys is often limited by their other characteristics: relatively low strength, hardness and wear resistance. A significant improvement in strength characteristics can be achieved by using a combination of strengthening strategies, for example, due to a significant modification of the chemical composition and transition to the so-called medium- and high-entropy compositions with high solid solution hardening, as well as by creating metal-matrix composites with ceramic reinforcing components. The best choice for titanium-based alloys is the use of TiB particles as a hardener, which adheres well to the titanium matrix without the formation of a transition region and has a similar coefficient of thermal expansion; in addition, due to its good thermal stability, TiB can provide strength even at elevated temperatures. The structure of NbTiZr/(NbTiZr) B composites is a function of many variables, including the production method and conditions (casting or powder metallurgy), the volume fraction of borides, and the parameters of further thermomechanical processing. These issues have been widely studied for titanium-based composites with an hcp lattice [1], to a much lesser extent for composites based on beta alloys [2], and have hardly been studied for metal-matrix composites with an MEA/HEA matrix. Therefore, the detailed analysis of the dependence of the structure and properties of NbTiZr/(NbTiZr)B composites on the volume fraction of borides, and the conditions for obtaining blanks is undoubtedly relevant, and can be of high practical importance.

In this work laboratory-scale NbTiZr/(NbTiZr) B composite ingots (20 g) were melted by vacuum arc remelting with a non-consumable electrode. For melting, pure (with a purity of at least 99.9%) elements that make up the matrix, as well as TiB_2 (titanium diboride) powder with an average particle size of 3-8 microns, were used. The weight proportion of TiB_2 in cast composite billets was 0.2, 2 and 4.5 mass. %. The main goal of introducing a minimum amount of borides was primarily to refine the structure during crystallization, while large amounts of the reinforcing component will cause the formation of strengthening boride particles. After uniaxial compression at room temperature the specimen of composite with 0.2 mass. % TiB_2 was not fractured even after 45% thickness reduction, while compression ductility for the conditions of composites with 2 and 4.5 mass. % TiB_2 was 25 and 9 %, respectively. The highest yield strength was shown by the state of the composite with 4.5 mass. % TiB_2 – 1010 MPa, while the conditions of the composite with 0.2 and 2 mass. % TiB_2 showed fairly similar values of the yield stress – 740 and 860 MPa, respectively. The apparent length of the (NbTiZr) B whiskers, heterogeneously distributed in the NbTiZr matrix, was 0.3 ± 0.2, 1 ± 0.5, 3 ± 1.8 μm for the three weight conditions of composites, respectively.

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HIGH TEMPERATURE OXIDATION RESISTANCE OF REFRACTORY HIGH ENTROPY ALLOYS

Ostovari M. A.[1*], Veselkov S. N.[1], Shaburova N. A.[1], Sudarikov M. V.[1], Samoilova O. V[1], Pratskova S. E.[2], Trofimov E. A.[1]

[1]South Ural State University, Chelyabinsk, Russian Federation
[2]Chelyabinsk State University, Chelyabinsk, Russian Federation
[*]ostovarim@susu.ru

High entropy alloys (HEAs) are defined as alloying system consisted of five or more principal elements with typically equiatomic or near equiatomic ratio, which occasionally exhibit extraordinary properties [1]. Among different types of HEAs, refractory HEAs (RHEAs) are considered as the most promising alloy systems to design new materials for high temperature applications beyond Ni based superalloys [2]. Besides, W-containing HEAs are potential candidate for high temperature applications such as plasma facing material in nuclear reactors owing to high melting temperature, high thermal conductivity and small tritium retention of tungsten. However, a systematic study on the oxidation resistance of W-containing HEAs is still lacking.

In this study, we investigated the oxidation resistance of several W-containing refractory HEAs at high temperatures to further examine the formation of complex oxides layer on the surface of these alloys. The equimolar WMoTiVCr, WMoTaTiCr, and WTiTaCr alloys were fabricated by arc-melting process under argon atmosphere using high purity (> 99.9 wt. %) metal powders. The as cast alloys exhibited a single BCC solid solution phase with dendritic microstructure and elemental segregation. Typically for all the alloys W and Ta segregated in the dendritic arms and Ti, Cr, Mo, and V segregated into the inter-dendritic regions. Oxidation behavior of the samples were studied at 1000 °C for 10 h in air atmosphere. WMoTiVCr alloy exhibited very low resistance against high temperature oxidation mainly due to the formation of a highly porous TiO_2 rich scale layer. By substituting V with Ta in WMoTaTiCr, a WO_3 and $CrTaO_4$ rich oxide layer was dominated and the oxidation resistance was improved. A similar oxide layer was also formed on the surface WTiTaCr alloy.

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AFFECT OF LASER SHOCK PEENING ON MICROSTRUCTURE EVOLUTION AND RESIDUAL STRESSES OF Ti-6Al-4V ALLOY

Ozerov M. S.*, Mironov S. Yu., Kalinenko A. A., Kashaev N. S., Plekhov O.A., Salishchev G. A., Zherebtsov S. V.

Belgorod National Research University, Belgorod, Russia
[*]ozerov@bsu.edu.ru

When designing aircraft, titanium alloys in particular Ti64 alloy are extremely in demand in the manufacture of a gas turbine engine fan and compressor blades, the critical characteristics of which are high fatigue strength and durability. The improvement in strength and fatigue

characteristics, especially of the surface zones, of this alloy is an extremely urgent task. These characteristics are largely determined by residual stresses, in this connection deformation proceedings or how they are called differently “residual-stress-based life extension techniques” which allow increasing of useful compressive stress in the surface area of the material have already been developed and continue to be developed. LSP represents a surface treatment that introduces compressive residual stresses with high penetration depth in critical regions susceptible to fatigue phenomena. Most studies of the effect of laser treatment on the microstructure of metals are concentrated on local areas of the surface treated zone, where the values of residual stresses are highest. However, the question of the LSP effect on the microstructure evolution at a greater laser power densities and, respectively, at a greater depth of shock waves penetration and the uniformity of the distribution over the depth of plastic deformation arising in the material during LSP is extremely intricate and poorly studied. Another interesting effect is the influence of the number of LSP overlaps on residual stresses and mechanical properties.

Samples of Ti-6Al-4V (Ti64) titanium alloy with a thickness of 6 mm, cut from a hot-rolled plate were used in this study. LSP was conducted using a Q-switched Nd:YAG laser operating at 10 Hz with a wave length of 1064 nm and a pulse duration of 10 ns. A diffractive optic was used to deliver 5 J in a square spot of 1 mm x 1 mm on a specimen surface covered with a steel foil, which led to a laser power density of 25 GW/cm^2. 1 and 3 numbers of overlapping LSP treatment were carried out.

It was found that one overlap of laser shock peening led to an increase in the value of residual stresses in comparison with the initial state, in which practically zero values of residual stresses were determined. After one overlap of LSP, the compressive residual stresses determined by the hole drilling method increase to a value of - 500 MPa down to a depth of 0.5 mm. It is shown that an increase in the number of LSP overlaps from 1 to 3 led to an increase in the magnitude of compressive residual stresses: - 200 MPa versus - 300 MPa on the surface; - 500 MPa versus - 700 MPa at a depth of 0.5 mm. After 1 overlap of LSP microstructural changes were small and manifested by accumulation of statistically-stored dislocations. After 3 overlaps of LSP was shown inhomogeneous microstructure distribution in both thickness and width directions (both effects could be explained in terms of the possible wave-type mechanism of the strain propagation) and microstructural changes: a formation of poorly-developed dislocation boundaries and subtle mechanical twinning.

HYDROGEN EMBRITTLEMENT OF 20FE-20CR-20MN-20NI-19CO-1X (X = N, C, AT. %) HIGH-ENTROPY ALLOYS

Panchenko M. Yu.[1*], Astafurova E. G. [1], Reunova K. A. [1], Melnikov E. V. [1], Astafurov S. V. [1], Moskvina V. A. [1], Nifontov A. S. [1,2]

[1]Institute of Strength Physics and Materials Science SB RAS, 2/4 Akademicheskii ave., 634055, Tomsk, Russia
[2]National Research Tomsk Polytechnic University, 30 Lenin ave., 634050, Tomsk, Russia
[*]panchenko.marina4@gmail.com

Hydrogen embrittlement of high-entropy FCC alloys doped with nitrogen and carbon atoms was studied. The following alloys were chosen for the investigation: 20Fe-20Cr-20Mn-20Ni-20Co (HEA), 20Fe-20Cr-20Mn-20Ni-19Co-1N, (N-HEA) and 20Fe-20Cr-20Mn-20Ni-19Co-1C (at.%) (C-HEA). The cast alloys were thermomechanically treated (TMT) to form the single-phase specimens. Electrochemical hydrogen-charging was carried out in the 3 % NaCl water-solution containing 3 g l^{-1} of NH_4SCN as a recombination poison at the current density of 10 mA/cm^2 for 50 h.

It was shown by X-ray diffraction analysis and electron microscopy that the HEA and N-HEA specimens have a single-phase coarse-grained austenitic structure after TMT (grain size of 150-250 μm). Carbon-alloyed C-HEA specimens have a smaller grain size of 50-80 μm and contain single undissolved carbides. Before hydrogen-charging, all initial specimens have good plasticity: δ_{HEA} = 62%, δ_N = 70%, and δ_C = 45%. The yield strength of the specimens depends on the content of interstitial atoms (nitrogen/carbon): $\sigma_{0.2}^{HEA}$ = 180 MPa, $\sigma_{0.2}^{N}$ = 285 MPa and $\sigma_{0.2}^{C}$ = 350 MPa.

Hydrogen-charging caused a change in the mechanical properties of all specimens. An increase in the $\sigma_{0.2}$, which is associated with solid-solution hardening by hydrogen atoms, was observed in all specimens. It is most pronounced in alloys doped with interstitial atoms ($\Delta\sigma_{0,2}^{HEA}$=10 MPa, $\Delta\sigma_{0,2}^{N}$=25 MPa и $\Delta\sigma_{0,2}^{C}$=32 MPa). Hydrogen embrittlement index I_H, which describes the hydrogen-induced loss of plasticity, is 25% in HEA specimens. I_H decreases to 10-15% in N- and C-HEA specimens. This can be due to the different diffusion rate and distribution of hydrogen atoms in the alloys, both directly during the hydrogen-charging and in the process of subsequent tensile deformation. Scanning electron microscopy revealed that a brittle hydrogen-assisted surface layer is observed on the fracture surface in hydrogen-charged specimens of all alloys. The wide brittle hydrogen-assisted layer is observed with a large inhomogeneity in depth and with an average thickness W_H^{HEA} = 95±40 μm in the HEA specimens. Transgranular and intergranular brittle elements are observed on the fracture surfaces of these specimens. In specimens with interstitial atoms (N- and C-HEA), the thickness of the brittle hydrogen-assisted layer decreases (W_H^{N} = 43±20 μm, W_H^{C}=65±35 μm). Alloying with nitrogen enhances the contribution from the transgranular fracture of hydrogen-assisted layer, while alloying with carbon leads to an increase in the contribution to intergranular fracture.

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NOVEL REFRACTORY HIGH ENTROPY ALLOYS WITH A BCC-B2 STRUCTURE

Panina E.S.*, Yurchenko N.Yu., Stepanov N.D., Zherebtsov S. V.

Belgorod National Research University, Belgorod, Russia
*panina_e@bsu.edu.ru

Recently, refractory high entropy alloys (RHEAs) have attracted attention as promising materials for high-temperature applications. Among them, so-called refractory high entropy superalloys (RHESAs) gained particular interest. Based on the Al-Mo-Nb-Ti-Ta-V-Zr system, RHESAs consist of coherent nanosized cuboidal bcc and B2 phases, imitating the microstructure design of nickel-based superalloys. However, in most RHEAs, the B2 phase serves as the matrix, leading to high strength but severe brittleness at room temperature. Attempts to regulate the mutual arrangement of the phases to get more balanced mechanical properties were successful only for a few RHESAs and elucidated a very narrow stability range of the Al-containing B2 phase.

This study utilizes another philosophy to design bcc/B2 RHEAs. Despite the general brittleness of most B2 phases applied as strengtheners in RHESAs, some B2 compounds were found to be inherently ductile. Particularly, Co-X (Ti, Zr, Hf) B2 intermetallics demonstrated decent ductility even in tension but inappropriate high-temperature strength. It seems reasonable to reinforce these B2 phases by secondary phases, for instance, bcc one. Here, the introduced $Nb_{30}Mo_{30}Co_{20}Ti_{20}$, $Nb_{30}Mo_{30}Co_{20}Zr_{20}$, and $Nb_{30}Mo_{30}Co_{20}Hf_{20}$ (at.%) alloys with a composite-like structure consisting of bcc and B2 phases, which structure-property relationships were comprehensively evaluated.

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WIRE ARC ADDITIVE MANUFACTURING AS FABRICATION METHOD FOR BLANKS FROM CHROMIUM BRONZE

G L Permyakov*, T V Olshanskaya, D N Trushnikov

Perm National Research Polytechnic University, Perm, Russian Federation
*gleb.permyakov@yandex.ru

Results are provided for a study of the additive manufacturing of blanks from chromium bronze using gas metal arc cladding with cold metal transfer (CMT). The main regularities of the formation of the structure, as well as the influence of the main parameters of the mode on the geometric characteristics of the formed walls made of heat-resistant bronze, were investigated, and a test surfacing of a thin-walled cone was carried out according to a three-dimensional model. Surfacing was carried out using Fronius TPS 320i CMT gas metal arc welding / cladding equipment installed on an ARC MATE 100iC robotic complex.

The use of CMT cladding makes it possible to implement a process with less spreading of metal and is suitable for growing small-sized workpieces of a given shape (the wall thickness of heat-resistant bronze was from 3 to 7 mm). Metallographic studies have shown that the technology of multilayer CMT cladding ensures high-quality metal formation with an almost complete absence of pores and discontinuities (there are only single pores of no more than 50 μm in size), the structure acquires a columnar structure, and transcrystallization of the metal is observed, i.e. germination of columnar grains through the deposited layers. To reduce this effect and to ensure a fine-grained equiaxed structure, methods based on the introduction of ultrasonic vibration effects into the melt and on the layer-by-layer deformation effect on the deposited metal will be tested in the near future.

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OBTAINING OF HEA NANOPARTICLES BY JOINT ELECTRIC EXPLOSION OF WIRES FROM DISSIMILAR METALS/ALLOYS

Pervikov A.V.*, Suliz K.V.

Institute of Strength Physics and Materials Science Siberian Branch of Russian Academy of Sciences, Tomsk, Russian Federation
*pervikov@list.ru

Combining multiple (five or more) metals in a single nanoparticle enables us not only to adjust the elementary composition but also control the interphase interface [1,2]. Despite the fact that some fields of application of heterophase high-entropy nanoparticles are at the very beginning of their development [3] in many times has been shown the opportunity of obtaining unique combination of physico-mechanical properties of materials based on these nanoparticles. It makes necessary to develop scalable ways to obtain them. This necessitates the development of their scalable obtaining methods, which are environmentally friendly, high productivity and the ability to vary within wide limits the average size, elemental and phase composition of nanoparticles [3].

In this work for obtaining of HEA nanoparticles was proposed a new approach that consists in the joint electric explosion of wires (EEW) from dissimilar metals/alloys. In comparison with other physical methods EEW has a series of important advantages, namely: relatively high

performance (up to 200 g/h), low energy consumption (25-50 kWh/kg) [4], wide opportunity to adjust nanoparticle size distribution and elementary composition, possibility to obtain complex composite nanoparticles in a single stage by altering buffer gas composition and the aggregate state of the buffer medium [6].

On the example of a joint electric explosion of wires of aluminum, copper, iron, and nichrome (Ni80Cr20) in an argon atmosphere, the possibility of obtaining HEA nanoparticles is shown for the first time. Analysis of the structural-phase state of the obtained samples showed that the average nanoparticle size is 49 ± 1 nm, and the crystal structure of the particles is represented by phases based on BCC and FCC lattices.

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MICROSTRUCTURE, MECHANICAL AND ELECTRICAL PROPERTIES OF COPPER ALLOY AFTER COLD PLASTIC DEFORMATION

Pilipenko A.G.[1*], Bodyakova A.I.[1,2]

[1]Belgorod State University, Belgorod, Russia
[2]National University of Science & Technology (MISIS), Moscow, Russia
[*]pilipenko.arina25@mail.ru

Nowadays copper alloys are the most used materials for the electrical industry. Microalloying and thermo-mechanical treatment provide the optimal combination of strength and electrical conductivity of these alloys. Alloying by element as Mg contributes to the solid solution strengthening and increase of work hardening. Plastic deformation by equal-channel angular pressing (ECAP) leads to an increase in hardness without significantly degradation of electrical conductivity.

The object of the present study was copper alloy Cu-0.25%Mg (wt.%). The original ingots were forged at 800 °C and rolled at 450 °C. This condition of samples was chosen as the initial state. The average grain size in the initial state was about 2.0 μm, dislocation density – 4.2×10^{14} m^{-2}.The yield strength (YS) and the ultimate tensile strength (UTS) achieved 375 and 425 MPa, respectively. Elongation was about 23%, electrical conductivity – 81% IACS. Then, the samples were subjected to ECAP to 1, 2 and 4 passes via route B_c with an intersection angle of the matrix channels of 90 ° at room temperature. The microstructure was studied by Nova NanoSEM 450 scanning electron microscope equipped with an electron backscattered diffraction (EBSD) analyzer. The samples were electro-polished in electrolyte with 25%HNO_3 and 75%CH_3OH at -20 °C and voltage of 10 V using a Tenupol 5 equipment. The microstructure parameters were

calculated using OIM Analysis software. The mechanical properties were investigated using an Instron 5882 machine with an initial strain rate of 2×10-3 c-1. The electrical conductivity was estimated by the eddy current method on the Constant K-6 equipment.

ECAP accompanied by elongation of initial grains. The 1st pass of ECAP led to the formation of the high density of low-angle boundaries (LAB) and a decrease in the average grain size to 0.9 μm. Increasing the number of ECAP passes was accompanied by the transformation of LAB to high-angle boundaries (HAB). Fraction of HAB was about 0.41 and 0.57 after 1 and 4 ECAP passes, respectively. The dislocation density achieved 9.8×10^{14} m^{-2} after 4 ECAP passes. The ultrafine-grained structure with an average grain size of about 0.6 μm was developed after 4 passes of ECAP.

Growth of strain led to an increase in the yield strength (YS) by 30-50 MPa and the ultimate tensile strength (UTS) by 40-50 MPa for each ECAP pass. The YS and UTS after 4 ECAP passes were 540 MPa and 560 MPa, respectively. Plasticity was slightly reduced after 1-2 ECAP passes. The 4th pass was accompanied by a sharp decrease in the elongation to 9.1%. The electrical conductivity was stable during 1-2 ECAP passes. After 4 ECAP passes the electrical conductivity decreased to 77.2 %IACS. These changes in the mechanical and physical properties were associated with grain refinement and an increase in the dislocation density.

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INTERNAL STRESSES AT POWER-LAW CREEP

Popov A.A.*, Boldin M.S., Chuvil'deev V.N.

Lobachevsky State University of Nizhny Novgorod, 23 Prospect Gagarina (Gagarin Avenue), Nizhny Novgorod, 603950, Russian Federation
*popov@nifti.unn.ru

The paper discusses a model of internal stresses under power-law creep. In the process of creep, as the transition from the unsteady stage of creep to the stationary stage occurs, the formation of subgrains occurs. The emitted lattice dislocations in the process of intragranular deformation quickly cross the subgrain and enter the subboundary. If the rate of generation of lattice dislocations corresponds to the rate of their "absorption" by subboundaries, then dislocations do not accumulate in the volume of subgrains. Thus, the kinetic equation [1] for the dislocation density in the subboundary in the presence of a lattice dislocation flux $I = \frac{\xi \dot{\varepsilon_v}}{b}$can be represented as:

$$\dot{\rho_s} = \frac{\xi \dot{\varepsilon_v}}{b} - \frac{\rho_s}{t_s} \quad (1)$$

where ξ - geometric coefficient, ρ_s - dislocation density in the subboundary, t_s - dislocation annihilation time, ε_v - deformation rate, $\dot{\rho_s}$ - rate of change in the dislocation density in the subboundary.

Defects accumulating in the subboundary create fields of internal stresses σ_i, which impede the motion of lattice dislocations that carry out intragranular deformation. The magnitude of internal stresses σ_i depends on the density of dislocations in the subboundary ρ_s. Thus, for the realization of power-law creep, the external applied stress σ must exceed the internal stress σ_i, by the value σ_{eff}:

$$\sigma_{eff} = \sigma - \sigma_i. \quad (2)$$

Thus, the strain rate can be written:

$$\dot{\varepsilon}_v = A_s \left(\frac{G\Omega}{kT}\right)\left(\frac{\sigma_{eff}}{G}\right)^3 \left(\frac{D_v}{b^2}\right) \quad (3)$$

where A_s - geometric coefficient, G - shear modulus, Ω - atomic volume, k - Boltzmann constant, $T = 0{,}5\ T_m$, D_v - bulk diffusion.

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EFFECT OF THERMOMECHANICAL TREATMENT ON THE STRUCTURE AND MECHANICAL PROPERTIES OF HIGH-ENTROPY ALLOYS OF THE FE-CO-NI-CR-C SYSTEM

Povolyaeva E. A.*, Shaysultanov D. G., Stepanov N. D. and Zherebtsov S. V.

Laboratory of Bulk Nanostructured Materials, Belgorod State University, 85 Pobeda Str., 308015, Belgorod, Russian Federation
*povolyaeva@bsu.edu.ru

The development of high-entropy alloys (HEAs) is of great interest, since such materials open the wide possibilities of creating materials with a set of desired properties for various industries. HEAs were identified by Yeh and Cantor in 2004 as equiatomic or nearly equiatomic alloys containing at least five basic elements. Recently, HEAs with TRIP / TWIP effects and an excellent combination of ultimate strength and ductility were developed; in some cases, lowering the temperature to cryogenic even increased the mechanical properties. At the same time, these alloys tend to have an insufficiently high yield strength. The increase in the yield strength without a noticeable deterioration in ductility can be achieved by alloying with interstitial elements like carbon. Such alloys are attractive from a practical point of view, especially for their use at extremely low temperatures.

$Fe_{(90-x)}(CoNi)_xCr_{9.5}C_{0.5}$ (x = 25; 30) HEAs were obtained by vacuum induction melting. The as-cast alloys were sheet rolled at room temperature to 80% thickness reduction and annealed at 800 and 1000 °C for 10 minutes with subsequent quenching in water. The $Fe_{60}(CoNi)_{30}Cr_{9.5}C_{0.5}$ alloy in the cold-rolled condition consisted of the fcc phase, an increase in the iron content by 5 at.% led to the formation of the secondary bcc phase. Subsequent heat treatment of the alloys led to a martensitic fcc→bcc transformation. In addition, annealing caused precipitation of $M_{23}C_6$ type carbides; an increase in the annealing temperature resulted in coarsening and more homogeneous distribution of carbides. Attractive tensile mechanical properties tensile tests and impact (KCV) toughness of the alloys at room and cryogenic temperatures was also revealed. It should be noted that a change in the temperature of the test does not significantly affect the KCV values; no brittle to ductile transition was observed in the temperature range from 20 to -196 °C.

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TEMPERATURE DEPENDENCE OF MECHANICAL PROPERTIES AND DEFORMATION MECHANISMS OF NITROGEN-CONTAINING HIGH-ENTROPY ALLOYS

Reunova K. A.[1*], Astafurova E. G[1]., Astafurov S. V.[1], Melnikov E. V.[1], Panchenko M. Yu.[1], Moskvina V. A.[1], Semeykina D. D.[2]

[1]Institute of Strength Physics and Materials Science SB RAS, 2/4 Akademicheskii ave., 634055, Tomsk, Russia
[2]National Research Tomsk Polytechnic University, 30 Lenin ave., 634050, Tomsk, Russia
[*]reunova.ksenya@mail.ru

The temperature dependence of mechanical properties and mechanisms of deformation in 20Fe-20Mn-20Cr-20Ni-20Co (at.%, 0N-HEA), 20Fe-20Mn-20Cr-20Ni-19Co-1N (1N-HEA) and 20Fe-20Mn-20Cr-20Ni-18.5Co-1.5N (1.5N-HEA) high entropy alloys have been investigated using the X-ray diffraction analysis, light, transmission and scanning electron microscopy, uniaxial tensile tests in the temperature range from 77K to 473K. All alloys have been subjected to a thermal-mechanical treatment for homogenization and refinement of grain structure.

It has been shown that all investigated alloys possess single-phase austenitic structure with FCC crystal lattice. Interstitial nitrogen causes a distortion of the crystal lattice and increases a lattice parameter of austenite from 0.3598 nm in nitrogen-free alloy to 0.3604 nm and 0.3607 nm in those with nitrogen concentrations of 1 and 1.5 at.%, respectively. The 0N-HEA is characterized by high tensile strength and ductility. The maximum values of the yield strength (YS) and elongation to failure (δ) are observed at the temperature T=77K (410MPa and 100%, respectively). In the high-temperature range, the properties of this alloy decrease with an increase in the test temperature, however, the ductility remains high (YS=130MPa, 53% at 473K). Nitrogen-alloying increases the YS and ultimate tensile stress (UTS) of the alloy, and these values are dependent on the nitrogen concentration. At T=77K, the yield strength YS=530MPa and 630MPa, UTS=1850MPa and 2050MPa for 1N-HEA and 1.5N-HEA, respectively. An increase in test temperature to 296K promotes a decrease in the value of YS down to 250MPa and 300MPa for 1N-HEA and 1.5N-HEA, respectively. The δ-value in nitrogen-alloyed alloys in low-temperature deformation regime are much lower than that in 0N-HEA (δ=60% and 50% for 1N-HEA and 1.5N-HEA, respectively) despite the fact that in high-temperature deformation region nitrogen-alloying weakly influences this value.

The 0N-HEA alloy characterized by ductile transgranular fracture independently on test temperature: numerous dimples are observed on the fracture surfaces. Nitrogen-containing alloys are characterized by ductile fracture as well. But after deformation at 77K, regions containing a distinct dimple fracture are observed in them as well as those, in which the dimples are slightly distinguishable. Such behavior of 1N-HEA and 1.5N-HEA is associated with an increase in the planarity of the dislocation structure in comparison with the initial alloy, and the activation of mechanical twinning in them.

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INFLUENCE OF SPD TREATMENT AND ANNEALING ON STRUCTURAL-PHASE TRANSFORMATIONS IN TITANIUM GRADE 4

Rezyapova L.R.[*], Usmanov E.I., Valiev R.R., Valiev R.Z.

Research Institute of Physics of Advanced Materials USATU, Ufa, Russia
[*]luiza.rezyapova.97@mail.ru

Titanium is one of the most promising materials in the medical industry. Its advantages are good biocompatibility and high corrosion resistance. To increase the strength characteristics,

titanium is alloyed with other elements that can weaken the corrosion resistance of the material and impair biocompatibility. In addition to alloying, it is possible to obtain high strength due to severe plastic deformations (SPD), due to which an ultrafine-grained (UFG) structure is formed [1].

This study is a process of high pressure torsion torsion (HPT) followed by annealing of commercially pure titanium Grade 4, which includes a minimum amount of alloying elements, one of which is iron - 0.4 wt%.

The deformation was carried out on an HPT SKRUZH-200 installation. Microhardness was measured using a «Duramin» device according to the Vickers method. A JEOL JEM-2100 transmission electron microscope (TEM) was used to obtain images of the fine microstructure. X-ray phase analysis (XRD) was performed using a Rigaku Ultima IV X-ray diffractometer on CuKα radiation (λ = 0.1540562 nm).

After HPT, an UFG structure was obtained with an average grain size of about 120 nm. To select the annealing temperature after HPT, the Grade4 alloy in the hot rolled and deformed state was subjected to various heat treatments. Thus, an annealing temperature of 700 ° C was chosen with a holding time of 30 minutes.

After annealing of the hot-rolled and deformed state, in addition to the α-phase, nanodispersed precipitates of various morphologies were present in the structure within the grains and along the boundaries. In the annealed hot rolled state, globular and acicular precipitates are 30-80 nm in size, and in the deformed annealed state, globular and ellipsoidal precipitates are 70-350 nm in size.

Research of titanium Grade 4, using TEM and XRD, revealed the formation of precipitates of second phases at temperatures above 650 °C, indicated as a Ti + Fe compound. After annealing titanium Grade 4 after HPT treatment, despite the growth of grains, the hardness does not drop to low values, but remains abnormally high for the annealed state, due to the precipitation of particles of the second phase.

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EVOLUTION OF THE PERLITE STEEL STRUCTURE AT MULTIPLE LONG-TERM DEFORMATION IMPACT

Kuznetsov R.V., Gromov V.E., Korochkin A.E.*, Rubannikova Y.A.

Siberian State Industrial University, Novokuznetsk, Russia
*korochk@rambler.ru

Railway rails are taken as an object, on the surface of which deformation has been posed repeatedly and for a long time. At present, at EVRAZ ZSMK JSC, rails are made of E76HF steel and, after accelerated cooling in a special unit, have pearlite structure.

Chemical composition is determined by TU 0921-276-01124323-2012.

The rails have been in operation at the Shcherbinka Experimental Range, and were seized after 1,769,037 thousand gross tons passing.

Macrostructure of the metal has been revealed by deep etching in a 50% aqueous solution of hydrochloric acid. The study of microstructure of metal of rails has been carried out by means

of optical and scanning electron microscopy. Defective substructure of the rail metal has been studied by transmission electron diffraction microscopy.

Study of the macrostructure has shown the absence of any internal defects, as well as discontinuities.

Investigations of microstructure of the rails metal, carried out on etched sections, has revealed grains of lamellar pearlite and, in a small amount, areas of ferrite; no bainite has been found in microstructure. It has been revealed that, with distance from the rolling surface, pearlite dispersion decreases, which is consistent with cooling conditions during thermal hardening.

More detailed study of microstructure of the rail head metal has been carried out on etched sections by scanning electron microscopy and transmission electron microscopy (thin foil method).

Scanning microscopy has shown that the main share of pearlite is regular colonies with regular alternation of cementite and ferrite plates.

Transmission electron microscopy has shown that as a result of repeated exposure to deformation, a significant transformation in steel structure occurs, namely, in state of lamellar pearlite grains. Impact of deformation, accompanied by destruction of cementite plates by cutting them with moving dislocations and by dissolving with the escape of carbon from the cementite lattice at dislocation lines, at low-angle and high-angle boundaries. At nanoscale level, formation of a subgrain structure containing nano-size cementite particles located at joints and along the boundaries of subgrains has been revealed. Subgrain sizes vary from 110 nm to 200 nm; the size of cementite particles is from 25 nm to 60 nm.

It has been found that transformation during rails operation under the deformation effect of pearlite structure of lamellar morphology relative to the central axis proceeds at a significantly slower rate compared to change in structure relative to the radius of fillet rounding. It has been shown that the subgrain structure is formed exclusively in surfacelayer of the rail metal. The relative content of subgrain structure in the surface layer of working fillet is 5 times higher than in the surface layer of rolling surface.

GLASS-FORMING ABILITY AND MAGNETIC SUSCEPTIBILITY OF CO-FE-SI-B-NB AMORPHOUS ALLOYS

Rusanov B. A.[1*], Sidorov V. E.[1], Mikhailov V. A.[1], Svec P. Sr.[2], Janickovic D.[2]

[1]Ural State Pedagogical University, Ekaterinburg, Russia
[2]Institute of Physics Slovak Academy of Sciences, Bratislava, Slovakia
[*]rusfive@mail.ru

Co- and Fe-based bulk metallic glasses (BMG) and amorphous ribbons are being actively studied due to their unique magnetic and electrical properties. Nowadays these alloys are used as highly sensitive sensors. Unfortunately, these alloys have a low glass-forming ability (GFA). In this work we investigated crystallization processes, GFA and magnetic susceptibility of Co-Fe-Si-B-Nb-R (R = Nd, Sm, Tb, Yb) alloys in amorphous and liquid states.

Base composition $Co_{48}Fe_{25}Si_4B_{19}Nb_4$ and alloys with small additions of rare-earth metals – Nd, Sm, Yb, Yb (1 at. % and 2 at. %) were prepared by remelting of pure initial components in induction furnace at 1900 K during half of hour in argon atmosphere. Amorphous ribbons (3-5 mm width and 37-40 μm thickness) were produced by planar flow casting method. BMG cylinders (2 mm in diameter and 25 mm height) were prepared by suction casting method. Amorphous structure of the alloys was checked by X-rays (Bruker D8 Advance Cu-Kα). Magnetic susceptibility of the alloys in solid and liquid states was measured by Faraday's method on an automated experimental set-up in helium atmosphere.

It was found that crystallization of these alloys goes in two stages and depends on rare-earth addition and its content in the alloy. GFA criteria were calculated. It was shown that the

paramagnetic Curie temperature of the alloys in liquid state can be used as an a-priori criterion of their GFA.

The most effective additions for increasing GFA of the base composition are 2 at. % of neodymium or samarium.

STRUCTURE OF THE HIGH-ENTROPY AL–TI–ZR–V-NB ALLOY

Russkih A. S.*, Zhilina E. M., Krasikov S. A., Ignatieva E. V.

Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences
*Russkih_A_S@mail.ru

Two decades ago, a fundamentally new concept of alloying was proposed, based on the creation of multicomponent alloys with a missing main element. Such alloys have been defined in scientific terminology [1] as high-entropy alloys (HES). One of the promising directions for the development of wind farms is the creation of compositions for high-temperature applications, the so-called heat-resistant wind farms.

In this paper, the structure of the synthesized alloy 36.5Al-15.6Ti-6.4Zr-20.4V-21.2Nb (at. %) was analyzed using aluminothermal reduction of metals from oxides. The use of aluminum as a reducing agent involves a partial transition of Al into an alloy and ensures the formation of compositions with the lowest density. In addition, aluminum not only helps to reduce the density, but also stabilizes [2] the solid solution.

The research methodology included conducting an Alumithermic reaction. The structure of the sample was studied using a scanning electron microscope. The analysis showed the presence of four phases, of which three phases were identified with a predominant aluminum content and one phase was characterized by a predominant amount of niobium. The phases had a uniform distribution over the entire volume of the ingot.

The work was carried out according to the state assignment for IMET UB RAS using equipment of the Collaborative usage centre "Ural-M"

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IMPROVING THE PHYSICAL AND MECHANICAL PROPERTIES OF THE FOIL FOR HIGH-VOLTAGE ELECTROLYTIC ANODES CAPACITORS BY INTRODUCING AN INTERMEDIATE ANNEALING

Sarkisov T.S.*, Akopyan T.K., Sarkisov S.S.

NUST MISIS, Moscow, Russia
*Tiksar@ya.ru

Oxide capacitor anodes are made of high purity aluminum (99.99 and 99.98%). The range of foil thicknesses is 0.05–0.1 mm. The criterion for its quality is the specific electrical capacity, determined for etched and oxidized (molded) foil. The amount of electrolytic capacity depends on the chemical composition, structure and texture of the foil. Foil made of high purity aluminum has

relatively low strength characteristics in comparison with foil made of aluminum of lower purity (99.7% or less).

The presence of a set of necessary mechanical and structural properties, as well as the level of physical properties (in this case, electrical capacity) is a mandatory requirement for this type of foil. This complex of properties is of particular importance for high-voltage capacitor foil. Here it is necessary to take into account the fact that high-voltage foil is supplied to capacitor plants in a soft, annealed state. During recrystallization annealing, the strength characteristics decrease even more, and the correct choice of annealing modes (intermediate and final) is one of the directions for obtaining the required set of physical and mechanical properties [1, 2].

In [3], studies were made of the effect of the final recrystallization annealing modes (temperature, heating rate and isothermal holding time) on the consumer properties (specific capacity and mechanical properties) of aluminum foil for anodes of electrolytic capacitors. The studies were carried out on samples of A99 aluminum foil obtained by cold rolling from a hot-rolled strip without intermediate annealing, which amounted to a total cold deformation of 98.75%. The influence of annealing modes on the structure, texture, specific capacity and temporary resistance was revealed [3]. We considered the case of introducing the initial low-temperature step into the final annealing mode, but the issue of reducing the degree of cold deformation or its alternation with intermediate annealing has not been studied. Intermediate annealing, along with obtaining plasticity for further rolling, as research shows, is the main tool for controlling the structure and texture of the finished product, which is revealed after the final annealing.

In this regard, the purpose of this work is to study the joint effect of intermediate and final annealing on the level of physicomechanical properties of foil for high-voltage capacitor anodes. A comparative analysis of the efficiency of thermal deformation treatment with the use of intermediate annealing and without it was carried out.

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MECHANICAL PROPERTIES OF ULTRAFINE-GRAINED TITANIUM ALLOY WITH VACUUM-PLASMA PROTECTIVE COATING

Savina Ya.N.[*], Valiev R.R., Modina Yu.M.

[1] *Ufa State Aviation Technical University, Ufa, Russia*
[*]Savina12@liveinternet.ru

Titanium alloys, due to their heat-resistant and high-strength properties, are widely used as structural materials in aircraft engine building [1-2]. A promising direction in the development of aircraft engine building is aimed at finding and improving methods for increasing the operational properties of materials from which parts of a gas turbine engine (GTE) are made. The combined approach, which consists in creating an ultrafine-grained (UFG) structure in the volume of the workpiece [3] and the deposition of a vacuum-plasma coating [4], makes it possible to increase the strength characteristics.

In this work, we present the results of a study of the mechanical characteristics and long-

term strength of cylindrical specimens made of VT6 alloy with an UFG structure with a vacuum-plasma TiVN coating.

The results show that at operating temperatures of 300 °C and 350 °C the long-term strength of coated specimens is higher (1000 MPa and 900 MPa) compared to uncoated specimens (900 MPa and 750 MPa).

Mechanical tests of specimens made of VT6 alloy with CG and UFG structure with a vacuum-plasma TiVN coating applied to the surface showed that the formation of an UFG structure in the alloy leads to an increase in strength characteristics both at a temperature of 20 °C and at a temperature of 400 °C.

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OXIDATION RESISTANCE AND MECHANICAL PROPERTIES OF HIGH ENTROPY CARBIDE BASED ON Hf-W-Mo-Ta-Ti-Nb-Zr-C

Sedegov A. S. [*], Moskovskikh D. O., Kuskov K. V., Korotickiy A. V., Sidnov K.

NUST «MISIS», Moscow, Russia
[*]a.sedegov@misis.ru

The object of this study is a new class of materials called high-entropy ceramics. Particular attention is paid to materials based on refractory elements - such as W, Hf, Ta, Ti, Nb, Zr. Due to the high melting temperatures of carbides based on elements of groups IV and V, they can also be classified as ultra-high-temperature materials, which are of increasing interest for use as a basis for ceramic-matrix composites used in hypersonic aircraft. High-entropy carbides also have high values of mechanical properties and good chemical high-temperature stability [1-3]. In this work, we investigated the equimolar compositions of high-entropy carbides (TaTiNbZrX) C (where X = Mo, W, Hf) obtained by SHS and spark plasma sintering [4].

For each of the compositions, comprehensive material science studies were carried out - by the methods of electron microscopy and X-ray phase analysis, the structural features of high-entropy materials were revealed depending on its components. A complex of mechanical and functional properties was studied - strength tests were carried out (hardness measurement, microindentation, bending strength), a number of functional properties were investigated - thermal conductivity and thermal linear expansion coefficients were measured, tests for static oxidative effects at high temperatures were carried out. Analysis and approximation of the kinetic curves of oxidation showed the logarithmic nature of the weight gain, which is a promising application for high-temperature applications.

We also compared the investigated mechanical characteristics with the results of modeling within the framework of the density functional theory, which showed good convergence of the results.

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EFFECT OF NITROGEN CONTENT ON THE STRUCTURE AND MECHANICAL PROPERTIES OF CO-CR-FE-MN-NI HIGH ENTROPY ALLOY

Semenyuk A. O.*, Klimova M. V., Salishchev G. A., Zherebtsov S. V., Stepanov N. D.

Belgorod State University, Belgorod, Russia
*semenyuk@bsu.edu.ru

High-entropy alloys (HEAs) with a face-centered cubic (FCC) structure are currently considered as promising structural materials. The Co-Cr-Fe-Mn-Ni system alloys have demonstrated a wide range of promising properties, for example, high ductility and fracture toughness at room and cryogenic temperatures, but generally they have low strength characteristics. It is well established that the addition of even small amounts of interstitial can strongly affect the phase stability, mechanical behavior, and properties of alloys. It was revealed that the addition of carbon can significantly improve the strength of any Cantor type alloys at room and cryogenic temperatures [1-2]. Meanwhile, information on the effect of other interstitial elements on the structure and properties of HEAs is quite limited. For example, nitrogen is known to be an efficient strengthener of austenitic (FCC) steels [3]; all so nitrogen doping is widely used in cryogenic steels [4-5]. However, systematic analysis of nitrogen influence on the structure and mechanical behavior of bulk fcc HEAs has not been performed so far. Therefore, in this work, the effect of nitrogen (0.5; 1.0; 2.0 at.%) on the structure and mechanical properties of the equiatomic CoCrFeNiMn.

Specimens of a CoCrFeMnNi high entropy alloy with different content of nitrogen (0.5-2.0 at.%) were prepared by induction melting. Microstructure and tensile mechanical behavior of the alloys in the as-cast condition were analyzed. The alloys with a low amount of N (0.5-1.0 at.%) had a single fcc phase coarse-grained microstructure. An increase in the content of N to 2.0 at.% resulted in the precipitation of a small amount (~1%) of Cr-rich M2N nitride particles. The yield strength of the alloys increased in proportion to the percentage of nitrogen by 117 MPa/at.% N at 293 K or by 316 MPa/at.% N at 77 K. The observed increase in strength was attributed to solid solution hardening. Ductility of the alloy with 0.5 or 1.0 at.% of N increased with a decrease in the testing temperature while ductility of the alloy with 2 at.% dropped from 67% at 293 K to 8% at 77K. Plastic deformation of the alloys at both 77 K or 293 K was mostly associated with planar dislocation slip. No signs of mechanical twinning were found even at 77K. Thermo-Calc software was used to produce a quasi-binary CoCrFeMnNi-N phase diagram for comparison the experimental and calculated results. The effect of N on strengthening and deformation mechanisms at different temperatures was discussed.

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CRYSTALLIZATION OF TI-NI-TA METALLIC GLASS SURFACE ALLOY FABRICATED ON TINI SMA SUBSTRATE BY ADDITIVE THIN-FILM ELECTRON-BEAM SYNTHESIS

Semin V.O.

Institute of Strength Physics and Materials Science SB RAS, Tomsk, Russia
viktor.semin.tsk@gmail.com

Recently, novel Ti-Ta-Ni [1] and Ti-Ta-Ni-Si [2] metallic glass (MG) surface alloys (SAs) possessing promising properties were successfully fabricated on TiNi substrates by pulsed melting of film/substrate systems. An increased thermal stability and a lower hardness of rejuvenated MGs was observed upon isothermal annealing at glass transition temperature. However, the relaxation phenomenon of amorphous matrix associated with annihilation of an excess free volume and transformation of medium-range order is poorly understood, so far. The significant achievements in the study of the atomic structure of MGs were made through implementation of nano-beam diffraction (NBD) technique [3]. In this regard, the present study aims to determine the structure of the short- and medium-range order in the glassy Ti-Ni-Ta SA after a low-temperature annealing by NBD.

Using the approved method of fabrication of surface alloys by means of a low-energy high-current electron beam, the ternary glassy Ti-Ni-Ta SA was produced [1]. The structure of samples was studied by high resolution transmission electron microscopy on JEM 2100F and in-situ X-ray diffraction technique on Shimadzu 7000S. To extract the radial distribution function, a series of NBD patterns were collected with a probe-beam diameter of 2 nm. The program package for crystal-chemical analysis ToposPro was utilized to reconstruct the scheme of phase transformation upon rejuvenation.

It has been found that the Ti-Ta-Ni SA shows completely amorphous structure represented by clusters of medium-range order. Devitrification of glassy state occurs at temperature of 673 K and accompanied by formation of metastable icosahedral phase. The concept of structural phase transformation is proposed describing the formation of a nanocrystalline composite structure by rearrangement of the structure of the medium-range order in the Ti-Ni-Ta SA.

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EFFECT OF CARBON CONTENT AND THERMOMECHANICAL TREATMENT ON STRUCTURE AND PROPERTIES OF INTERSTITIAL TRIP HIGH-ENTROPY ALLOYS

Shaysultanov D. G.*, Povolyaeva E. A., Stepanov N. D. and Zherebtsov S. V.

Laboratory of Bulk Nanostructured Materials, Belgorod State University, 85 Pobeda Str., 308015, Belgorod, Russian Federation
*Shaysultanov@bsu.edu.ru

In recent years, high-entropy alloys (HEAs) have attracted considerable attention, because of their exceptional properties [1]. In particular, $Fe_{60}(CoNi)_{30}Cr_{10}$ HEA [2] demonstrates a TRIP effect, resulting in significant strain hardening, and very high ultimate strength and ductility. Meanwhile HEAs with TRIP effect often possess rather low yield stress. To overcome this problem without a noticeable deterioration of ductility, alloying with interstitial elements, in particular, carbon, can be used. Although the positive effect of carbon on the mechanical properties of the single face-centered cubic (fcc) phase HEAs is well known, its influence on the structure and properties of TRIP HEAs require further study. In addition, many aspects of the effect of thermomechanical treatments on the structure and properties of such alloys remain unclear. Thus, in this work, we studied the effect of carbon content (0.5 at.%) on structure and properties of the $Fe_{65}(CoNi)_{25}Cr_{10}$ alloy in the cast condition; besides the influence of thermomechanical treatment on the alloy with 0.5 at.% C was examined.

The program alloys $Fe_{65}(CoNi)_{25}Cr_{10}$ and $Fe_{65}(CoNi)_{25}Cr_{9.5}C_{0.5}$ were obtained by vacuum arc melting. High-purity elements (≥99.9 wt.%) were used as starting materials. The $Fe_{65}(CoNi)_{25}Cr_{9.5}C_{0.5}$ alloy was additionally subjected to cold rolling up to 80% and annealed at temperatures of 700-900°C for 10 min with further water quenching. Microstructure of the alloys in the as-cast conditions had a two-phase structure consisting of fcc and a body-centered (bcc) solid solutions. An increase in the carbon content from 0 to 0.5 at.% led to a decrease in the bcc phase amount from 90% to 35%. Besides the carbon addition resulted in higher ductility without significant loss in strength. Cold rolling of the $Fe_{65}(CoNi)_{25}Cr_{9.5}C_{0.5}$ alloy to 80% thickness reduction leads to an increase in the bcc phase amount up to 40%. Subsequent annealing at 700-900°C for 10 min. led to the development of a recrystallized microstructure with an increased volume fraction of the bcc phase, and the precipitation of $M_{23}C_6$-type carbides. Relationships between the chemical composition, processing, structure, and mechanical properties of alloys are briefly discussed.

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ENTROPY FORMING ABILITY DESCRIPTOR FOR MODELING OF N METALLIC CARBIDES

Sidnov K. P.*, Vorotilo S., Sedegov A. S.

National University of Science and Technology MISiS, Moscow 119049, Russia
*k.sidnov@misis.ru

High-entropy materials are of great interest for materials science due to a combination of unique properties, and predicting the possibility of their obtaining, as well as their properties using ab initio methods, is one of the most promising areas of modeling and development of new materials.

The development of modern computational methods and tools has led to the emergence of new ways of describing disordered systems within the framework of the electron density functional theory. One of these methods is the recently proposed method for the statistical description of the configurational disorder in solid solutions and alloys. This method is based on the energy distribution spectrum calculation of disordered structures, representing a set of ordered ones - a method for calculating the entropy forming ability (EFA). This descriptor evaluates the possibility of the coexistence of different states with the same composition and type of crystal lattice near the ground state and quantitatively determines the configurational disorder capable of stabilizing high-entropy homogeneous phases [1].

In this paper, we consider the possibility of using the described methodology, originally proposed by the authors for carbides with 5 metals on a cationic sublattice for modeling disordered refractory carbides of 2, 3, 4 and 5 metals. Within the framework of this work, we also calculated the mechanical properties (hardness, Young's modulus, bulk modulus, shear modulus), compared the obtained characteristics with the results of experimental studies, and proposed a method for screening studies of the hardness and fracture toughness (K1C) of materials based on the structural representation of a disordered structure as a combination of ordered structures and the Mazhnik-Oganov model [2].

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X-RAY STUDY OF THE PHASE HOMOGENEITY OF TUNGSTEN CARDIBE CERAMICS PRODUCED BY THE SPARK PLASMA SINTERING METHOD

Smetanina K.E.*, Andreev P.V., Nokhrin A.V., Lantsev E.A., Vostokov M.M.

Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia
*smetanina@nifti.unn.ru

Tungsten carbide (WC) hard alloys are widely used as material for metal-cutting tools because of their unique combination of high strength and cracking resistance.

Spark plasma sintering (SPS) of powders is one of the most promising methods of producing hard alloys. The sintering process takes place in a graphite mold with millisecond pulses of high-power current are passed through. It was shown, that the intense diffusion of carbon from the mold into the surface layers of sintered samples takes place during sintering. It helps to reduce the intensity of the brittle phase particle formation (W_2C phase in the case of sintering WC ceramics and η-phases (Co_3W_3C etc.) – in the case of sintering WC-Co alloys) [1, 2]. Despite the positive effect of this phenomenon on the mechanical properties of the sample, it leads to an inhomogeneous distribution of crystal phases in its various sections.

The purpose of this work is to study of the effect of the initial WC powder parameters and the application of BN coating on the inner surfaces of the mold on the homogeneity of the ceramic phase composition obtained by the SPS method.

The objects of this study were four WC powders with different particle sizes: 50 nm (obtained in IMET RAS by plasma chemical synthesis and containing 2.6 ± 0.2% wt. of W), and three powders produced by JSC «KZTS»: 0.8 μm (contains 1.7 ± 0.2% wt. of W_2C), 3 μm (contains 2.5 ± 0.2% wt. of W_2C), 14 μm (contains 1.0 ± 0.2% wt. of W_2C).

SPS of eight ceramics (in BN-coated graphite mold and not) was performed on «Dr. Sinter model SPS-625» (SPS Syntex, Japan) in a vacuum. Heating rate = 50°C/min., P = 70 MPa, sintering temperature = 1400-1600°C (depending on the initial powder). The technique of layer-by-layer X-ray phase analysis (XRPA) is described in [1]. XRPA was carried out after each stage of the ceramic surface treatment on a diffractometer «XRD-7000» (Shimadzu, Japan, CuKα, λ = 1.54 Å). Five stages of the surface treatment have been carried out.

During the first three steps (the total layer removed was ~ 100-150 μm) the «reaction products» of the inner parts of the mold with the powder surface – graphite and WB (in the case of sintering with BN) were removed. In these stages, W_2C phase (or W, in the case of 50 μm powder) was not detected in any of the ceramic samples. It is assumed that the carbon diffuses from the mold and reacts with W (in the case of 50 μm powder): $2W + C \rightarrow W_2C$ and with W_2C phase: $W_2C + C \rightarrow 2WC$. In the subsequent polishing steps (the total layer removed → 200 μm), W_2C phase was detected in ceramics sintered from 50 nm, 0.8 μm, and 3 μm powders. No traces of W_2C phase were observed in ceramics sintered from 14 μm powder.

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SOLUTION DEPOSITION OF BIOACTIVE CALCIUM PHOSPHATE COATINGS ON TITANIUM IMPLANTS

Smirnov I. V.*, Teterina A. Yu., Mikheeva P. V., Kalita V.I., Barinov S.M., Komlev V.S.

Baikov Institute of Metallurgy and Materials Science RAS,
Russia, Moscow, Leninskiy prospect, 49, 119334
*baldyriz@gmail.com

High strength characteristics combined with neutral biological properties make titanium-based implants indispensable for bone tissue high mechanical stress defects replacement. Implants made of titanium and its alloys do not lead to the rejection reactions, but the possibility of corrosion

may cause secondary operations. Methods of combining different materials in one product are an urgent task for researchers. Such materials summarize the positive properties of each other and minimize the disadvantages. The use of calcium phosphates (CP) as a coating on a titanium implant significantly increases the biological properties of the final product, biocompatibility and osseointegration.

In this research a method of the multiphase coatings formation based on CP modifications has been investigated. The plasma deposition method of coatings formation based on high-temperature modifications hydroxyapatite (HA) and α-tricalcium phosphate (α-TCP) on a titanium substrate with an intermediate layer TiCaO followed by a subsequent transformation of the surface layer into low-temperature octacalcium phosphate (OCP) has been realised.

The necessity for multiphase coatings creation based on the difference in properties of the intermediate layers. The first layer TiCaO promotes high bonding of the titanium substrate with HA and α-TCP coatings. The densely sintered coating (HA and α-TCP) prevents corrosion reactions of the titanium implant. The formation of the final layer OCP increases bioactivity, since OCP has a high degree of resorption. OCP is a precursor of the biological hydroxyapatite (HA) and promotes the new bone tissue formation in low regenerative potential areas, that contributes the rapid strong bondings between the implant and the patient's bone tissue. The DCPD coating plays the intermediate role for OCP formation. It has been obtained by precipitation from a solution. The solution containing Ca^{2+} and PO_4^{3-} in the required concentrations reacts with a sprayed layer of HA or α-TCP, that leads to the formation and growth of DCPD crystals uniformly over the surface. The OCP-based surface layer was formed by transforming the pre-deposited DCPD coating under the buffer system conditions according to the reaction:

$CaHPO_4 \cdot 2H_2O \leftrightarrow Ca^{2+} + HPO_4^{2-} + 2H_2O$

$HPO_4^{2-} \leftrightarrow PO_4^{3-} + H^+$

$8Ca^{2+} + 2HPO_4^{2-} + 4\,PO_4^{3-} + 5H_2O \leftrightarrow Ca_8(HPO_4)_2(PO_4)_4{}^*5H_2O$

The method, which combines the plasma spraying and transformation processes, makes it possible to create variously composited coatings in different ratios depending on the task at hand. In this research, the technique of the bioactive coatings creating in the HA / OCP and TCP / OCP systems has been investigated. It can significantly change the final properties of a titanium implant. Such coatings help to increase the osseointegration, reduce the rejection reactions occurance, and the number of reoperations.

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THERMODYNAMICS OF VAPORIZATION PROCESSES IN THE GEO_2–ZNO SYSTEM

Smirnov A. S.*, Smorchkov K. G., Gribchenkova N. A., Alikhanyan A. S.

Kurnakov institute of general and inorganic chemistry of the Russian Academy of Sciences, Moscow, Russia

*prostreet02@rambler.ru

The GeO_2 and ZnO oxides can be used simultaneously in a complex ceramic [1]. Different methods of materials synthesis as well as exploitation conditions are often associated with high temperatures. Therefore, thermal stability and vaporization thermodynamics of the GeO_2–ZnO system are of great importance. Up to date, vaporization processes in the GeO_2–ZnO system have not been studied.

In the present work, thermodynamics of heterogeneous equilibria was investigated by Knudsen effusion mass spectrometry at temperatures 1140-1280 K . The GeO_2–ZnO system samples in the whole composition range were obtained by the solid-state synthesis in air at 1173 K. In accordance with XRD analysis, the only complex oxide Zn_2GeO_4 and equilibrium mixtures [Zn_2GeO_4 +ZnO] and [GeO_2 + Zn_2GeO_4] were obtained. These samples' vaporization was examined by Knudsen effusion method using a high-temperature mass spectrometer for the effusing gas analysis. Registered mass spectra were interpreted and the qualitative and quantitative vapor composition were found. The incongruent character of vaporization in the GeO_2–ZnO system was determined and the direction of shifting of the system figurative point during vaporization in an open volume was established.

The obtained partial pressures of vapor species were used for calculation of the equilibrium constants of several reactions occurring during vaporization in the GeO_2–ZnO system and the system components activity in different phase fields of the system phase diagram. The enthalpies of reactions and the enthalpy of formation of Zn_2GeO_4 were calculated from the experimental data obtained. A graphical interpretation of the results was given as the *p–x*-section of the GeO_2–ZnO system phase diagram at 1260 K.

The obtained data can be used for prediction of thermal behavior and side interactions with other materials for the GeO_2–ZnO system.

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THERMODYNAMICS OF COMPLEX COMPOUNDS BASED ON ZNO AND NB_2O_5

Smorchkov K.G. *, Smirnov A.S., Gribchenkova N.A., Alikhanyan A.S.

IGIC RAS, Moscow, Russia
*strelok1304@yandex.ru

Ceramics based on zinc niobates are promising materials in microwave electronics due to its electromagnetic parameters. To obtain functional materials with specified physical and physicochemical properties, knowledge of their thermodynamic characteristics, as well as the thermodynamics of vaporization processes, is required. In this regard, we carried out high-temperature study of the vaporization processes and thermodynamic properties of the ZnO – Nb_2O_5 system. This study was carried out by the Knudsen effusion method with mass spectral analysis of the gas phase in the temperature range 1200–1500 K. Mass spectral analysis showed that the saturated vapor over the studied system in the entire range of compositions consists mainly of zinc atoms and oxygen molecules. Applying equation Hertz-Knudsen and conditions of congruent sublimation of ZnO allowed us to calculate the partial pressure of zinc atoms and oxygen molecules. The standard enthalpies of some heterophase reactions were calculated, by the 2nd and 3rd laws of thermodynamics (Table 1). The standard enthalpies of formation of zinc niobates from simple oxides and elements were calculated, by Hess's law, using the obtained values of the enthalpies of the reactions and known literature data on the standard enthalpies of formation of Nb_2O_5(cr), Zn(g). (Table 2).

Table 1. Standard enthalpies of heterophase reactions (kJ/mol), calculated according to the 2nd and 3rd laws of thermodynamics.

Reaction	2-law	3-law
$ZnO(cr) = Zn(g) + 0.5O_2$	483.7±15.5	484.7±7.0
$Zn_3Nb_2O_8(cr) = ZnNb_2O_6(cr) + 2Zn(g) + O_2$	941.3±35.7	991.5±16.0
$ZnNb_2O_6(cr) = Nb_2O_5(cr) + Zn(g) + 0.5O_2$	509.4±13.0	529.1±7.5
$ZnNb_2O_6(cr) = 1/17\ Zn_2Nb_{34}O_{87}(cr) + 15/17\ Zn(g) + 15/34\ O_2$	481.6±24.6	467.2±7.5
$Zn_2Nb_{34}O_{87}(cr) = 17Nb_2O_5(cr) + 2\ Zn(g) + O_2$	1061.5±5.3	1077.1±16.0

Table 2. Standard enthalpies of formation of zinc niobates (kJ/mol)

Compound	$-\Delta_fH_{298.15}$ (from oxides)	$-\Delta_fH_{298.15}$
$Zn_3Nb_2O_8(cr)$	50.1±32.1	2992.0±30.2
$ZnNb_2O_6(cr)$	48.3±21.3	2292.4±19.9
$Zn_2Nb_{34}O_{87}(cr)$	89.7±19.4	33056.1±15

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THE EFFECT OF INTERLAMELLAR SPACING ON STRENGTH AND DUCTILITY OF β-SOLIDIFIED γ -TIAL BASED ALLOY

Sokolovsky V.S. *, Panov D.O., Volokitina E.I., Salishchev G.A.

Belgorod National Research University, Belgorod, Russia
*sokolovskiy@bsu.edu.ru

β-solidified γ-TiAl based alloys are considered as promising high-temperature lightweight materials for the manufacturing of aircraft and automotive engines due to a favorable combination of specific strength, stiffness, and creep resistance [1]. To increase the room temperature ductility, alloying and refine structure were used [2, 3]. For instance, some alloying elements like boron, carbon, silicon or rare-earth elements allow to significantly refine structure of as-cast alloys [4, 5]. Considerable improvement of ductility can be received in alloys with colony size below 50 μm [6]. Colony size and interlamellar spacing can be controlled by heat treatment [7], including quenching from α-phase field and subsequent aging at temperatures of (α_2+γ)-phase field.

The effect of interlamellar spacing on mechanical properties, deformation mechanisms and fracture behavior of the β-solidified Ti-43.2Al-1.9V-1.1Nb-1.0Zr-0.2Gd-0.2B alloy under tension and compression was studied. Ingot in the as-cast condition was subjected to thermomechanical and subsequent two-step heat treatment to obtained conditions with different interlamellar spacing. The interlamellar spacing was ranged from 10 to 800 nm, remaining the same colony size of 25μm. The tensile and compression stress-strain curves and the resulting mechanical properties were obtained. The alloy with λ~100 nm demonstrates the maximum values of strength and ductility under tensile and compression loading. Both increasing and decreasing of interlamellar spacing resulted in significant drop in the ductility. The fracture surfaces of the program alloy obtained after tensile and compression testing was investigated. A transition from transcrystalline fracture to intercrystalline transcrystalline fracture was found. Post-mortem transmission and scanning electron microscopy of surface further identified deformation structures for different mode orientations of colonies. Mechanical behavior and deformation mechanisms occurring in a lamellar colony with orientation relative to the loading direction were discussed.

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Lecturer of the Young Scientists School

STRUCTURE AND MECHANICAL PROPERTIES OF HIGH ENTROPY ALLOYS FOR STRUCTURAL APPLICATIONS

Stepanov N.D., Eleti R.R.

Laboratory of Bulk Nanostructured Materials, Belgorod State University, Belgorod, Russia
stepanov@bsu.edu.ru, rajeshwar.eleti@gmail.com

The so-called high-entropy alloys (HEAs) have attracted the attention of researchers from all over the world, largely because of their attractive mechanical properties. However, despite over a dozen years of research, it is still unclear if some practical alloys can come out of this idea. In the present work, recent results on development of HEAs based on 3d transition metal or refractory metals are presented. Specific attention was paid to the following aspects: (i) Prediction of structure using phenomenological criteria and CALPHAD method; (ii) Thermomechanical processing to tailor the structure and properties; (iii) Deformation and strengthening mechanisms; (iv) Examples of alloys with promising mechanical characteristics. Some suggestions for future research directions are given.

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EFFECT OF TEMPERING ON FRACTURE TOUGHNESS OF B-ADDED 9%CR MARTENSITIC STEELS

Tkcahev E.*, Borisova Yu.

Belgorod State University, Belgorod, Russia
*tkachev_e@bsu.edu.ru

The present work characterize the fracture toughness of a modified 9%Cr steels with high B and low N contents after tempering at different temperatures. The load-deflection curves were used to evaluate the values of maximum load P_f during the impact tests.

The studied steels Fe-0.1C-9Cr-1.8W-0.6Mo-3Co-0.05Nb-0.2V-0.012B-0.007N (%wt.) (hereafter B-added steel) and Fe-0.1C-9Cr-1.8W-0.6Mo-3Co-0.05Nb-0.2V-0.013B-0.007N-

0.085Ta (hereafter TaB-added steel) are similar in chemistry except in Ta content. The B-added and TaB-added steels were normalized at 1060°C for 0.5h and 1050°C for 0.5h respectively and then tempered at 500, 750 and 780°C for 3 h. The Charpy impact tests were performed on standard V-notch specimens at room temperature using Instron IMP460 machine with a 300 J capacity.

The toughness of the normalized TaB-added steel is 24 J/cm^2 which is lower than that of B-added steel (43 J/cm^2). This may result from difference in prior austenite grain (PAG) size since the mean PAG size in TaB-added steel is about twice lower than that in B-added steel [1,2]. Both steels are characterized by significant drop in impact toughness below 10 J/cm^2 after tempering at 500°C. Tempered martensite embrittlement of studied steels is accompanied by decrease in the maximum load P_f from 33.5 to 13.4 kN for B-added steel and from 28.8 to 6.4 kN for TaB-added steel. The increase in tempering temperature to 750°C led to change in fracture mode in B-added steel from brittle to ductile with high toughness of 244 J/cm^2. In contrast the impact toughness of TaB-added steel tempered at 750°C is only 32 J/cm^2. However, further increase in tempering temperature to 780°C leads to increase in impact energy of TaB-added steel to 135 J/cm^2. The corresponding value of impact toughness of the B-added steel after the same heat treatment is 265 J/cm^2.

Such difference in impact toughness of studied steels tempered at 780°C can be attributed to the decreased value of P_f=21.6 observed for TaB-added steel as compared to that for B-added steel P_f=27.3. Since the value of maximum load during impact test represents the ease of the initiation of the crack, it was concluded that the decreased toughness of the studied Ta-added 9% Cr steel is associated with reduced critical stress required for crack initiation.

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SUPESTRENGTH OF NANOSTRUCTURAL TITANIUM OBTAINED BY COMBINED DEFORMATION-HEAT TREATMENT

Usmanov E.I. *, Rezyapova L.R., Valiev R.R., Valiev R.Z.

Research Institute of Physics of Advanced Materials USATU, Ufa, Russia
*usm4nov-emil@yandex.ru

As is known, commercially pure titanium is one of the most widely used materials for the manufacture of medical implants due to its high corrosion resistance, biocompatibility, and the absence of harmful alloying elements. However, with the active development of medicine, the requirements for the mechanical properties of implants also increase. For this purpose, technically pure titanium has an insufficiently high complex of mechanical properties. For this reason, the direction of further development of methods of deformation-heat treatments remains relevant. And one of the most promising ways to increase the strength properties of commercially pure titanium while maintaining its biocompatibility is the formation of an ultrafine-grained (UFG) structure in it by the methods of severe plastic deformation (SPD) [1].

In this work, various combinations of heat-deformation treatments are investigated in order to further improve the mechanical properties of commercially pure titanium Grade 4. Deformation processing was carried out by the method of high-pressure torsion (HPT), which is the most effective in refining the structure to a nanoscale state [2]. Heat treatment was carried out by annealing at various temperature and time conditions. The mechanical behavior of the material was investigated by testing small samples for uniaxial tension on an Instron 5982 system (Nanotech Center for Collective Use, USATU) at room temperature with a tensile rate of 10^{-4} sec^{-1}.

When processing commercially pure titanium Grade 4 using the combined mode: HPT + annealing at 700 ° C + HPT + annealing at 350 ° C, it was possible to achieve a record strength value (σ_u > 1500 MPa), while maintaining satisfactory ductility. Using the data of structural studies, the report discusses the nature of the high mechanical properties of the obtained material.

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SYNTHESIS OF HIGH ENTROPY CARBIDE OF TRANSITION METALS IN A MOLTEN SALT

Varaksin A.V.*, Petrova S.A., Rempel A.A.

Institute of Metallurgy UB RAS, Yekaterinburg, Russia
*vorax@yandex.ru

In this paper, the possibility of synthesis of high-entropy carbide (TiZrNbHfTa)C in the salt melt is considered. The method is based on the phenomenon of no-current transfer of metal to carbide of another metal through the salt melt.

When comparing the electrode potentials of the metals Ti, Zr, Hf, Nb and Ta relative to the reference chlorine electrode in the NaCl-KCl melt (1:1 mol.) at 1000 K [1], it becomes that the most electropositive metal is niobium, and the most electronegative metal is hafnium. The intermediate position in the electropotential series is occupied by titanium.

Therefore, when titanium carbide powder is placed in an ionic melt containing metallic tantalum and niobium and a salt of one of these metals, the mass transfer of tantalum and niobium as a more electronegative metal to titanium carbide as a more electropositive electrode is realized with the formation of a diffusion coating on the surface in the form of a ternary carbide (TiNbTa)C. The ternary carbide obtained in this way is placed in a salt melt to conduct a reaction with the following metals in the electropotential series – zirconium and hafnium. As a result, the product of such a sequential synthesis and subsequent high-temperature sintering is a high-entropy carbide (TiZrNbHfTa)C.

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INCREASED EROSION RESISTANCE OF UFG TITANIUM ALLOYS WITH PROTECTIVE ION-PLASMA COATING

Valiev R.R.*, Savina Ya.N., Modina Yu.M.

Ufa State Aviation Technical University, Ufa, Russia
*rovaliev@gmail.com

Parts made of titanium alloys used in aircraft engine building are subject to high loads and erosive surface wear [1]. The creation of an ultrafine-grained (UFG) structure by SPD methods [2] in the bulk of the material and the deposition of protective coatings [3-4] on its surface can improve the service properties of parts.

This work presents recent results of erosion tests of a vacuum-plasma protective TiVN coating on substrates of VT6 and VT8M-1 titanium alloys obtained by various SPD methods - equal channel angular pressing (ECAP) and rotary swaging.

According to the results of erosion tests, the application of a vacuum-plasma protective TiVN coating made it possible to significantly reduce the carryover of the sample mass, thereby increasing the wear resistance under conditions of erosive wear.

Thus, the combination of the UFG structure in the bulk of the material and the deposited protective coating on its surface is a very promising direction for the development of modern aircraft engine building.

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RESEARCH ON THE MICROSTRUCTURE AND STRENGTHENING MECHANISM OF COCRFENISIX (X=0, 0.25, 0.5, 0.75) BASED ON ARC ADDITIVE MANUFACTURING

Wang J., Chen X. *

Wenzhou University, College of Mechanical and Electrical Engineering, Wenzhou 325000, China
*chenxizhang@wzu.edu.cn

In recent years, the performance and strengthening mechanism of non-metallic elements for medium and high entropy alloys have gradually increased. However, in the field of additive manufacturing, the influence of the non-metallic element Si on the microstructure and properties of high-entropy alloys is still unclear. In this paper, taking the non-metal element Si as the starting point, the effect of adding Si element to the CoCrFeNi alloy on its microstructure changes and material properties is studied. CoCrFeNiSix (x=0, 0.25, 0.5, 0.75) high-entropy alloy is formed by arc additive manufacturing technology. X-ray diffractometer (XRD) was used to analyze that the

inside is mainly FCC phase. But with the increase of Si element content, the precipitates gradually grow up and are evenly distributed in the FCC phase. When the molar ratio of Si element reaches 0.75, the inside is mainly BCC phase. The valence electron structure of Si element is more likely to react with Cr element. This further affects the reaction of Cr element and Ni element. X-ray diffractometer (XRD) and EDS energy spectrum analysis revealed that the precipitated phases are mainly Cr2Ni3 and Cr3Ni5Si2 phases. The results show that Si element can increase the precipitation of -Cr-rich phase to improve the tensile strength of the material. But with the increase of Si element, the tensile strength has not been continuously strengthened. At the same time, the ductility of the material is greatly reduced, and the hardness continues to increase.

PREPARATION, MICROSTRUCTURE AND THERMOELECTRIC PROPERTIES OF MEDIUM-ENTROPY BiSbTe1.5Se1.5 AND PbSnTeSe ALLOYS

Yaprintseva E.N.[1,2], Yaprintsev M.N.[2], Vasil'ev A.E.[1], Ivanov O.N.[1*]

[1]Belgorod State Technological University named after V.G. Shukhov, Belgorod 308012, Russia
[2]Belgorod State University, Belgorod 308015, Russia
[*]Ivanov.Oleg@bsu.edu.ru

Developing high-entropy and medium-entropy alloys is effective approach of modern thermoelectric materials science [1-3]. Owing to effective scattering of phonons by lattice disorder, which is formed in the high-entropy and medium-entropy alloys, these alloys possess intrinsically low lattice thermal conductivity. This feature is very important to enhance the thermoelectric efficiency of materials. Currently, medium-entropy *n*-type $BiSbTe_{1.5}Se_{1.5}$ and *p*-type PbSnTeSe alloys are ones of promising thermoelectric alloys. To prepare single-phased grained $BiSbTe_{1.5}Se_{1.5}$ and PbSnTeSe samples, we applied self-propagating high-temperature synthesis and spark plasma sintering. The density of the samples was equal to ~6.87 ($BiSbTe_{1.5}Se_{1.5}$) and ~7.07 $g \cdot cm^{-3}$ (PbSnTeSe). Similarly to grained Bi_2Te_3-based materials, $BiSbTe_{1.5}Se_{1.5}$ samples were found to be textured, whereas no texturing observed in PbSnTeSe samples. Average grain size was estimated as ~3.3 ($BiSbTe_{1.5}Se_{1.5}$) and ~18.9 μm (PbSnTeSe). For both materials, specific electrical resistivity is gradually growing with increasing temperature. This behavior due to temperature change in carriers mobility is characteristic of metals and degenerate semiconductors. In accordance with type of majority carriers, sign of the Seebeck coefficient for both materials is opposite (negative for $BiSbTe_{1.5}Se_{1.5}$ and positive for PbSnTeSe). The lowest value of the total thermal conductivity was equal to ~0.64 ($BiSbTe_{1.5}Se_{1.5}$) and ~1.2 W/m·K (PbSnTeSe). The thermoelectric properties of the medium-entropy $BiSbTe_{1.5}Se_{1.5}$ and PbSnTeSe alloys can be considered as promising enough. The highest thermoelectric figure-of-merit was estimated as ~0.43 for $BiSbTe_{1.5}Se_{1.5}$ and ~0.35 for PbSnTeSe.

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DEVELOPMENT AND INVESTIGATION OF EUTECTIC Al-Cr-Nb-Ti-Zr REFRACTORY HIGH ENTROPY ALLOYS

Yurchenko N. Yu. [*], Panina E. S., Zherebtsov S. V., Stepanov N. D.

Laboratory of Bulk Nanostructured Materials, Belgorod National Research University, Belgorod, Russia
[*]yurchenko_nikita@bsu.edu.ru

Metals and metallic alloys are still the most suitable materials of choice for many structural applications. However, the conventional alloy design strategy relied on one base element almost eliminates the further breakthrough in mechanical properties. New multicomponent alloys, so-called high entropy alloys (HEAs), often demonstrate more advanced performance than traditional materials [1]. For instance, eutectic high entropy alloys (EHEAs) usually based on the late transition elements showed an excellent strength-ductility combination and good corrosion resistance, making them the attractive candidates for marine usage [2].

Stable up to melting point lamellar structure with alternating "hard" and "soft" phases is the reason for the good mechanical properties of EHEAs. It seems interesting to implement a similar microstructure design for refractory high entropy alloys (RHEAs). RHEAs are considered potential substitutes for nickel-based superalloys in future gas turbine engines due to their outstanding high-temperature strength [3]. The regular arrangement of the phases with carefully selected characteristics offered by EHEA's concept is believed to improve the creep resistance and/or ductility of RHEAs already in the as-cast state.

In this study, we aimed at the development of new lightweight eutectic RHEAs (ERHEAs) based on the Al-Cr-Nb-Ti-Zr system. Note, the obtaining of eutectic structures in RHEAs is a non-trivial task. Many methods used for searching such a microstructure type are exclusive for EHEAs based on late transition metals, and none of them is adapted for ERHEAs. Nevertheless, a CALPHAD (CALculation of PHAse Diagrams) is the most suitable and time-saving approach due to quantitative and qualitative evaluation of phase composition of different potential EHEAs. Here, we used the CALPHAD to design a palette of different ERHEAs, for which structure-property relationships and deformation mechanisms were analyzed thoroughly.

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EFFECT OF GRAIN REFINEMENT ON CRYOGENIC BEHAVIOR OF AN AL-MG-SC-ZR ALLOY

Yuzbekova D. Y.[*], Mogucheva A. A., Kaibyshev R. O.

Belgorod State National Research University, Belgorod, Russia
[*]yuzbekova@bsu.edu.ru

Al-Mg-Sc-Zr alloys are attractive for cryogenic applications due to superior combination of strength and ductility [1]. The mechanical properties of the Al-Mg-Sc-Zr alloys at cryogenic

temperatures are already well studied [1-3]. However, the effect of grain size on temperature dependencies of strength and ductility is scarcely known. It was recently shown that fully recrystallized structures with an average grain size of ~1 □m could be produced using the method of equal channel angular pressing (ECAP) in this type alloys [4]. In order to identify the effect of grain refinement on cryogenic behavior, namely on temperature dependencies of strength and ductility, the tensile tests were carried out at temperatures ranging from 25ºC to –196ºC for the 1545K aluminum alloy before and after ECAP. ECAP was utilized to grain refinement and it's performed at 300ºC to strains ~12 via route B_C (the samples are rotated by 90º along the same direction after each pass).

It was found that the grain refinement promotes to increase yield stress with decreasing temperature while increment in the elongation-to-failure at cryogenic temperatures tends to decrease with decreasing grain size. The elongation-to-failure is determined by ultimate dislocation density which is feasible to be accumulated in an aluminum alloy without failure. The investigated alloy before ECAP exhibits continuous yielding. As a result, the deformation curves of the alloy in this state have a general parabolic shape until necking. After ECAP, alloy exhibit discontinuous yielding and Piobert–Lüders plateau. Thus, the grain refinement leads to transition from continuous yielding to discontinuous one. Dimple fracture was found to occur in whole temperature range for both material conditions. It was revealed that the grain refinement restrains to propagation of cracks nucleated on lateral surfaces and microcrack coalescence.

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YIELD STRENGTH ANOMALY IN A B2 MATRIX AlNbTiVZr0.25 REFRACTORY HIGH ENTROPY ALLOY

Yurchenko N. Yu.*, Panina E. S., Zhilina M. A., Salishchev G. A., Stepanov N. D.

Laboratory of Bulk Nanostructured Materials, Belgorod National Research University, Belgorod, Russia
*yurchenko_nikita@bsu.edu.ru

During the last fifty years, intermetallics are considered substitutes for existing high-temperature materials in gas turbine engines [1]. However, despite the excellent specific high-temperature strength, oxidation, and wear resistance, intermetallics have some critical drawbacks, like notorious brittleness and scattered properties, hindering their massive utilization as bulk structural materials. Among numerous strategies, alloying is the most convenient and effective approach to balancing the performance of intermetallics [2].

The vast compositional space of the recently introduced high entropy alloys (HEAs) concept offers new horizons in tuning the properties of intermetallics and their formation in unexpected systems [3]. For instance, unable to appear in binary Al-ETM (ETM-early transition metal) system, an Al-containing B2 phase becomes stable in refractory high entropy alloys (RHEAs), which are new

potential high-temperature materials. In RHEAs, the B2 phase can play the role of either matrix or secondary phase, replicating the successful microstructure design of nickel-based superalloys [4].

However, many aspects of the mechanical behaviour and deformation mechanisms of the multicomponent B2 phase in RHEAs remain unexplored. One such feature is yield strength anomaly (YSA). YSA is a positive temperature dependence of strength, which is typical for some materials, including B2 compounds [5]. This study evidenced the YSA in a B2 matrix $AlNbTiVZr_{0.25}$ RHEA in the temperature interval of 600-800°C. The reasons responsible for YSA were carefully addressed.

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THE USING ZR, SN, ZN AS NEW COMPONENTS OF THE HIGH-ENTROPY PHASE WITH THE M-TYPE HEXAFERRITE STRUCTURE

Zaitseva O. V.*, Zhivulin V. E., Punda A. Y., Trofimov E. A.

South Ural State University, Chelyabinsk, Russian Federation
*nikonovaolga90@gmail.com

The aim of our research (for example, [1]) is to obtain new high-entropy oxide phases with the M-type hexaferrite structure by solid-phase synthesis in systems that have not previously become an object of research in terms of creating high-entropy phases, as well as to study the structure, composition, and characteristics of the samples obtained.

This work is devoted to the experimental preparation of new high-entropy phases with the M-type hexaferrite structure, the composition of which (qualitative and quantitative) reflects the formula $BaR_{12}O_{19}$. In this formula, the R components, along with the previously used ones – Fe, Mn, Al, Ga, In, are used a number of new, previously unused for these tasks, components – Zr, Sn, Zn.

The elements most often acting as a doubly charged cation in the formation of a hexaferrite structure, in this case, are Ba. Also, according to the literature data [2], the possibility of replacing iron in M-type hexaferrites was proved, first of all, by such elements as Al, Mn, and Ti. Zr is an electronic analogue of Ti, and was previously successfully used to replace ferric iron in hexaferrites, Sn, Zn are also mentioned in the literature as possible participants in substituted hexaferrite structures. All this refers to the simultaneous doping with one or two elements, however, it gives us reason to believe that Zr, Sn, Zn can also be used to obtain a high-entropy material with an M-type hexaferrite structure.

At this stage of the work, samples of the following compositions were studied: $Ba(Fe, Mn, Zr, Ga, Al)_{12}O_{19}$; $Ba(Fe, Sn, Zn, Ga, Al)_{12}O_{19}$.

In the first case, it was planned to establish whether Zr can act as a component of the high-entropy phase with the M-type hexaferrite structure. The second composition made it possible to establish whether Sn and Zn could be used together as such components (it was assumed that the

combination of Sn^{4+} and Zn^{2+} makes it possible to achieve mutual compensation of the charges of the ions of these metals, having obtained an average value of $^{+3}$).

The experimental samples were obtained by solid-phase synthesis. In order to determine the optimal temperature of solid-phase synthesis, samples of a given composition were sintered in an oxidizing atmosphere (in air) at temperatures of 1200 °C, 1300 °C and 1400 °C for 5 hours. Then the obtained samples were cooled and studied by MRSA and XRD methods.

Investigation of the structure and chemical composition of samples of the Ba(Fe, Mn, Zr, Ga, Al)$_{12}O_{19}$; Ba(Fe, Sn, Zn, Ga, Al)$_{12}O_{19}$ systems obtained by solid-phase synthesis showed the possibility of the formation of high-entropy microcrystals with the M-type hexaferrite structure.

In the course of the study, it was found that in the composition of the high-entropy phase of $BaR_{12}O_{19}$, a number of new components, previously not used by anyone for these tasks, can be used as R components – Zr, Sn, Zn.

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SYNTHESIS OF THE LA($CR_{0.2}MN_{0.2}FE_{0.2}CO_{0.2}NI_{0.2}$)$O_3$, ND($CR_{0.2}MN_{0.2}FE_{0.2}CO_{0.2}NI_{0.2}$)$O_3$, ($LA_{0.5}ND_{0.5}$) ($CR_{0.2}MN_{0.2}FE_{0.2}CO_{0.2}NI_{0.2}$) O_3 HIGH-ENTROPY OXIDES

Zhivulin V. E.*, Trofimov E. A., Gudkova S. A., Punda A. Y., Zaitseva O. V., Vinnik D. A.

South Ural State University, Chelyabinsk, Russian Federation
*splav.zlat@mail.ru

Functional materials with controlled properties based on many composite oxides are of great interest. Transition metal ions based complex oxides are widely discussed among researchers and find various practical applications. Substituted manganites with general formula ABO_3 (where A^{3+}–rare earth element such as Ln = La, Pr, Nd or substituted element; B–Mn) have a perovskite-like structure. Interest in manganites is due to the strong correlation of chemical composition, structural, magnetic and electrical parameters, and the ability to influence physical properties by changing the chemical composition. One of the main approaches to improving the properties of manganites is chemical substitution of Mn^{3+} ions by diamagnetic and paramagnetic ions. In addition, in recent years, the prospects of the development and application of high-entropy systems with perovskite-like structures were discussed in many papers [1-2].

The aim of our work is to study the possibility of synthesizing a high-entropy oxides with a perovskite-like structure ABO_3 (where A – La, Nd or $La_{0.5}Nd_{0.5}$; B – $Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2}$) [3].

The ceramic samples were produced by the solid-state reactions method. The initial components for the preparation of samples were powders of lanthanum (III)(La_2O_3) and neodymium (III) (Nd_2O_3) oxides, iron (III) oxide (Fe_2O_3), chromium (III) oxide (Cr_2O_3), manganese (III) oxide (Mn_2O_3), cobalt (II) oxide (CoO) and nickel (II) oxide (NiO). All the chemicals used were of analytical grade (99.999%).

The initial components (oxides) were mixed in the appropriate stoichiometric proportions and ground during 3 h in a ball mill. Mixed powders were compacted in pellets (diameter and height were 1 cm) at 3 tons/cm^2. In the course of the experiment, weighed portions of the resulting mixture were heated and kept in an oven at 1300 ˚C in air for 10 h. The heating rate was 400 ˚C/h.

The cooling rate was 100 °C/h. The phase composition and crystal structure were investigated utilizing X-ray powder diffraction (XRD) in Cu-Kα radiation. The measurements were performed on a diffractometer Rigaku Ultima IV in the angular range from 10° to 80° with the speed of 2°/min. The average chemical composition was controlled using the scanning electron microscope (SEM) Jeol JSM7001F with energy dispersive spectrometer Oxford INCA X-max 80 by energy-dispersive X-ray spectroscopy (EDX).

As a result, $La(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$, $Nd(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$ and $(La_{0.5}Nd_{0.5})(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$ HEOs with perovskite-like structure were produced by solid-state reactions. Based on XRD data, all produced samples are single phase and can be described by the SG: R-3c ($La(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$) and SG: Pnma ($Nd(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$ and $(La_{0.5}Nd_{0.5})(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$).

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