ANNOTATION
dissertation for the degree of Doctor of Philosophy (PhD)
according to the educational program 8D07202 - "Metallurgy of ferrous and non-ferrous metals"
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CREATION OF A PHYSICOCHEMICAL MODEL OF THE STRUCTURAL STATE OF THE FE-SI-AL-MN-CR SYSTEM FOR THE DEVELOPMENT OF SCIENTIFIC FOUNDATIONS FOR OBTAINING COMPLEX FERROALLOYS BASED ON THE BJERRUM-GUGGENHEIM CONCEPT

The aim of the dissertation workis to thermodynamically justify the solubility of aluminum in complex alloys based on their phase diagrams through the Bjerrum-Guggenheim osmotic coefficient and to determine the optimal ratios of elements in these alloys, at which complete assimilation of aluminum by the melt will occur.

Research objectives
to thermodynamically justify the compositions of silicon-aluminum alloys with an increased aluminum content of the Fe-Si-Al system.

to establish, using the method of thermodynamic-diagrammatic analysis, the effective compositions of complex alloys based on iron, manganese, chromium and aluminum with the construction of diagrams of phase relationships of individual parts in the Fe-Si-Al-Cr-Mn system.

thermodynamic-diagrammatic analysis of the Fe-Si-Al-Mn system with the construction of phase relationship diagrams.

thermodynamic-diagrammatic analysis of the Fe-Si-Al-Cr system with the construction of phase relationship diagrams.

identification of patterns and study of the structural state of highly effective complex alloys based on their phase diagrams from the standpoint of the Bjerrum-Guggenheim concept.

Research methods
The following research methods were used in completing the dissertation:

thermodynamic modeling of the process of smelting complex ferroalloys was carried out;

studies were conducted using the Gauss method;

research was conducted using the matrix method with a fourth-order determinant;

research was conducted on the mathematical apparatus for describing lines of monovariant phase equilibria based on the Bjerrum-Guggenheim concept;

Tests were conducted on the smelting of aluminosilicon chrome and aluminosilicon manganese alloys in an ore-thermal furnace with a capacity of 300 kVA.

The main provisions (proven scientific hypotheses and other conclusions that are new knowledge) submitted for defense

results of thermodynamic modeling of the smelting process of aluminosilicon chrome and aluminosilicon manganese alloys;

results of data on composition and temperature taken from the crystallization fields of liquidus and solidus lines to the reference point for the Cr-Al, Mn-Al and Cr-Mn systems;

results of mathematical expressions of crystallization fields of phases of binary systems Cr-Al, Mn-Al and Cr-Mn on a single analytical basis;

The results of the study, based on the thermodynamic-diagrammatic analysis of the Al-Mn-Fe-Si system, determined the range of alloy compositions that meet the requirements for steel processing and use for metallothermic reduction;

results of large-scale laboratory tests of the process of smelting aluminosilicon chrome and aluminosilicon manganese in an ore-thermal furnace with a capacity of 300 kVA.

Description of the main results of the study

As a result of theoretical and experimental research:

From a thermodynamic point of view, the crystallization fields of phases of boundary binary systems of tetrahedrons are considered: Fe-Si-Al-Mn and Fe-Si-Al-Cr.

Initial data on the composition and temperature were formed, taken from the crystallization fields of the liquidus and solidus lines to the reference point for the Cr-Al, Mn-Al and Cr-Mn systems.

The regularities of the behavior of the Bjerrum-Guggenheim osmotic coefficient on the activity ratio for the liquid and solid phases in the form of correlation dependencies were revealed.

The nature of the change in the Bjerrum-Guggenheim osmotic coefficient for particular systems along the crystallization line of phases is shown.

Mathematical expressions of crystallization fields of phases of binary systems Cr-Al, Mn-Al and Cr-Mn are proposed on a single analytical basis.

Based on the thermodynamic diagrammatic analysis of the Al-Mn-Fe-Si system, the range of alloy compositions was determined that meets the requirements for steel processing and use for metallothermic reduction.

It was established that the calculated compositions of the AlSiMn alloy are in the $FeSi-Fe_3Al_{11}Si_6-Si-MnSi$ tetrahedron.

It was established that the calculated compositions of the AlSiCr alloy are in the $Al-Si-Fe_3Al_{11}Si_6-Cr_5Si_3$ tetrahedron.

Optimum compositions of aluminosilicomanganese (AlSiMn) alloy have been determined for its use in steel processing or metallothermic reduction smelting of refined grades of ferromanganese.

Three variants of AlSiMn alloy compositions are proposed, in which compositions with increased silicon and aluminum content are supposed to be used for metallothermic smelting of medium- and low-carbon ferromanganese, and alloys with increased manganese content and the sum of silicon and aluminum of no more

than 50% for steel processing. Variants of the experimental AlSiMn alloy compositions: AlSiMn-10 (Fe-15%, Si-50%, Al-25%, Mn-10%), AlSiMn-20 (Fe-20%, Si-45%, Al-15%, Mn210%), AlSiMn-30 (Fe-20%, Si-40%, Al-10%, Mn-30%).

Tests of smelting of aluminosilicochrome alloy were conducted using coals of the Sary-Adyr deposit with different ash content and high-carbon ferrochrome screenings. During the 3 stages of smelting, three types of alloy grade composition were obtained - AlSiCr-10/50/25, AlSiCr-15/45/25 and AlSiCr-20/40/25.

Justification of the novelty and importance of the results obtained

Thermodynamic substantiation of compositions of silicon-aluminum alloys with increased aluminum content in the Fe-Si-Al system has been carried out. Effective compositions of complex alloys based on iron, manganese, chromium and aluminum have been established with the construction of phase relationship diagrams for individual parts in the Fe-Si-Al-Cr-Mn system. Regularities have been revealed and the structural state of highly effective complex alloys has been studied based on their phase diagrams from the standpoint of the Bjerrum-Guggenheim concept. Detailed studies of the $\Phi'AxBy$ graphs at the melting point of a congruently melting compound have been carried out and the nature of stratification in the liquid phase during melting for metallic Fe-Cr and Fe-Mn systems has been established.

Compliance with scientific development directions or state programs

The topic of the dissertation corresponds to the priority "Rational use of natural resources, including water resources, geology, processing, new materials and technologies, safe products and designs" of the National Scientific Council under the Government of the Republic of Kazakhstan.

In carrying out the dissertation work, part of the research work was carried out within the framework of grant funding (GF), on the project "Identification of patterns and study of the structural state of highly effective complex alloys based on their phase diagrams from the standpoint of the Bjerrum-Guggenheim concept" (within the framework of the GF of scientific and (or) scientific and technical projects for 2020-2022, IRN AP08855453), in which the doctoral student is the responsible executor. Applicant: Branch of the RSE on the Right of Economic Management "National Center for Integrated Processing of Mineral Raw Materials of the Republic of Kazakhstan" of the Committee for Industrial Development and Industrial Safety of the Ministry of Industry and Infrastructure Development of the Republic of Kazakhstan " Zh. Abishev Chemical and Metallurgical Institute".

Description of the doctoral student's contribution to the preparation of each publication

The author's personal contribution consists of carrying out the main volume of theoretical and experimental research presented in the dissertation, including the development of theoretical models, experimental research methods, conducting

research, analyzing and presenting the results in the form of publications and scientific reports.

On the topic of the dissertation, 6 scientific papers have been published, including: 4 (four) articles in peer-reviewed scientific publications in the scientific direction of the dissertation topic, indexed in the Science Citation Index Expanded of the Web of Science database (Clarivate Analytics) and by CiteScore in the Scopus database (Elsevier), 2 (two) articles in the collection of the International Scientific and Practical Conference.

Information on the main publications in peer-reviewed scientific journals in the scientific direction of the dissertation topic, indexed in the Science Citation Index Expanded of the Web of Science (Clarivate Analytics) database and by CiteScore in the databaseScopus (Elsevier)

Yerekeyeva, G.,Zhumagaliev, YE,Nurumgaliyev, A., Mongolkhan O.,Davletova, A.,Sagynbekova, G./ THERMODYNAMIC-DIAGRAM ANALYSIS OF THE Fe-Si-Al-Cr SYSTEM WITH THE CONSTRUCTION OF DIAGRAMS OF PHASE RELATIONS // Metalurgija. – 2022. Vol 61, Iss. 3-4. – P. 825-827;

Yerekeyeva, G., Tolokonnikova, VV,Baisanov, S.O.,Narikbayeva, GI/ Regularities of phase equilibria based on the Bjerrum-Guggenheim concept for the Fe-Al binary system // CIS Iron and Steel Review. – 2022. Vol 24, Iss. 2. – P. 79-83;

Yerekeyeva, G., Tolokonnikova, VV,Baisanov, S.O.,Narikbayeva, GI, Korsukova I. / THERMODYNAMIC-DIAGRAM ANALYSIS OF THE Fe-Si-Al-Mn SYSTEM WITH THE CONSTRUCTION OF DIAGRAMS OF PHASE RELATIONS // Metalurgija. – 2022. Vol 61, Iss. 3-4. – P. 828-830;

Yerekeyeva, G., Nurumgaliyev, A.,Zhuniskaliyev, T.,Shevko, V., Mukhambetgalyev Ye., Kelamanov B., Kuatbay Ye., Badikova A.,Volokitina, I./ Modeling and development of technology for smelting a complex alloy (ligature) Fe-Si-Mn-Al from manganese-containing briquettes and high-ash coals // Scientific Reports-2024. Vol 14(1), P. 7456.

Information about the report presented and discussed on the results of the dissertation work at the International Scientific and Practical Conference:

Yerekeeva G.S.,Tolokonnikova V.V., Nurumgaliev A.Kh., Zayakin O.V. BJERRUM-GUGGENHEIM COEFFICIENTS OF THE FE-SI RANGE OF DISSOCIATION DEVELOPMENT // "Youth, Science and Technology: Ways of Improvement and Integration": LIII Republican Scientific and Practical Conference. Proceedings of the International Scientific Conference – Temirtau;

Yerekeeva G.S.,Nurumgaliev A.Kh., Baysanov S., Tolokonnikova V.V. Theoretical analysis of smelting refined grades of ferrochrome // Proceedings of the XI International Beremzhanovsky Congress on Chemistry and Chemical Technology 2021, November 19-20 - Almaty