ABSTRACT

of the dissertation for the degree of the doctor of philosophy (PhD)
on the specialty 6D060600 – Chemistry

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Production of high-strength alloys of the TiAl system using metal hydrides

The thesis is devoted to the study of the influence of SC, Y, Dy, and Ta doping on the microhardness, microstructure, and phase composition of the titanium-aluminum system.

In this paper, the physicochemical characteristics, microhardness, and structural-phase state of TiAl-Me (Me=Sc, Y, Dy, Ta) systems synthesized using the "hydride technology" are studied in detail. The Rietveld method determined the content of the main phases in the initial system Ti:Al= 1:1, as well as TiAl-Month 2% microadditives Sc, Y, Dy, Ta with high accuracy.

Relevance of the dissertation research topic. Ti-Al alloys have a number of useful properties, in particular increased strength characteristics combined with low density, as well as high heat resistance and a tendency to passivation. Due to these properties, such alloys are widely used in the aerospace, chemical and petrochemical industries. There are several classifications of titanium-aluminum alloys, which are based on structures in the cooled and quenched state.

Intermetallic alloys of the Ti-Al system are also more promising materials for new-generation engines. They have high specific heat resistance, oxidation resistance, high modulus of elasticity and low density. In the Ti-Al system, intermetallides Ti3Al (α2-phase) and TiAl (γ-phase) are formed on the titanium side, from which it is possible to create scale-resistant heat-resistant alloys of a new type. Aluminum and titanium-containing alloys based on it can also be used in various fields of mechanical engineering. Thanks to the development of large-scale optimized production, they have become more affordable and cost-effective materials.

The key problem in the development of γ-TiAl alloys remains their low technological properties, primarily low ductility/fracture toughness in a wide temperature range and insufficient mechanical processing. Improved ductility can be achieved by micro-and macro-alloying, as well as by obtaining a specific alloy structure and optimizing the chemical composition. Therefore, the main attention of researchers of γ-TiAl alloys in the last two decades has been focused on achieving an optimal combination of mechanical properties by varying the

elemental composition and microstructure with different colony/grain size and plate thickness.

One of the "young" methods of powder metallurgy is the hydride method. Hydride technology is a new environmentally friendly technology for producing complex functional materials. Powders and ingots of metals are used as starting materials. From them, the corresponding hydrides are obtained in the hydrogen current. The resulting hydrides were mixed together and pressed under pressure. At the output, a tablet is formed and annealed in a vacuum system. It is important to achieve the most complete dehydrogenation of the product blanks in the sintering process to achieve high mechanical properties.

The advantage of this method is its relative cheapness, the use of refractory materials, and the production of materials with high purity. To obtain alloys by hydride technology, a high-temperature flow furnace is required in order not to obtain intermetalides at an insufficient temperature. A review of the literature data showed the prospects and wide application of hydride technology in the production of functional materials.

The degree of development of the problem. Fairly wide range of sources was involved in the process of writing, which can be divided into three blocks (voluminous literary works on the theory and development of Ti-Al alloys, publications in foreign journals, and conference reports). For completeness of the study and comparison, special programs were used, which are a repository of data on the structures of organic and inorganic compounds. As reference lattices, we used crystallographic data from the COD database, as well as model structures of the Ti-Al system predicted by the USPEX program code with the SIESTA outer shell.

Modern methods of production of binary and multicomponent alloys are based on melting technologies (induction, electric arc or electron beam), or powder metallurgy. Each of these areas is characterized by significant labor intensity and hardware difficulties (the use of high vacuum and the creation of an inert environment at high temperatures, the duration and multiplicity of processes, etc.). Methods of powder metallurgy are characterized by a special duration, since the rate of interaction of metals in the initial mixtures is mainly determined by the rates of diffusion in the solid state. Specific difficulties in obtaining high-quality alloys are also associated with the presence of a dense passivating film on the surfaces of refractory metal particles, which prevents mutual diffusion processes. In this regard, the search for new effective methods for obtaining binary and multicomponent alloys with specified physical and technical properties is relevant in the applied field.

The aim of this work is to study the effect of alloying additives Sc, Y, Dy, Ta on the structural and phase state of the titanium-aluminum system obtained using the "hydride technology".

To achieve this goal, the following tasks were defined:

- obtain a two-component alloy in the equimolar Ti-Al ratio using the "hydride technology" and select the temperature regime of experiments.

- select alloying additives and their quantitative content, as well as alloying conditions to improve the mechanical properties of Ti-Al alloy.

- to study the microstructure and localization of alloying elements in the structure of alloys by scanning electron microscopy and x-ray spectral microanalysis

- to determine the effect of alloying additives Sc, Y, Dy, Ta on the qualitative and quantitative phase composition of the ti–Al alloy, as well as three–component systems Ti49–Al49–Sc2, Ti49–Al49–TA2, Ti49–Al49–Y2, Ti49–Al49-Dy2.

- conduct model experiments to determine thermodynamically stable crystal structures in three-component systems using the USPEX-SIESTA program using the evolutionary code and compare the obtained theoretical parameters of crystal lattices with experimental data;

- to calculate the energy of the crystal lattices of the formed phases and use the obtained data for qualitative and quantitative analysis of the phase composition by the Rietveld method.

- to determine the effect of alloying additives Sc, Y, Dy, Ta in Ti-Al alloys obtained by "hydride technology" on microhardness.

The subject of this study is the microstructure and phase composition, as well as the physical and mechanical properties of tial and TiAl-Me alloys (Me=Sc, Y, Dy, Ta).

The scientific novelty of the results of the dissertation submitted for defense is determined by the fact that the author for the first time:

- for the first time at the "hydride technology" provided unique alloy with a lamellar structure on the basis of intermetallic phases: Ti50–Al50, Ti49–Al49–Sc2, Ti49–Al49–TA2, Ti49–Al49–Y2, Ti49–Al49–Dy2 with additions of Sc, Y, Dy, Ta, up to 2 at.%;

- for the first time carried out a systematic study of the effect of alloying elements Sc, Y, Dy, Ta on the microstructure, qualitative and quantitative phase composition and localization of the alloying elements

- it was first established that the addition of a third alloying element in the tial-REM and TiAl-TA systems leads to an increase in the binding energy of atoms in the crystal lattice and a significant stabilizing effect due to the formation of solid solutions of REE and TA in the intermetallic phase of TiAl and additional phases

(Ti3(Al, Sc), YAl2, DyAl2, TaTi, Ta39Al69, Ti0, 96Ta0,04,Ta161, 8Al282,2, (TaTi66)0.33, (ti, TA) AL3).

- for the first time, an increase in the microhardness of three-component Ti49-Al49-Sc2, Ti49-Al49-Y2 and Ti49-Al49-Ta2 alloys obtained using the "hydride technology" due to solid-phase and dispersion hardening was established.

Theoretical significance of the results: new data on the effect of SC, Y, Dy, and Ta additives on the structure and properties of Ti-Al alloys obtained by the GT method using x-ray phase analysis, scanning and transmission electron microscopy, and x-ray spectral microanalysis can be used to improve the mechanical properties of γ-TiAl alloys and are recommended for use in industry.

The practical significance of the research presented in this dissertation is to obtain new unique alloys with a layered structure for successful application in aviation technology, materials science, etc.

Conclusions of the study:

1. for the First time, an alloy in the equimolar Ti–Al ratio was obtained using the "hydride technology" and unique layered compositions based on intermetallic phases and alloying additives Sc, Y, Dy, Ta. the temperature intervals of hydrogenation and annealing were Established: hydrogenation of Sc, Y, Dy, Ta was performed at 450, 420, 420, 550 °C, respectively; the annealing temperature for samples Ti50–Al50, Ti49–Al49–Sc2, Ti49–Al49–TA2, Ti49–al49–Y2, ti49–al49–dy2 was 1150 °C.

2. it is Established that the metals Sc, Ta, Y, Dy with a content of no more than 2 at%can act as effective alloying additives.

3. the distribution of alloying elements in local sections of the alloy structure was studied and it was found that the alloying elements are distributed in the matrix of intermetallic phases with a simultaneous increase (2 p) in the layer thickness and/or form separate phases: Sc, Ti3(Al, Sc), YAl2, DyAl2, TaTi, Ta39Al69, Ti0, 96Ta0,04,Ta161, 8Al282,2, (TaTi66)0.33, (TA, Ti)Al3,located on dislocations or on grain boundaries And/or grain volume.

4. quantitative and qualitative analysis of the phase composition of the obtained two-and three-component systems is Carried out. It was found that the initial Ti50-Al50 system contains the main phases Ti3Al, TiAl, TiAl2; when the third component is added, new phases Ti3(Al, Sc), YAl2, DyAl2, TaTi, Ta39Al69, Ti0, 96Ta0,04,Ta161, 8Al282,2, (TaTi66)0.33, (TA, Ti)Al3 are formed in the Ti49-Al49-Ta2,Ti49-Al49-Dy2 systems.

5. the USPEX-SIESTA Program uses an evolutionary code to model crystal lattices of thermodynamically stable phases formed during doping of the Ti-Al system, the parameters of which are consistent with experimental data.

6. it is Established that the introduction of additives of alloying elements in the internode is possible and it leads to an increase in the binding energy of atoms in the lattice and to a significant stabilizing effect in the TiAl-REM and TiAl-TA systems. It is shown that TA and Y additives significantly increase the effective energy of Ti49-Al49-Ta2 and Ti49-Al49-Y2 systems, and dy additives lead to a significant stabilizing effect of Ti49-Al49-Dy2 relative to the initial Ti50-Al50 alloy.

7. it was Found that ti49-Al49-Sc2, Ti49-Al49-Y2, and Ti49-Al49-Ta2 alloys have the highest microhardness, which is associated with an increase in the set of phases in three-component systems, the formation of solid solutions, and changes in the morphology of layers.

The main provisions for protection:

1. using the "hydride technology" method, unique alloys with a layered structure based on intermetallic phases are obtained: Ti50-Al50, Ti49-Al49-Sc2, Ti49–Al49–TA2, Ti49–Al49–Y2, Ti49–Al49–Dy2.

2. the Addition of a third alloying element in the tial-REM and TiAl-TA systems leads to an increase in the binding energy of atoms in the crystal lattice and a significant stabilizing effect due to the formation of solid solutions of REE and TA elements in TiAl and additional phases (Ti3(Al,Sc), YAl2, DyAl2, TaTi, Ta39Al69, Ti0,96Ta0,04, Ta161,8Al282,2, (TaTi66)0.33, (Ti,TA)Al3).

3. three-Component alloys Ti49-Al49-Sc2, Ti49-Al49-Y2 and Ti49-Al49-Ta2 obtained by "hydride technology" are characterized by increased microhardness due to solid-phase and dispersion hardening due to an increase in the set of phases and changes in the microstructure of layers.

Connection of work with the plan of state scientific programs. The dissertation work was carried out as part of joint research work conducted at the Department of chemistry of the L. N. Gumilyov Eurasian national University and The laboratory of chemical technology of Tomsk state University with the financial support of the TSU competitiveness program (research project of the national research University of Russia 8.2.10.2018 L, 2018-2020)

Testing the work. The results of the dissertation work were presented at the following conferences: VI Russian-Kazakh youth scientific and technical conference "New materials and technologies" (Moscow Barnaul, Russia, 2018), XVI international conference "Prospects for the development of fundamental Sciences" (Tomsk, Russia, 2019), XVII international conference "Prospects for the development of fundamental Sciences" (Tomsk, Russia, 2020), international conference "Multifunctional chemical materials and technologies" (Tomsk, Russia, 2019), 61st international research conference "Promising directions for the development of modern science" (Moscow, Russia, 2020) and XVI international

school-seminar "evolution of defective structures in condensed media" (Barnaul, Russia, 2020).

The personal contribution of the applicant consists in the analysis of literary data, household and conducted experimental honor. The author participated in the development of the implementation plan for the dissertation work, participated in the discussion of the results and in the preparation of publications on the topics of the dissertation work.

Main results of the dissertation research. The main results of the thesis are reflected in 10 publications, including 1 article published in international scientific journal with impact factor (IF=2,2 Q2) according to the databases Web of Science Core Collection, 3 articles published in journals recommended by the Committee of the Ministry of education of Kazakhstan and 6 volumes of proceedings of international conferences.

Volume And structure of the dissertation. The thesis is presented on 109 pages of computer text, includes 53 figures and 22 tables. The dissertation consists of an introduction, the main honor, in which presentation of this literary review, experimental honor, results of generalization of experimental data, conclusions, a list of exploited Easterners from 191 titles.