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THERMODYNAMIC PREDICTION OF THE TECHNOLOGICAL CONDITIONS FOR PRODUCING THE TI-10V-2FE-3AL ALLOY BY VACUUM ARC REMELTING

Abstract. This paper presents the results of a thermodynamic analysis of equilibrium phase diagrams for systems relevant to the ternary-melt ***Ti-10V-2Fe-3Al*** alloy, along with calculations of thermodynamic parameters and a staged thermodynamic prediction of the technological conditions for vacuum arc remelting (VAR). Three remelting stages are justified thermodynamically: the first melt removes coarse ***Fe***, ***V***, and ***Al*** oxides; the second melt breaks down most ***FeTi/Fe₂Ti*** intermetallics and transfers part of the titanates into slag; the third melt brings the system close to equilibrium, minimizing oxide and intermetallic inclusions. Practical recommendations were developed based on the thermodynamic analysis, including the required vacuum level **($pO_2 \leq 10^{-20}–10^{-22}$)**, control of ***O***, ***N***, and ***H*** impurities, requirements for alloying additions, conditions for ternary remelting, and β-homogenization.

Key words: *vacuum arc remelting, titanium alloys, process thermodynamics, ternary remelting, prediction, stable compounds.*

Ti-10V-2Fe-3Al қорытпасын вакуумдық-доға балқыту әдісімен өндіру технологиясының шарттарын термодинамикалық болжау

Аңдатпа. Бұл мақалада үш рет балқытылатын ***Ti-10V-2Fe-3Al*** титан қорытпасына сәйкес жүйелердің тепе-теңдік диаграммалары бойынша жүргізілген термодинамикалық талдау нәтижелері, термодинамикалық параметрлердің есептеулері, сондай-ақ вакуумдық-доға балқыту (ВДП) технологиясы шарттарын кезеңдік термодинамикалық болжау берілген. Үш реттік ВДП балқытудың термодинамикалық негіздемесі көрсетілді: бірінші балқыту – ***Fe***, ***V***, ***Al*** ірі оксидтерін жою; екінші балқыту – ***FeTi/Fe₂Ti*** интерметаллидтерінің басым бөлігін ыдыратып, титанаттардың бір бөлігін қожға шығару; үшінші балқыту – жүйені тепе-теңдікке жақын күйге жеткізу, оксидтік және интерметаллидтік қосылыстарды барынша азайту. Термодинамикалық талдау негізінде практикалық ұсынымдар жасалды: вакуум деңгейі **($pO_2 \leq 10^{-20}–10^{-22}$)**, ***O***, ***N***, ***H*** қоспаларын бақылау, лигатураға қойылатын талаптар, үш реттік балқыту шарттары, β-гомогенизация.

Түйінді сөздер: *вакуумдық-доға балқыту, титан қорытпалары, процестің термодинамикасы, үш реттік балқыту, болжау, тұрақты қосылыстар.*

Термодинамическое прогнозирование условий технологии получения сплава Ti-10V-2Fe-3Al методом вакуумно-дуговой плавки

Аннотация. В статье приведены результаты термодинамического анализа диаграмм равновесного состояния систем, соответствующих сплаву тройного переплава ***Ti-10V-2Fe-3Al***, расчеты термодинамических параметров и стадиальное термодинамическое прогнозирование условий технологии вакуумно-дуговой плавки (ВДП) получения сплавов тройного переплава: 1 переплав – удаление грубых оксидов ***Fe***, ***V***, ***Al***; 2 – разрушение большей части интерметаллидов ***FeTi/Fe₂Ti*** и вывод части титанатов в шлак; 3 – доведение системы до состояния, близкого к равновесному, с минимальной долей оксидных и интерметаллидных включений. Разработаны практические рекомендации согласно термодинамическому анализу, глубина вакуума **($pO_2 \leq 10^{-20}–10^{-22}$)**; контроль ***O***, ***N***, ***H***, требования к лигатуре; условия тройного переплава, β-гомогенизация.

Ключевые слова: *вакуумно-дуговая плавка, титановые сплавы, термодинамика процесса, тройной переплав, прогнозирование, устойчивые соединения.*

Introduction

In recent decades, titanium alloys have accounted for approximately 15–30% of the mass of airframes and gas-turbine engines in modern aircraft, reaching even higher levels in certain load-bearing and landing-gear components due to their unique combination of high specific strength, corrosion resistance, and performance at elevated temperatures [1, 2]. The growing share of titanium is driven by its exceptional property suite-high thermal stability, bifunctional behavior under cyclic loading, and compatibility with next-generation composite materials. These characteristics allow significant weight reduction, increased service life of components, and enhanced aircraft safety. The growing share of titanium is driven by its exceptional property suite-high thermal stability, bifunctional behavior under cyclic loading, and compatibility with next-generation composite materials.

The current state and future prospects of the titanium industry, along with the key physical-metallurgical principles governing the formation of structure and properties in titanium alloys, are comprehensively reviewed in the seminal work by Banerjee and Williams [1], which emphasizes a shift from empirical processing selection toward science-based alloy and process design.

Metastable β- and (α+β) alloys occupy a special place among structural titanium materials, offering high strength while maintaining adequate fracture toughness and fatigue resistance [1, 3]. A classical representative of this group is the ***Ti-10V-2Fe-3Al (Ti-10-2-3)*** alloy, widely used in aerospace applications (landing-gear components, load-bearing airframe parts) due to the ability to finely tune its microstructure (volume fraction and morphology of the α phase, β matrix, α″ martensite, ω phase) through thermomechanical processing and ageing [4–7]. Modern studies show that this alloy exhibits a broad spectrum of deformation mechanisms –from stress-induced martensitic transformation to TRIP/TWIP effects – providing new opportunities for further improving the strength-ductility balance [3–5, 7].

However, translating laboratory-scale processing to an industrial ternary (multiple) vacuum arc remelting (VAR) route requires thermodynamically grounded control of impurity content (***O***, ***N***, ***H***, ***C***) and phase composition in the ***Ti–V–Fe–Al*** system. Reviews on high-strength titanium alloys for aerospace applications [2] and on metastable β alloys [3, 8] emphasize that melt purification, management of β stabilizers, and controlled phase transformations (β→α, β→α″, β→ω) are the key factors governing the reliability and service life of critical components. The increasing use of ***Ti-10-2-3*** presents new challenges for metallurgical enterprises, especially in countries where industrial production of such β alloys has not previously been implemented. Achieving industrial-quality ingots of ***Ti-10-2-3*** requires: a deep understanding of the thermodynamic features of the ***Ti–V–Fe–Al*** system; development of optimal

VAR and ternary-remelting regimes; strict control of gaseous impurities (***O***, ***N***, ***H***) that determine brittleness and durability of the β phase; formation of a homogeneous microstructure free of dendritic segregation and intermetallic inclusions; and adaptation of downstream deformation and heat-treatment routes to the required final properties [9, 10].

Against this background, improving the technology for producing ***Ti-10-2-3*** ternary-remelt ingots by vacuum arc melting – using modern modeling and experimental approaches –constitutes an important scientific and practical task aimed directly at increasing the share of domestically produced titanium alloys in critically loaded aerospace components.

The aim of the present study was thermodynamic prediction of the technological conditions for producing the ***Ti-10V-2Fe-3Al*** alloy by vacuum arc melting, as well as analysis of microstructural evolution during heat treatment and stabilization of structural features and gas content ***(O/N/H)*** in the system.

Materials and methods of research

Initial materials

The object of the study was a ternary-remelting ***Ti-10V-2Fe-3Al*** ingot produced by vacuum arc melting (VAR) according to the customer-specified composition: ***Al*** 2.60–3.40%, ***V*** 9.00–11.00%, ***Fe*** 1.60–2.20%, ***O*** max. 0.13%. Thermodynamic calculations and phase-diagram modelling were performed for this composition.

The production of this ingot involved the following input materials, whose chemical compositions are presented in Tables 1–3:

Research Methods

For the thermodynamic calculations, the HSC Science software (Phase Diagram module) by Outokumpu Oy was used. For technological prediction of the ternary VAR (vacuum arc remelting) process, it is appropriate to select temperature ranges associated with specific stages of the process: the melting region / VAR molten pool (1750–1950 °C), corresponding to removal of ***O***, ***N***, ***H***, ***Cl***, and Mg and melt-gas-oxide equilibrium; the β-region and ingot homogenization (900–1100 °C), corresponding to β-homogenization, dissolution of intermetallic phases, and chemical uniformity; the α+β region and ageing (700–900 °C), corresponding to the formation of the working α+β microstructure of ***Ti-10-2-3***; and the oxidation / α-case region (600–900 °C), corresponding to the behavior of the ***Ti-Al-***O system and the growth of the oxygen-enriched layer.

These temperature intervals are of technological interest for intensifying and predicting the process; therefore, an analysis of the predominant and thermodynamically stable phases in the systems was carried out.

Results and their discussion

Equilibrium-state diagrams were obtained for the following systems: ***Ti-V-O***, ***Ti-Fe-Al***, *Ti-Fe-O*, and ***Ti-Al-O*** (Fig. 1).

For the ***Ti-V-O*** system, it was established that at high temperatures (≈1800–3000 °C), not only titanium oxides but also a sequence of vanadium oxides (VO_2, V_2O_3, V_3O_5, etc.) remain stable at very low pO_2 (Fig. 1a). This indicates that vanadium in the ***Ti-10-2-3*** alloy thermodynamically behaves as an oxygen «getter»: when oxygen is introduced, ***V*** oxidizes preferentially over ***Ti***, and the resulting vanadium oxides transfer into slag/inclusions. Consequently, during VAR melting of ***Ti-10-2-3***, part of the vanadium effectively behaves as a deoxidizer, which reduces the activity of oxygen in the metallic phase but simultaneously leads to a loss of effective V due to its conversion into oxides.

Analysis of the ***Ti-V-O*** diagram shows that under conditions characteristic of vacuum arc melting, vanadium is the most thermodynamically favorable oxygen acceptor. This results in preferential formation of vanadium oxides and a reduction in

Table 1

Composition of aluminum granules

Кесте 1

Алюминий түйіршіктерінің құрамы

Таблица 1

Состав алюминиевых гранул

Element	*Al*	*Zn*	*Si*	*Fe*	*Mn*	*Mg*	*Ni*	*Pb*	*Sn*	*Ti*	*Cr*	*Cd*	*Be*	*Cu*	*C*
№	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Content, %	99,8	0,003	0,025	0,113	0,02	0,0002	0,0051	0,001	0,0007	0,007	0,001	0,0001	0,0001	0,0004	0,002

Table 2

The composition of the V-Al-Fe ligature

Кесте 2

V-Al-Fe лигатурасының құрамы

Таблица 2

Состав лигатуры V-Al-Fe

Element	*V*	*Al*	*Fe*	*B*	*C*	*Cr*	*Cu*	*Mo*	*P*	*S*	*Si*	*N*	*O*
№	1	2	3	4	5	6	7	8	9	10	11	12	13
Content, %	66,6	21,1	12,1	0,001	0,001	0,01	0,002	0,01	0,001	0,003	0,10	0,03	0,03

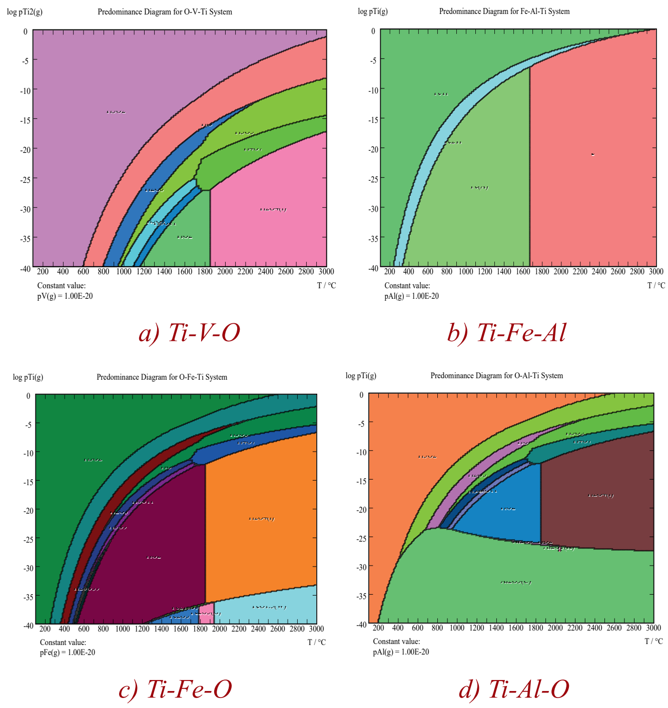

Figure 1. Equilibrium state diagrams of systems.
Сурет 1. Жүйелердің тепе-теңдік күй диаграммалары.
Рис. 1. Диаграммы равновесного состояния систем.

oxygen activity in the metallic phase, but is accompanied by the transfer of vanadium into the slag phase. This factor must be considered when balancing V in the charge and selecting the number of remelting cycles.

For the ***Ti–Fe–Al*** system, the stable states ***FeTi***, ***Fe_2Ti*** and elemental Fe were identified, with iron dominating in the high-temperature region: at ≈2000 °C and low partial pressures of ***$Ti_2(g)$*** and ***$Al_2(g)$***, the ***FeTi*** and ***Fe_2Ti*** fields occupy a significant portion of the diagram (Fig. 1b). This shows that iron does not merely remain as elemental Fe but tends to form very stable intermetallics ***FeTi*** and ***Fe_2Ti*** with titanium; this thermodynamically explains why insufficient homogenization and an insufficient number of remelts lead to brittle ***FeTi*** inclusions and ***Fe***-rich dendrites in titanium ingots.

The predominance of ***FeTi*** and ***Fe_2Ti*** in the ***Ti-Fe-Al*** diagram at ≈2000 °C indicates the high thermodynamic stability of these intermetallics even in the liquid pool of VAR. This justifies the requirement for multiple (at least ternary) remelting of ***Ti-10V-2Fe-3Al*** and subsequent β-homogenization to break down ***FeTi*** particles and redistribute iron into the β matrix. It was also established that, from a VAR-process optimization standpoint, any excess Fe in the charge immediately increases the fraction of ***$FeTi/Fe_2Ti$***; therefore strict control of ***Fe*** to ≤ 2% combined with ternary remelting is necessary to minimize intermetallics.

For the ***Ti-Fe-O system***, the diagram shows that oxide phases such as ***$FeTiO_3$***, ***Fe_2TiO_4***, ***Fe_2TiO_5*** and ***$FeO{\cdot}TiO_2$*** are stable over a very wide range of temperatures and oxygen partial pressures (Fig. 1c). These phases represent thermodynamically favorable traps for both oxygen and iron. Thus, in the presence of oxygen, part of the ***Fe*** and ***Ti*** is consumed to form these stable complex oxides, which remove oxygen from the metallic phase (advantage) but simultaneously deplete the alloy in ***Ti*** and ***Fe*** (drawback). Almost all of these oxide phases are in equilibrium with nearly pure iron under certain conditions, meaning that iron can be readily segregated into slag as titanates if oxygen is not sufficiently suppressed.

Thermodynamic analysis of the ***Ti-Fe-O*** system showed that at 1100–1600 °C, complex oxides such as ***$FeTiO_3$***, ***Fe_2TiO_4***, ***Fe_2TiO_5*** and ***$FeO{\cdot}TiO_2$*** remain stable, simultaneously binding iron and oxygen. These phases act as thermodynamic sinks for ***Fe*** and ***O*** in the slag; however, their formation is accompanied by the loss of titanium and iron from the melt. This imposes strict constraints on the oxygen content in the charge and justifies the requirement for deep vacuum during VAR remelting.

Furthermore, ***O_2*** levels in both the metal and chamber must be kept sufficiently low so that these ternary oxides do not enter their stability fields; otherwise, ***Ti*** and ***Fe*** losses to slag may occur.

For the ***Ti-Al-O*** system, analysis of the diagram shows that ***Al_2O_3*** and ***$Al_2O_3{\cdot}TiO_2$*** are extremely stable even at high temperatures (Fig. 1d). This means that any oxide film on aluminum in the charge will not be reduced under VAR conditions. At very low ***pO_2*** and high titanium activity, aluminum tends to form the intermetallic phase ***AlTi*** rather than oxides, meaning that ***Al*** behaves as an α-stabilizer provided it has not already oxidized to ***Al_2O_3***. The combined stability of ***Al_2O_3*** and ***TiO_2*** explains the formation of α-case and oxide inclusions if heat treatment is performed outside of vacuum or inert atmosphere.

Thermodynamic analysis of the ***Ti-Al-O*** diagram showed that ***Al_2O_3*** and mixed oxides ***$Al_2O_3{\cdot}TiO_2$*** possess extremely high thermodynamic stability in the 1600–2000 °C range. Under vacuum arc melting conditions, these phases are practically non-reducible, meaning that any oxide film on the aluminum master alloy will fully transfer into non-metallic inclusions. Therefore, the oxygen purity of the aluminum feedstock is a critical factor for the quality of ***Ti-10V-2Fe-3Al*** ingots. It was also determined that aluminum master alloy must be etched and cleaned from its oxide film, and that heat treatment of the ingots must be conducted only in vacuum or high-purity ***Ar***, otherwise α-case (***TiO_2*** + oxygen-enriched α layer) will form.

Thermodynamic calculations for β-annealing temperatures (1000–1100 °C) are summarized in Table 3.

It was established that at β-annealing temperatures (1000–1100 °C), the thermodynamically most stable phases are ***Al_2O_3***, ***TiO_2***, and the mixed titanate ***$Al_2O_3{\cdot}TiO_2$***. Aluminum oxide and aluminum titanate are therefore extremely stable and, once introduced into the ***Ti-10V-2Fe-3Al*** melt, are not reduced under vacuum arc remelting conditions. These phases are retained in the alloy as persistent non-metallic inclusions, making reliable prediction of their formation essential for effective melt control.

Table 5 presents the general technological recommendations derived from the thermodynamic analysis of the VAR process (Table 4).

Based on the thermodynamic analysis of equilibrium systems relevant to vacuum arc remelting of ternary-remelted alloys, a framework for thermodynamic forecasting of technological conditions has been developed and practical recommendations have been formulated:

Table 3

Standard Gibbs energy ΔG° of formation of oxides and titanate in the Ti-Al-O system (β-annealing temperature range of Ti-10V-2Fe-3Al)

Кесте 3

Ti-Al-O жүйесіндегі оксидтер мен титанаттың түзілуінің стандартты Гиббс энергиясы ΔG° (Ti-10V-2Fe-3Al β-күйдіру температура диапазоны)

Таблица 3

Стандартная энергия Гиббса ΔG° образования оксидов и титаната в системе Ti-Al-O, (диапазон температур β-отжига Ti-10V-2Fe-3Al)

Reaction	Temperature, °C	ΔG°, kJ/mol	Comment
$2Al(s) + 3/2\ O_2(g) \rightarrow Al_2O_3(s)$	1000 °C	≈ –1304	Very high thermodynamic stability of Al_2O_3
$2Al(s) + 3/2\ O_2(g) \rightarrow Al_2O_3(s)$	1100 °C	≈ –1276	Slight decrease in the absolute value of ΔG° with increasing T, but Al_2O_3 remains extremely stable
$Ti(s) + O_2(g) \rightarrow TiO_2(s)$	1000 °C	≈ –672	Stable titanium oxide, but significantly «weaker» in ΔG° than Al_2O_3
$Ti(s) + O_2(g) \rightarrow TiO_2(s)$	1100 °C	≈ –656	Formation energy in absolute value is almost twice lower than that of Al_2O_3

Table 4

General technological recommendations according to thermodynamic analysis of the vacuum arc melting process

Кесте 4

Вакуумдық доғалық балқыту процесінің термодинамикалық талдауы бойынша жалпы технологиялық ұсыныстар

Таблица 4

Общие технологические рекомендации согласно термодинамическому анализу процесса ВДП

Factor / Diagram / Stage	Physical Meaning	Technological Requirement	Practical Consequence
Stage I VAR: melting	Formation of the liquid β-phase	Stable arc, required superheat	Uniform electrode melting
Stage II VAR: degassing	Removal of ***H***, ***N***, ***O***	Deep vacuum 10^{-2}–10^{-3} Pa	Reduction of gases in the ingot
Stage III VAR: solidification	Formation of β / α+β structure	Control of cooling rate	Minimal dendritic segregation
Stage IV: remelting	Approach to equilibrium	Necessity of ternary remelting	Homogeneous structure
Stage V: ingot homogenization	Chemical composition leveling	Soaking in the β-region	Absence of intermetallics

– control of vanadium behavior as an internal deoxidizer: according to the ***Ti-V-O*** phase diagram, vanadium is the most thermodynamically favorable oxygen acceptor, resulting in preferential formation of vanadium oxides and a reduction in oxygen activity in the alloy. This necessitates accounting for vanadium losses during vacuum arc remelting and adjusting its content in the charge accordingly;

– high thermodynamic stability of ***FeTi/Fe₂Ti*** intermetallics: the ***Ti-Fe-Al*** diagram at $T \approx 2000$ °C demonstrates the predominance of ***FeTi*** and Fe_2Ti stability fields, confirming the thermodynamic inevitability of iron-titanium intermetallic formation even at low ***Fe*** concentrations. This substantiates the necessity of ternary VAR remelting and subsequent β-homogenization to disrupt intermetallic regions and ensure chemical uniformity;

– ternary ***Fe-Ti-O*** oxides as traps for ***Fe*** and ***O***: the ***Ti-Fe-O*** diagram shows the stability of $FeTiO_3$, Fe_2TiO_4, Fe_2TiO_5, and $FeO\cdot TiO_2$ phases, which bind iron and oxygen in the slag phase. While this allows the slag to act as an effective scavenger for ***Fe*** and ***O***, it simultaneously imposes an upper limit on permissible oxygen content in order to minimize titanium losses;

– irreducible stability of Al_2O_3 and $Al_2O_3\cdot TiO_2$: according to the ***Ti-Al-O*** diagram, aluminum oxide and aluminum titanates are practically non-reducible under VAR conditions. Consequently, the oxide film on the aluminum master alloy represents a critical source of persistent non-metallic inclusions in ***Ti-10V-2Fe-3Al***;

– justification for the ternary remelting scheme: the combined analysis of all four systems shows that the first remelt removes coarse ***Fe-***, ***V-***, and ***Al***-based oxides; the second remelt breaks down the majority of ***FeTi/Fe₂Ti*** intermetallics and transfers part of the titanates into the slag; and the third remelt brings the system close to thermodynamic equilibrium, minimizing the content of oxide and intermetallic inclusions;

– process regimes and limitations for industrial production of ***Ti-10V-2Fe-3Al***: thermodynamic diagrams enable formulation of the following practical recommendations: maintenance of deep vacuum during VAR with effective $pO_2 \leq 10^{-20}$–10^{-22}; strict control of ***O***, ***N***, and ***H*** in the charge (particularly in the aluminum master alloy and ferrovanadium); mandatory ternary remelting combined with β-homogenization; and heat treatment exclusively in vacuum or high-purity argon to prevent α-case formation.

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