DIFFUSION AND OXIDATION KINETICS OF β AND γ PHASES IN REFRACTORY METALS ALLOYED TI-AL SYSTEM

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To,

Maa and Baba

CERTIFICATE

This is to certify that the thesis entitled **"Diffusion and oxidation kinetics of β and γ phases in refractory metals alloyed Ti-Al system"** is being submitted by **Mr. SHIVANSH MEHROTRA** to the Indian Institute of Technology Delhi for the award of the degree of **DOCTOR OF PHILOSOPHY**. This is a record of bonafide research work carried out by him under my supervision and guidance. The matter presented in this thesis has not been submitted, in part or in full to any other University or Institute for the award of any degree or diploma.

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SHIVANSH MEHROTRA

Abstract

Titanium aluminide alloys have garnered significant attention as materials that offer comparable or superior high-temperature performance while substantially reducing the weight of critical jet engine components, such as low-pressure turbine blades, valves, and nozzles, which operate under extreme conditions. The aerospace sector relentlessly works to enhance the performance and efficiency of aircraft engines. These components present considerable potential for not only weight reduction but also substantial improvements in engine performance, efficiency, and long-term durability. This thesis provides a comprehensive investigation into the high-temperature oxidation behaviour and diffusion kinetics of β- and γ-based Ti-Al alloys by focusing on the role of refractory elements in modifying the microstructure, enhancing oxidation resistance, and influencing diffusion parameters.

This study begins by investigating the isothermal oxidation mechanism of pure Ti within the temperature range of 600 °C to 1200 °C, by calculating activation energies for two distinct oxide growth regimes. A quantitative growth model is developed, that yielded an activation energy of 155 kJ/mol for the stable parabolic growth regime. Marker-based experiments reveal that oxygen ions are the dominant species driving the growth of TiO_2. Based on these findings, a temperature-dependent isothermal oxidation mechanism for titanium is proposed, integrating both experimental observations and thermodynamic analyses.

Oxidation response of Group V (V, Nb and Ta) and Period V (Zr, Nb and Mo) refractory metals alloyed γ-TiAl phase has also been studied at 1000 °C in air by conducting a systematic comparison-based study where the atomic percentages of Al, Ti, and the refractory alloying element have been kept consistent across all alloys. An external oxide zone develops for all the alloys comprising of three distinctive layers: (i) innermost (Al_2O_3 dominantly) (ii) intermediate (Al_2O_3 + TiO_2) and (iii) outermost (TiO_2 + small pockets of Al_2O_3). However, tiny amounts of

refractory based oxides of Nb_2O_5, Ta_2O_5, ZrO_2 and MoO_2 also formed for the respective alloyed γ-TiAl. An internal oxide region of (Al_2O_3+Ti_3Al) developed in the case of binary γ-TiAl and Nb-alloyed, while (Ti, Zr) complex oxides had formed in the Zr alloyed γ-TiAl. Mo- and Ta-alloyed γ-TiAl produced no internal oxide layer, but segregation of Mo and Ta was observed at the alloy/oxide interface. The Group V elements had good solubility in TiO_2 and oxidation resistance of the alloys increased down the Group V in the sequence of Ta>Nb>V. While a sequence of Nb>Mo>Zr was observed for the Period V elements with no specific trend. The Ta-alloyed γ-TiAl exhibited the highest oxidation resistance because of an increase in the vacancy formation energy of oxygen in TiO_2. The oxygen vacancy formation energy of TiO_2 was concluded to be the most crucial factor governing the oxidation resistance of alloyed γ-TiAl phase compared to the valence of the alloying elements. The oxidation mechanism of the alloyed γ-TiAl has been delineated considering the oxide phase evolution and the associated thermodynamic phase stability of the respective oxides.

Based on the oxidation studies on γ-TiAl, Ta and Nb were selected as the alloying elements for high temperature oxidation studies on β-Ti(Al) alloys. The addition of Ta to β-Ti(Al) alloys was found to significantly reduce oxidation rate constants in both linear and parabolic growth regimes. Synergistic alloying of β-Ti(Al) with both Nb and Ta demonstrated highest oxidation resistance, as the (Nb+Ta)-containing alloy exhibited the lowest weight gain and slowest parabolic oxidation rate compared to alloys containing only Nb or Ta. Oxide phase evolution revealed that Ta-containing β-Ti(Al) alloys developed a multi-layered external oxide zone (EOZ), with Ta-rich TiO_2 and β-Ta_2O_5 forming in the inward region, and Ta-free TiO_2 and α-Al_2O_3 in the outward region. Additionally, these alloys exhibited the formation of α-Al_2O_3 lamellae within the internal oxide zone (IOZ) at 1200 °C, with adjacent regions transforming into Ti_3Al.

Inert marker experiments showed oxygen as the primary diffusing species in Ta-free β-Ti(Al), while for Ta-containing β-Ti(Al), oxide formation involved both oxygen and metallic ion diffusion. Presence of columnar and equiaxed TiO_2 grains forming on either sides of the β-Ta_2O_5 grains within the EOZ was observed, which again proved the participation of both oxygen and metallic ions in the oxide growth process. DFT analysis attributed the improved oxidation resistance of Ta-containing β-Ti(Al) to modifications in TiO_2 defect concentrations, where Ta increased the formation energy of oxygen vacancies and decreased titanium vacancy formation energy, thereby suppressing TiO_2 growth. Finally, a Ti-Al-Ta-O phase diagram at 1200 °C was established, and a comprehensive oxidation mechanism was proposed, integrating both experimental and computational insights.

To assess the diffusion parameters of Ti and Al in the β-phase, which are the major diffusing species during high temperature oxidation of β-Ti(Al) alloys, diffusion studies were conducted using the diffusion couple technique. An increase in interdiffusion coefficients with an increase in Al content in binary β-Ti(Al) is rationalized by a decreasing trend of activation energy for interdiffusion and an increase in driving force for diffusion. Higher activation energy of impurity diffusion coefficient of Al in β-Ti than that of self-diffusion coefficient of β-Ti may further suggest lower interaction tendency of vacancies with Al atoms in the β-Ti(Al) phase.

The effects of Ta and Nb on the diffusion kinetics of the β-Ti(Al) solid solution phase were also examined using the pseudo-binary diffusion couple technique at temperatures ranging from 950 to 1100 °C. Both β-Ti(Al, Ta) and β-Ti(Al, Nb) systems exhibited consistently higher interdiffusion coefficients compared to the binary β-Ti(Al) system. This increase is attributed to the reduced activation energy for interdiffusion and an increase in the thermodynamic factor with Al content. The decrease in activation energy is linked to higher vacancy concentrations and easier atomic migration due to the addition of Ta or Nb. A reduction in the pre-exponential factor with addition of Ta/Nb was also observed, which was attributed

to a decrease in the correlation factor. Additionally, the increased impurity diffusion coefficients of Al in β-Ti(Ta) than Ta-free β suggest a stronger interaction between vacancies and Al in the presence of Ta. Kirkendall marker experiments revealed that Ti has a higher intrinsic diffusion coefficient than Al in the β-Ti(Al, Nb) system, which was explained by Lazarus' valence model. The effect of vanadium (V) on diffusion parameters in the β-phase was also explored, revealing that V enhances interdiffusion in the β-Ti(Al) phase at 1000 °C.

सारांश

टाइटेनियम एलुमिनाइड मिश्रधातुओं ने उच्च तापमान पर उत्कृष्ट प्रदर्शन के साथ-साथ जेट इंजन के महत्वपूर्ण घटकों—जैसे कि लो-प्रेशर टरबाइन ब्लेड, वॉल्व और नोज़ल—के वज़न में उल्लेखनीय कमी लाने की उनकी क्षमता के कारण व्यापक ध्यान आकर्षित किया है। एयरोस्पेस क्षेत्र लगातार एयरक्राफ्ट इंजनों के प्रदर्शन और दक्षता को बेहतर बनाने का प्रयास करता है। ये घटक न केवल वज़न घटाने की दिशा में बल्कि इंजन की कार्यक्षमता, दक्षता और दीर्घकालिक टिकाऊपन में सुधार की संभावनाएँ भी प्रस्तुत करते हैं। यह शोध β- और γ-आधारित Ti-Al मिश्रधातुओं के उच्च तापमान पर ऑक्सीकरण व्यवहार और विसरण गतिकी की गहन जाँच प्रस्तुत करता है, विशेष रूप से रिफ्रैक्टरी तत्वों की भूमिका पर ध्यान केंद्रित करते हुए, जो सूक्ष्मसंरचना को संशोधित करते हैं, ऑक्सीकरण प्रतिरोध बढ़ाते हैं, और विसरण मापदंडों को प्रभावित करते हैं।

इस अध्ययन की शुरुआत शुद्ध टाइटेनियम की समतापी ऑक्सीकरण क्रिया की जाँच से होती है, जो 600°C से 1200°C तापमान सीमा में की गई, जिसमें दो भिन्न ऑक्साइड वृद्धि क्षेत्रों के लिए सक्रियण ऊर्जा की गणना की गई। एक मात्रात्मक वृद्धि मॉडल विकसित किया गया, जिसने स्थिर पैराबोलिक वृद्धि क्षेत्र के लिए 155 kJ/mol की सक्रियण ऊर्जा प्रदान की। मार्कर-बेस्ड प्रयोग यह दर्शाते हैं कि TiO_2 की वृद्धि में ऑक्सीजन आयन प्रमुख भूमिका निभाते हैं। इन निष्कर्षों के आधार पर, प्रयोगात्मक अवलोकनों और ऊष्मागतिकीय विश्लेषणों को एकीकृत करते हुए टाइटेनियम के लिए तापमान-निर्भर समतापी ऑक्सीकरण तंत्र प्रस्तावित किया गया।

समूह V (V, Nb, Ta) और कालक्रमानुसार V (Zr, Nb, Mo) के रिफ्रैक्टरी धातुओं से मिश्रधातुकृत γ-TiAl चरण की 1000°C पर वायु में ऑक्सीकरण प्रतिक्रिया की भी व्यवस्थित तुलनात्मक अध्ययन के माध्यम से जाँच की गई, जहाँ Al, Ti और रिफ्रैक्टरी तत्व की परमाण्विक प्रतिशतता सभी मिश्रधातुओं में समान रखी गई। सभी मिश्रधातुओं में एक बाह्य ऑक्साइड क्षेत्र विकसित हुआ जिसमें तीन विशिष्ट परतें थीं: (i) सबसे भीतरी (मुख्यतः Al_2O_3), (ii) मध्यवर्ती (Al_2O_3 + TiO_2), और (iii) बाह्यतम (TiO_2 + अल्प मात्रा में Al_2O_3)। साथ ही Nb_2O_5, Ta_2O_5, ZrO_2 और MoO_2 जैसे रिफ्रैक्टरी तत्वों के ऑक्साइड भी संबंधित मिश्रधातुओं में कम मात्रा में बने। γ-TiAl और Nb-मिश्रित मामलों में (Al_2O_3 + Ti_3Al) का आंतरिक ऑक्साइड क्षेत्र विकसित हुआ, जबकि Zr-मिश्रधातु में (Ti, Zr) जटिल ऑक्साइड बने। Mo और Ta मिश्रित γ-TiAl में कोई आंतरिक ऑक्साइड परत नहीं बनी, परंतु मिश्रधातु/ऑक्साइड इंटरफेस पर Mo और Ta के पृथक्करण (segregation) का अवलोकन किया गया।

Group V तत्वों की TiO_2 में अच्छी घुलनशीलता पाई गई और ऑक्सीकरण प्रतिरोध Ta>Nb>V के क्रम में बढ़ता गया। जबकि Period V तत्वों के लिए Nb>Mo>Zr का क्रम प्राप्त हुआ, पर कोई विशिष्ट प्रवृत्ति

नहीं पाई गई। Ta-मिश्रित γ-TiAl ने सर्वोच्च ऑक्सीकरण प्रतिरोध प्रदर्शित किया, जो TiO_2 में ऑक्सीजन रिक्तियों की निर्माण ऊर्जा में वृद्धि के कारण था। यह निष्कर्ष निकाला गया कि मिश्रधातुकृत γ-TiAl चरण के ऑक्सीकरण प्रतिरोध को नियंत्रित करने वाला सबसे महत्वपूर्ण कारक TiO_2 की ऑक्सीजन रिक्तियों की निर्माण ऊर्जा है, न कि मिश्रधातु तत्वों का संयोजक मान (valence)। मिश्रधातुकृत γ-TiAl के ऑक्सीकरण तंत्र को ऑक्साइड चरणों के विकास और संबंधित ऊष्मागतिकीय स्थिरता के आधार पर स्पष्ट किया गया।

γ-TiAl पर आधारित इन ऑक्सीकरण अध्ययनों के आधार पर Ta और Nb को उच्च तापमान ऑक्सीकरण अध्ययन के लिए β-Ti(Al) मिश्रधातुओं में मिश्रधातु तत्व के रूप में चुना गया। β-Ti(Al) मिश्रधातुओं में Ta की उपस्थिति ने दोनों—रेखीय और पैराबोलिक—वृद्धि क्षेत्रों में ऑक्सीकरण दर स्थिरांकों को काफी हद तक घटा दिया। Nb और Ta दोनों के सम्मिलन से प्राप्त β-Ti(Al) मिश्रधातु ने सर्वोच्च ऑक्सीकरण प्रतिरोध प्रदर्शित किया, क्योंकि (Nb+Ta) युक्त मिश्रधातु में वज़न वृद्धि सबसे कम और पैराबोलिक ऑक्सीकरण दर सबसे धीमी रही। ऑक्साइड चरणों के विकास से यह ज्ञात हुआ कि Ta युक्त β-Ti(Al) मिश्रधातुओं ने एक बहु-स्तरीय बाह्य ऑक्साइड क्षेत्र (EOZ) विकसित किया, जिसमें अंदरूनी भाग में Ta-समृद्ध TiO_2 और β-Ta_2O_5 और बाहरी भाग में Ta-रहित TiO_2 और α-Al_2O_3 बने। इसके अतिरिक्त, इन मिश्रधातुओं में 1200°C पर आंतरिक ऑक्साइड क्षेत्र (IOZ) के भीतर α-Al_2O_3 लैमेलों का निर्माण हुआ, जिनके आस-पास के क्षेत्र Ti_3Al में परिवर्तित हो गए।

इनर्ट मार्कर प्रयोगों से यह ज्ञात हुआ कि Ta-रहित β-Ti(Al) में ऑक्सीजन प्रमुख विसरण प्रजाति है, जबकि Ta-युक्त β-Ti(Al) में ऑक्साइड निर्माण में ऑक्सीजन और धात्विक आयनों दोनों का योगदान रहा। EOZ के भीतर β-Ta_2O_5 अनाजों के दोनों ओर बनने वाले columnar और equiaxed TiO_2 अनाजों ने एक बार फिर यह प्रमाणित किया कि ऑक्साइड वृद्धि में ऑक्सीजन और धातु आयनों दोनों की भागीदारी है। DFT विश्लेषण से यह पाया गया कि Ta-युक्त β-Ti(Al) मिश्रधातु में TiO_2 दोष सांद्रता में परिवर्तन के कारण ऑक्सीकरण प्रतिरोध बेहतर हुआ; जिसमें Ta ने ऑक्सीजन रिक्तियों की निर्माण ऊर्जा को बढ़ाया और टाइटेनियम रिक्तियों की ऊर्जा को घटाया, जिससे TiO_2 की वृद्धि दब गई। अंततः, 1200°C पर एक Ti-Al-Ta-O चरण आरेख (phase diagram) स्थापित किया गया और एक समग्र ऑक्सीकरण तंत्र प्रस्तावित किया गया, जिसमें प्रयोगात्मक और संगणनात्मक (computational) अंतर्दृष्टियों का समावेश है।

β-चरण में Ti और Al की विसरण विशेषताओं का मूल्यांकन करने के लिए, जो β-Ti(Al) मिश्रधातुओं के उच्च तापमान पर ऑक्सीकरण के दौरान प्रमुख विसरण प्रजातियाँ हैं, विसरण युग्म (diffusion couple) तकनीक का प्रयोग किया गया। द्विघटक β-Ti(Al) में Al की मात्रा बढ़ने पर इंटरडिफ्यूजन गुणांक में वृद्धि को सक्रियण ऊर्जा में गिरावट और विसरण प्रेरक बल (driving force) में वृद्धि के माध्यम से व्याख्यायित किया

गया। β-Ti में Al का अशुद्धता विसरण गुणांक, β-Ti के स्वयं विसरण गुणांक से अधिक होने के कारण यह संकेत मिलता है कि β-Ti(Al) में रिक्तियों की Al परमाणुओं से कम पारस्परिक क्रिया होती है।

Ta और Nb का प्रभाव भी β-Ti(Al) ठोस विलयन चरण की विसरण गतिकी पर 950°C से 1100°C तक तापमान पर स्यूडो-बाइनरी विसरण युग्म तकनीक से जाँचा गया। β-Ti(Al, Ta) और β-Ti(Al, Nb) दोनों प्रणालियों में द्विघटक β-Ti(Al) की तुलना में इंटरडिफ्यूजन गुणांक अधिक रहा। यह वृद्धि सक्रियण ऊर्जा में कमी और Al सामग्री के साथ ऊष्मागतिकीय कारक (thermodynamic factor) में वृद्धि के कारण हुई। सक्रियण ऊर्जा की कमी उच्च रिक्ति सांद्रता और Ta या Nb की उपस्थिति में परमाणुओं की आसान गतिशीलता से जुड़ी थी। साथ ही, Ta/Nb के सम्मिलन से पूर्व-घातांकी गुणांक (pre-exponential factor) में कमी भी देखी गई, जिसे सहसंबंध कारक (correlation factor) में गिरावट से जोड़ा गया। इसके अतिरिक्त, Ta-युक्त β-Ti(Al) में Al के अशुद्धता विसरण गुणांक में वृद्धि दर्शाती है कि रिक्तियों और Al के बीच अधिक मजबूत पारस्परिक क्रिया होती है। किर्केंडॉल मार्कर प्रयोगों से यह स्पष्ट हुआ कि β-Ti(Al, Nb) प्रणाली में Ti का अंतर्निहित विसरण गुणांक Al की तुलना में अधिक है, जिसे लाजारस के संयोजक मॉडल (Lazarus' valence model) द्वारा समझाया गया। β-चरण में V के प्रभाव का भी अध्ययन किया गया, जिससे यह पता चला कि V, 1000°C पर β-Ti(Al) चरण में इंटरडिफ्यूजन को बढ़ावा देता है।

Chapter-wise summary

Chapter 1 gives a brief review of the importance of titanium aluminide alloys as an alternative to superalloys in aerospace industry and the role of refractory alloying elements (V, Nb, Ta, Zr, and Mo) in enhancing oxidation resistance of β-Ti(Al) and γ-TiAl alloys, while emphasizing the need for a systematic study to understand their role.

Chapter 2 articulates the motivation and objectives of the research work. The study aims to systematically investigate the effects of Group V and Period V refractory elements on the high temperature oxidation behaviours and diffusion kinetics of β-Ti(Al) and γ-TiAl alloys, focusing on the oxide phase evolution and the mechanisms of oxide growth. Ultimately, the goal of the research is to identify effective alloying elements amongst the Group V and Period V refractory elements that improve oxidation resistance and understand their influence on atomic mobility. The research aims to investigate the effects of specific refractory elements on oxidation mechanisms and diffusion kinetics in β-Ti(Al) and γ-TiAl alloys, focusing on phase evolution during high-temperature exposure.

Chapter 3 details the experimental approach used in this study. The text outlines a series of experimental studies aimed at understanding high-temperature oxidation and diffusion behaviours of the γ and β alloys. The study employs Thermogravimetric Analyzer (TGA) and calibrated muffle furnace techniques to investigate oxidation responses, while alloy compositions are strictly controlled for comparative analysis. The alloys are prepared through vacuum arc melting, followed by homogenization, and subjected to isothermal oxidation experiments at various temperatures. In addition to oxidation studies, pseudo-binary diffusion couple experiments are conducted on β-phase alloys, and various characterization techniques, including X-ray diffraction and electron microscopy, are utilized to analyze the oxide phases formed during oxidation. Density functional theory (DFT) calculations using Vienna Ab initio

Simulation Package (VASP) provide atomistic insights into the role of Ta in oxidation resistance.

Chapter 4 discusses the results of the isothermal oxidation of pure titanium at temperatures ranging from 600 °C to 1200 °C to understand the kinetics and transport behaviour of titanium and oxygen in the oxide phases. Through various experimental techniques, including XRD and SEM, the study establishes the formation of rutile as the predominant oxide phase and explores the mechanisms of oxidation, including the interface-controlled linear and diffusion-controlled parabolic growth regimes of the oxide layer. The findings indicate that oxygen plays a dominant role in the growth of the oxide layer, with significant implications for the performance and longevity of titanium-based components in high-temperature environments.

Chapter 5 investigates the effects of various refractory elements on the oxidation behaviour of γ-TiAl. The study focuses on the high-temperature oxidation response of γ-TiAl alloys that are alloyed with several refractory elements from Group V and Period V of the periodic table, including Vanadium (V), Niobium (Nb), Tantalum (Ta), and others. Experimental techniques such as XRD and FE-SEM are employed to analyze the microstructures and phase compositions of the alloys before and after oxidation. The oxidation kinetics are assessed through TGA at 1000 °C, revealing that the addition of different alloying elements influences the weight gain and oxidation resistance of the alloys. The research identifies the formation of oxide phases such as TiO_2 and Al_2O_3, impacting the overall oxidation kinetics. The study concludes that Ta provides the highest oxidation resistance, followed by Nb, while V and Zr are detrimental to oxidation resistance. The research highlights that the valence of alloying elements plays a crucial role in determining the vacancy formation energy, which is a key factor in the oxidation kinetics.

Chapter 6 investigates the impact of alloying elements, specifically tantalum (Ta) and niobium (Nb), on the high-temperature oxidation resistance of β-Ti(Al) alloys. The incorporation of Ta and Nb into β-Ti(Al) alloys significantly enhances their oxidation resistance. The study shows that increasing Ta content reduces oxidation rates effectively, as weight gain during oxidation decreases. This highlights the critical role of alloying elements in developing materials with improved high-temperature stability. The oxidation of β-Ti(Al) alloys leads to the formation of a distinct oxide phase structure, including TiO_2 and α-Al_2O_3. The study shows that in Ta-containing alloys, the internal oxide zone (IOZ) evolves differently compared to Ta-free alloys, with the presence of Ta promoting the formation of β-Ta_2O_5. This showcases how alloy composition influences oxide phase characteristics. The study quantifies oxidation rate constants for various alloys, revealing that the addition of Ta reduces both the linear and parabolic oxidation rate constants. This correlation provides valuable data for predicting the service life and performance of alloys in high-temperature applications. By correlating experimental results with DFT analysis, the study elucidates the defect chemistry governing oxidation processes. It demonstrates that the formation energy of oxygen vacancies is altered by the presence of Ta, suggesting that alloying strategies can be optimized to enhance oxidation resistance through targeted defect engineering. This chapter contributes to a deeper understanding of the oxidation mechanisms in β-Ti(Al) alloys and underscores the importance of alloying strategies in developing materials for high-temperature applications. Future research can build on these findings to explore additional alloying elements or composite structures that may further enhance the performance of these materials in demanding environments.

Chapter 7 provides a comprehensive exploration of the interdiffusion behaviour in β-Ti(Al) solid solution phases, utilizing advanced techniques and significant analytical frameworks. The insights gained from this study are invaluable for advancing the understanding of Ti-Al alloy

systems, particularly in high-temperature contexts where diffusion plays a critical role in determining material performance. Key findings include the linear increase of interdiffusion coefficients with Al content, variations in activation energy, and the role of vacancies in influencing diffusion behaviour. The implications of this research extend beyond theoretical understanding, offering practical pathways for optimizing material properties in various engineering applications.

Chapter 8 discusses the influence of refractory elements, particularly Niobium (Nb) and Tantalum (Ta), on the diffusion kinetics of β-Ti(Al) alloys. It highlights the importance of understanding how these elements affect the diffusion behaviour of the β-Ti(Al) system, especially during high-temperature service conditions. A pseudo-binary diffusion couple approach is employed to quantitatively analyze the diffusion kinetics of these alloys. The results show that the presence of Nb and Ta enhances the oxidation resistance and increases interdiffusion coefficients compared to the binary Ti-Al system. Additionally, the chapter examines the effects of Vanadium (V) on diffusion and provides insights into how the atomic size and lattice distortion of these elements contribute to changes in diffusion behaviour. The chapter provides a comprehensive analysis of the effects of Nb and Ta on the diffusion kinetics of β-Ti(Al) alloys, highlighting their potential in enhancing material performance under high-temperature conditions. The insights gained from this study could pave the way for the development of advanced titanium alloys with improved mechanical properties and resistance to oxidation.

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List of Abbreviations

BCC	Body-Centered Cubic
HCP	Hexagonal Close-Packed
XRD	X-ray Diffraction
TGA	Thermogravimetric Analysis
DFT	Density Functional Theory
EPMA	Electron Probe Microanalyzer
WDS	Wavelength Dispersive Spectroscopy
EDS	Energy Dispersive Spectroscopy
FE-SEM	Field Emission Scanning Electron Microscope
EBSD	Electron Backscatter Diffraction
BSE	Backscattered Electron
XPS	X-ray Photoelectron Spectroscopy
UPS	Ultraviolet Photoelectron Spectroscopy
UHV	Ultra-High Vacuum
IDZ	Interdiffusion Zone
IOZ	Internal Oxide Zone
EOZ	External Oxide Zone
PB	Pseudo-Binary (Diffusion Couple method)
VAM	Vacuum Arc Melting
TIG	Tungsten Inert Gas
CALPHAD	Calculation of Phase Diagrams
k_p	Parabolic Rate Constant
Φ	Thermodynamic Factor
BE	Binding Energy
Φ_{SA}	Work Function of the Sample
JCPDS	Joint Committee on Powder Diffraction Standards