



Analyzing Thermodynamic Modeling and Phase Stability in Ultra-High-Temperature Ceramics for Space Exploration: A Review

Hayder Abdulhasan Lafta¹, Mustafa M. Mansour^{2*}, Alaa M. Lafta³

Department of Mechanical Engineering, College of Engineering, University of Thi-Qar, Thi-Qar 64001, Iraq

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ABSTRACT

This review aims to comprehensively evaluate the thermodynamic properties and phase stability of ultra-high-temperature ceramics (UHTCs) using the CALPHAD (CALculation of PHase Diagrams) approach. UHTCs exhibit exceptional properties, including high melting points, superior hardness, and thermal shock resistance, making them promising materials for aerospace applications and high-temperature scientific instrumentation. The study focuses on phase equilibria in binary systems, including Zr–B, Hf–B, Ta–B, Mo–B, Zr–C, Hf–C, Ta–C, and Mo–C, as well as multicomponent Zr–Hf–(Ta,Mo)–C systems. Despite their technological importance, comprehensive thermodynamic assessments remain limited, particularly due to insufficient experimental data and incomplete coverage in existing thermodynamic databases. The primary objective is to assess thermodynamic properties, including Gibbs energy of formation, enthalpy of formation, heat capacity, and phase stability, through computational thermodynamic modeling. The CALPHAD methodology is employed to calculate component activities, construct phase diagrams, and map phase equilibria across different compositions and temperatures. Temperature-dependent Gibbs energy functions are used to predict equilibrium phase relationships, phase transformations, and critical equilibrium points. The analysis integrates available experimental information with computational models to establish consistent thermodynamic descriptions of relevant ceramic systems. Furthermore, the review identifies knowledge gaps and highlights the need for additional experimental investigations to improve thermodynamic databases and validate predicted phase equilibria. Ultimately, this assessment provides a theoretical foundation for optimizing UHTC compositions, understanding high-temperature phase behavior, and supporting the development of advanced ceramic materials with enhanced thermal and mechanical performance for extreme operating environments, particularly in aerospace engineering..

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1. INTRODUCTION

Thermodynamic fundamentals of ultra-high-temperature materials are essential for analyzing and understanding different systems, such as metal-carbon systems, and are fundamental for developing hypersonic vehicles and rocket engines. In hypersonic aerodynamics, the main requirement in materials science is to build a thermal-absorbing tip that can withstand high temperatures and thermomechanical loads. Researchers expect materials to perform in an ultra-high temperature environment of above 3000 K. Most of the high melting point materials are carbides, borides, and nitrides of transition metals, such as zirconium (Zr), hafnium (Hf), niobium (Nb), tantalum (Ta), vanadium (V), and tungsten (W). These materials exhibit exceptional oxidation resistance compared with conventional refractory alloys. For example, ZrB₂–SiC and HfB₂–SiC composites can maintain structural integrity at temperatures exceeding 2000–2200°C through the formation of protective oxide layers

*Corresponding Author

Email: mustafa.muhammedali@utq.edu.iq

consisting primarily of SiO_2 , ZrO_2 , and HfO_2 . In contrast, conventional nickel-based superalloys typically experience severe oxidation and degradation above approximately 1100–1200°C. The oxidation rates of UHTCs are therefore significantly lower under extreme aerospace thermal environments, making them attractive candidates for thermal protection systems and hypersonic vehicle applications. The exceptional properties of hafnium carbide (HfC) and tantalum carbide (TaC) have motivated extensive molecular dynamics (MD) investigations. These simulations have been employed to evaluate atomic-scale diffusion mechanisms, thermal stability, melting behavior, defect evolution, thermal conductivity, and mechanical responses under extreme temperature conditions. Such studies provide valuable insight into the behavior of UHTCs in environments relevant to hypersonic flight and atmospheric re-entry applications [1]. In material research and engineering, temperature is an essential thermodynamic parameter determining its physical and chemical properties. Thermodynamic properties and phase diagrams of materials are essential and serve as the foundation for exploring new ultra-high-temperature materials for space exploration [2]. For the early phase of material research and development (R&D), a thermodynamic equilibrium condition can be considered by knowing and analyzing thermodynamic quantities such as change of enthalpy (ΔH), Gibbs free energy (ΔG), and entropy (ΔS), which determine the phase stability or instability of materials [3]. Thermodynamic modeling is fundamentally based on the minimization of Gibbs free energy (G), which determines the equilibrium state of a system. Here, H represents enthalpy, T is the absolute temperature, and S denotes entropy ($G=H-TS$). At equilibrium, the stable phase assemblage corresponds to the minimum Gibbs free energy under specified temperature, pressure, and composition conditions. In engineering, the phase diagram allows one to determine the state of the material with a specific change in composition and temperature. A proposition of the phase diagram and thermodynamic modeling of carbide ultra-high-temperature ceramics like zirconium is fundamental for several fields. To this end, this study reviews the thermodynamic modeling and analysis of phase stability of ultra-high-temperature ceramics and carbides.

2. BACKGROUND AND SIGNIFICANCE

Over the years, a good amount of research has been done on understanding phase diagrams, thermo-physical properties, reactions, and the limitations of refractory materials, particularly ultra-high-temperature ceramics. These materials are the best choice for thermal protection of spacecraft re-entry into the Earth's atmosphere. Our understanding of computational thermodynamics has also evolved from calculations of only the activity of stable or solid solutions for zircon or pyrochlore, perovskite, etc.) to the understanding of the occurrence of multiple stable primary phases, such as the Laves phase of Zr_2Ti in ZrO_2 at lower temperatures or Hf_2Zr in HfO_2 at higher temperatures, or other ceramic phases at higher temperatures. The number of these primary stable phases increases with the variation of composition [4]. The annual number of published papers (Scopus data) on Ultra-High-Temperature Ceramics from 2010 to 2024, is illustrated in Figure 1. General workflow of CALPHAD-based thermodynamic modeling for ultra-high-temperature ceramics, illustrating the integration of experimental thermodynamic data, Gibbs-energy optimization, Integrated framework showing the complementary roles of first-principles calculations, CALPHAD thermodynamics, and experimental validation in predicting phase stability and qualifying UHTCs for aerospace applications phase-diagram

Integrated Thermodynamic Modeling Framework for UHTCs, Thermodynamic strategy for predicting equilibrium phases and evaluating oxidation resistance and mechanical stability of ultra-high-temperature ceramics under extreme aerospace environments

Understanding the role of the other oxides in these systems is also vital. For instance, the role of ThO_2 in stabilizing the pyrochlore structure in the $\text{ZrO}_2\text{-Y}_2\text{O}_3$ and the $\text{HfO}_2\text{-Y}_2\text{O}_3$ systems at lower temperatures (below 2345-2415 K), and in stabilizing the fluorite structure at still lower temperatures (below 1573 K) [5]. Furthermore, it is also realized that though the liquid phase can call the shots inside the materials in terms of inducing super-/i-liquidity, which is not larger compared to the solidus temperature of the eutectic, it may not always be the L/E equilibrium, and often could be L/S or S/L, or L-discontinuous reaction. Except for SiC, as shown Figure 1, ultra-high-temperature ceramics are almost in shambles today [6]. Low-density SiC foams, generally doped with B₄C or AlB₁₂, have been explored for thermal insulation, low cost, high radiative effusivity, and survivability in thermal protection systems.

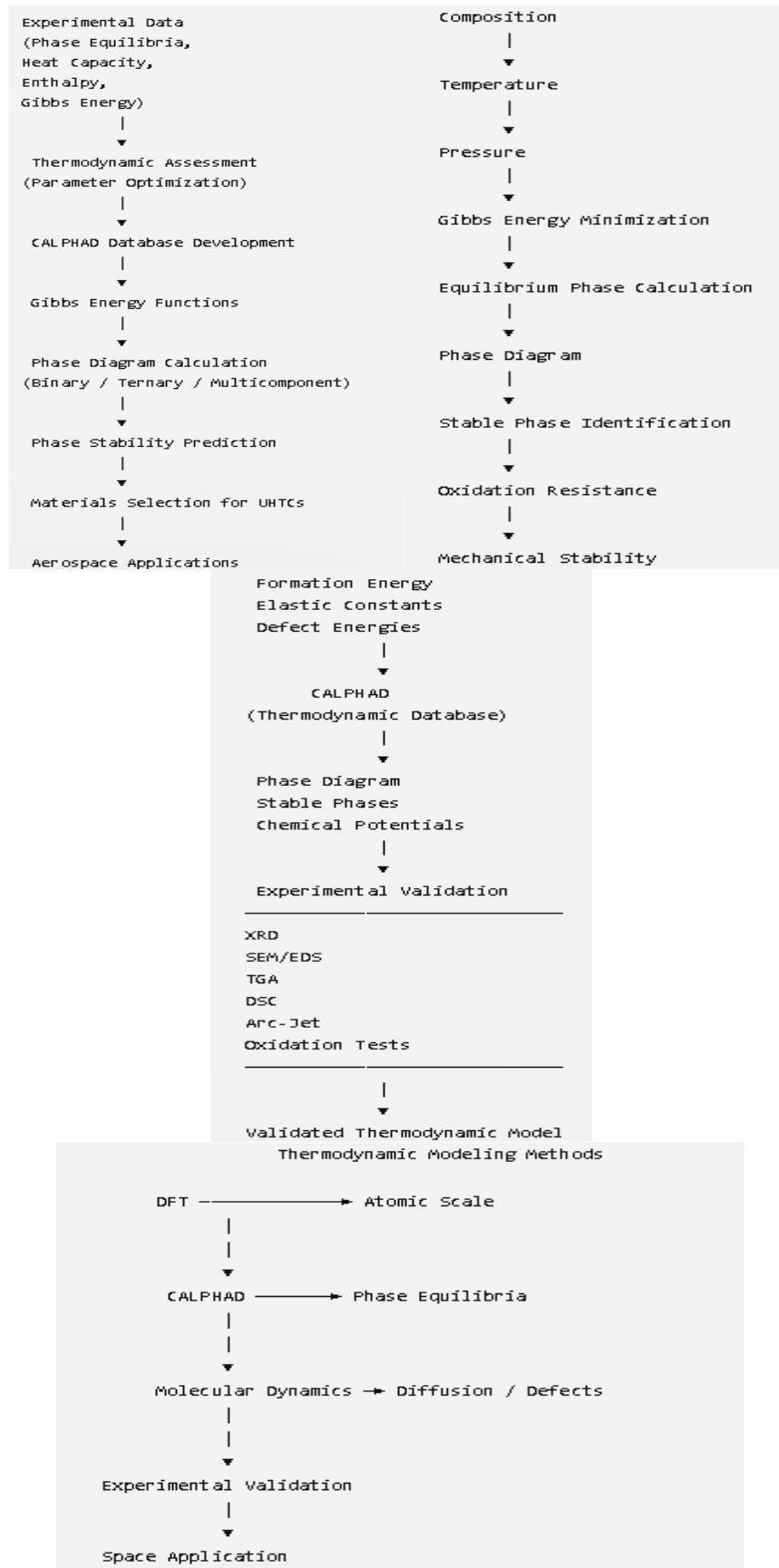


Figure 1. CALPHAD-Based Thermodynamic Modeling Workflow

Figure 2. Keywords Network Visualization Based on Web of Science Database

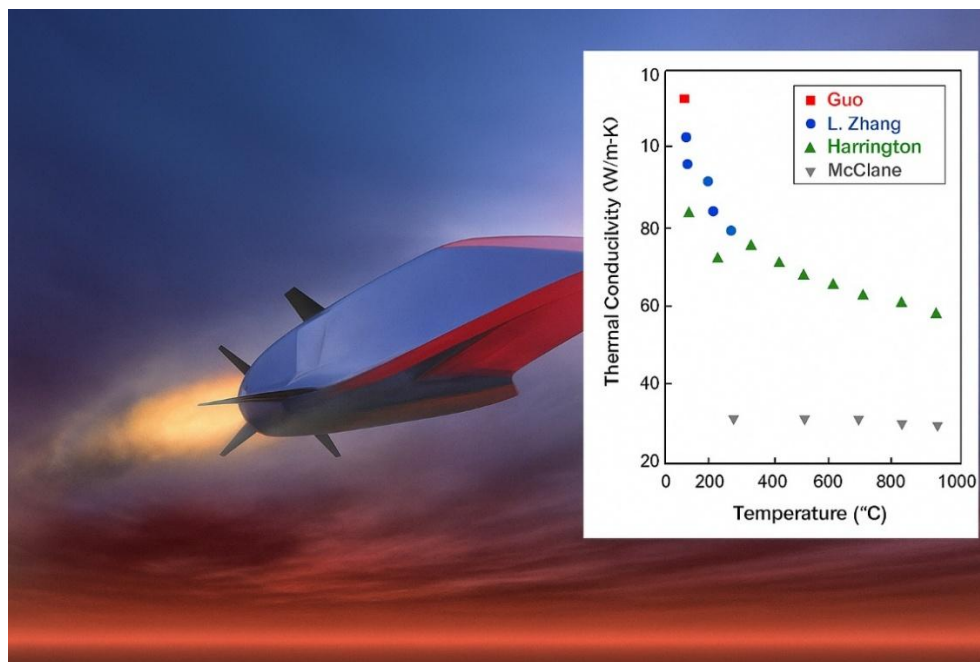


Figure 3. Ultra-High Temperature Ceramics: Materials for Extreme Environments [6]

3. BASIC PRINCIPLES OF THERMODYNAMIC MODELING

The degree of similarity between a set of atoms and an ideal crystal structure for an element or compound is a robust indicator of phase stability. In an ideal world, our models and computer simulations could calculate this 'driving force' for metastability and give us a direct, quantitative estimate of phase equilibrium [7].

The driving force for phase transformation is commonly defined as the difference in Gibbs free energy between competing phases. A phase transformation becomes thermodynamically favorable when the Gibbs free energy of the product phase is lower than that of the parent phase. In UHTCs, temperature, pressure, composition, and defect concentration significantly influence the magnitude of this driving force and therefore determine phase stability and transformation behavior. [8].

The change in these parameters with composition, the so-called mixing enthalpy (ΔH_{MIX}) and molar volume (ΔV_{MIX}) of mixing, can be modeled in several ways, the most basic of which uses the regular solution model for the Gibbs free energy, standard deviations, 'site fractions' and the concept of randomness from deletion-insertion of atoms or order-to-disorder transitions.

To begin with, Figure 2 generalizes this function to multi-component UNC ceramics. For these 'virtual' elements, the formation enthalpy $\Delta f_{SM} T$, with respect to TMO at $P_g = 0$ bar, is a function of GR+SR absorption. Isotropic polymers have been calculated with excellent results; the deviations are mostly less than 2% [9].

As shown in Figure 4, the annual number of publications related to UHTCs increased substantially between 2010 and 2024. The growth trend reflects increasing research interest driven by aerospace applications, hypersonic technologies, and advanced thermal protection systems. The sharp increase observed after 2018 also highlights the emergence of high-entropy ceramics and computational thermodynamics as active research directions.

4. THERMODYNAMIC DATABASES AND SOFTWARE TOOLS

Thermodynamic databases are datasets representing the Gibbs free energy of systems at various composition-temperature-pressure conditions. These databases are used by several software tools that can calculate equilibrium compositions for different systems, either standalone or in equilibrium with other phases, and are a necessary first step for combining them with diffusion mobility databases. Several databases have been developed and optimized for different material systems such as elements, binary, ternary, quaternary, and internal oxidation. At most, these include unary (single element), binary (2 elemental systems), and ternary (three element systems) [10]. The accuracy of these databases is benchmarked using calculated and acceptable experimental data to determine the effectiveness and applicability of the model. As such, researchers can only calculate a finite number of systems of importance. Several thermodynamic databases are widely used for CALPHAD-based modeling of advanced ceramic systems.

These include the Thermo-Calc TCS databases, FactSage FToxid and FTmisc databases, Pandat PanEngine databases, SGTE thermodynamic databases, and NIST-JANAF thermochemical datasets. These resources provide thermodynamic descriptions of phases and enable accurate prediction of phase equilibria, phase transformations, and oxidation behavior in UHTC systems. Many pieces of software are capable of utilizing these databases, and several studies are benchmarking code relative to one another. However, releasing quality databases and software tools that facilitate the construction of custom and compatible databases can significantly aid thermodynamic modeling worldwide [11].

Thermodynamic databases and computation tools have become standard software throughout materials science and technology applications, working with significantly more phases than those of interest to the space community. However, special purpose-built tools and databases for UHTC-Tr systems and supporting systems will increase the accuracy and efficiency of modeling used to inform and accelerate experiments and ultimately qualify critical components that achieve planetary entry and return.

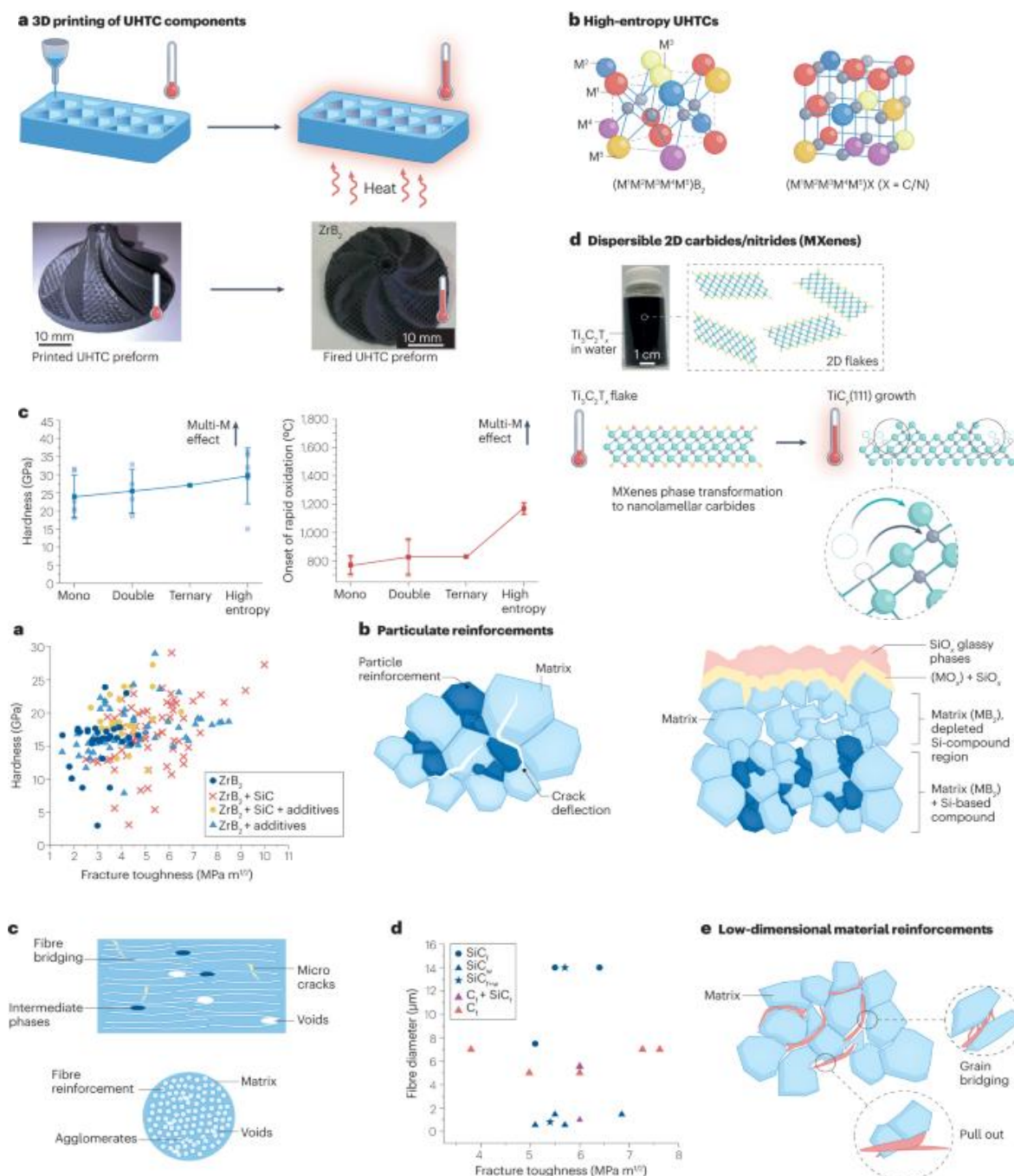


Figure 4. Ultra-High Temperature Ceramics: Materials for Extreme Environments [9]

5. APPLICATIONS OF THERMODYNAMIC MODELING IN MATERIALS SCIENCE

The field of application of thermodynamic modeling in materials science ranges from the study of equilibrium, metastable, and non-equilibrium phenomena in materials, for the synthesis of new materials or designing a substitute for conventional materials, to aiding the development of technologies, etc [12]. This versatile and vivid behavior of materials is represented by their phase stability calculations, which depict the different phases of the materials existing under a relatively wide range of temperatures, pressures, and concentrations of an element in a system in an equilibrium state. In metallurgy, the center of interest lies in understanding the phase transformations occurring during recrystallization, grain growth of materials, and the corresponding changes in mechanical, electrical, and magnetic properties. In materials science, these kinds of phase separations explain the tendency to synthesize materials through different routes [13].

In oxide ceramics applications, with increasing temperatures or space applications, these ceramics can be transformed from one phase to another with the change in concentrations of various elements under wide temperature ranges. Also, "isentropic plot (spall strength of materials like metals as a function of sound velocity and shock wave velocity) indicates the equivalent variability of ceramics with that of metals at higher temperatures" [14]. In designing advanced materials like metal matrix composites (MMC's), where the ceramic property (i.e., point defects, divacancy layer states) is influenced by the addition of non-metallic elements like nitrogen (N), the thermodynamic modeling also helps in predicting the phase formation, chemical composition, and thermal behavior of the N-type MMC's. The thermodynamic model results practically demonstrate the above-mentioned applications [15].

Tabel 1. Application

Application Area	Role of Thermodynamic Modeling	Importance of Phase Stability	Example Materials	Benefits
Thermal Protection Systems (TPS)	Predict heat flux, oxidation resistance at reentry conditions	Ensures materials maintain structure at >2000°C [16]	ZrB ₂ , HfB ₂ with SiC additives	Reduced ablation, increased lifetime, reliable atmospheric reentry
Rocket Nozzles and Thrusters	Evaluate phase behavior under rapid heating and cooling	Avoids phase transformation and degradation under fluctuating temperatures [17]	HfC, TaC, ZrC	High erosion resistance, thermal shock protection
Hypersonic Vehicles Leading Edges	Model temperature gradients and phase diagrams for steady flight	Prevents structural failure under prolonged heating [18]	ZrB ₂ -SiC, HfB ₂ -SiC composites	Maintains aerodynamic integrity, reduces thermal damage
Aeroshells for Planetary Entry	Design optimal composition for minimal oxidation and thermal stress	Avoids formation of porous or unstable oxides	UHTC matrix with oxide-dispersed phases	Better thermal barrier efficiency, low mass loss
Nuclear-Powered Spacecraft Shields	Simulate neutron-induced phase changes	Maintains mechanical integrity under radiation [19]	Carbide-rich UHTCs (e.g., TaC-ZrC)	Enhanced durability, radiation shielding
Satellite Components (e.g., thruster walls)	Predict long-term stability in vacuum and orbital heating	Avoids sublimation or decomposition	HfN, ZrN coatings	Minimal mass loss, consistent performance
Additive Manufacturing of UHTC parts	Helps select sintering conditions and stable compositions	Prevents cracking or unwanted phase segregation	UHTC-based powders with dopants	Enables complex shapes, tailored properties

6. PHASE STABILITY IN UHTCs

Ultra-high-temperature ceramics (UHTCs) are generally exposed to extreme external conditions such as high temperatures and reduced pressure. Their exposure to the space environment can lead to oxidation due to plasma or atmospheric interactions, ultimately resulting in thin, dense oxide scales. Mechanical behavior, is mainly an interest for in-space applications. High-temperature mechanical behavior is dominated by different microstructural states. The phase stability at high temperatures controls their microstructural development. At low temperatures, the materials can have metastable, essentially strain-free phases [20]. With increasing temperature or longer annealing times, the UHTCs tend towards their thermodynamically stable phase. A first-order transition depends on both the driving stress needed for developing the phases and the mechanism length scale and kinetics. Table 1 highlights the broad applicability of thermodynamic modeling across aerospace-related UHTC systems. A common feature among these applications is the need to maintain phase stability and oxidation resistance under extreme thermal environments. For example, ZrB₂-SiC and HfB₂-SiC composites benefit from thermodynamic predictions of oxide-layer formation, whereas carbide-based systems such as HfC

and TaC rely on phase stability calculations to minimize material degradation at ultra-high temperatures. These examples demonstrate that thermodynamic modeling is not only a theoretical tool but also a practical framework for materials selection and design in aerospace engineering.

The temperature where this transition occurs increases with dimension, and the configurational entropy at the transition, often denoted Kelvin temperature, can be written as follows: $T_0 = \Delta H_v / \Delta A$. Here, ΔH_v is the molar volume of transformation, and ΔA represents the Gibbs free energy difference between the transformed and parent phase per degree of freedom [21]. At larger temperatures than T_0 , the materials only consist of the most stable phase. The ultimate stable phase due to phase transitions and low driving stress indicates that the phase thermodynamically can coexist at higher temperatures. The high-temperature phase stability is determined by the temperature, pressure, and component concentration at high temperatures.

Tabel 2 (a). Methodology in UHTC Research

Methodology	Purpose	Tools/Techniques	Applications in UHTC Research
CALPHAD Modeling	Thermodynamic database development, phase diagram prediction [22]	Thermo-Calc, Pandat, FactSage	Predicts stable phases, phase equilibria, oxidation resistance
First-Principles Calculations (DFT)	Atomic-level phase stability, enthalpy of formation [23]	VASP, Quantum ESPRESSO, CASTEP	Evaluates phase transformation, defect behavior, bond strength
Experimental Thermogravimetric Analysis (TGA)	Oxidation kinetics, weight change with temperature	TGA instruments under oxygen/vacuum atmospheres	Determines oxidation onset, mass loss rate, stability temps
Differential Scanning Calorimetry (DSC)	Measures phase transformation temperatures and enthalpy [24]	DSC devices with high-temperature range	Identifies melting, solidification, and phase change points
X-ray Diffraction (XRD)	Identifies phases present after heat treatments [25]	Powder XRD, synchrotron radiation	Confirms predicted phases from CALPHAD/DFT
Scanning Electron Microscopy (SEM/EDS)	Microstructure and elemental distribution after oxidation [26]	SEM + Energy-dispersive X-ray spectroscopy (EDS)	Examines oxidation layers and diffusion mechanisms
High-Temperature Oxidation Testing	Simulates environmental conditions (reentry, hypersonic flow)	Tube furnaces with controlled atmospheres (O ₂ , vacuum, etc.)	Validates performance predictions from models
Ablation Testing	Determines material loss rate under plasma/high heat flux	Arc-jet testing, plasma wind tunnel	Evaluates TPS suitability, verifies modeling predictions
Phase Field Modeling	Predicts microstructural evolution during phase transitions	COMSOL Multiphysics, OpenPhase	Simulates grain growth, diffusion, and interfacial reactions
Finite Element Analysis (FEA)	Thermo-mechanical response modeling under stress	ANSYS, Abaqus	Predicts cracking, delamination, and mechanical failure during use

7. EXPERIMENTAL TECHNIQUES FOR STUDYING PHASE STABILITY

The phase and chemical stabilities of UHTCs are of critical importance for engineering applications such as aerospace and nuclear. As mentioned in the previous section, thermodynamic modeling can predict the phase stability and liquid formation during processing or high temperature exposure. The predicted phase stability must be validated using phase stability experiments to ensure the accuracy of the modeling. Numerous research papers have been written on phase stability. However, the precise thermodynamic quality and comparison between these experiments utilizing diverse modeling methods are rare [27]. Knowing the phase stability results are crucial in accurately predicting the performance and lifetime of UHTC materials. This section reviews various experimental techniques used to measure phase stability for UHTCs.

There are numerous experimental techniques to study phase stability. All techniques occurred under vacuum and at temperatures ranging from approximately 500 °C to 4000 °C, encompassing the melting points of UHTC materials. High-temperature/high-vacuum mechanical testing is a common approach for performing difficult experiments at high temperatures and vacuums [28]. For example, diffusion couple measurement is employed to investigate phase stability under temperature and pressure and acute pressure gradients using material samples. These high-temperature/high-vacuum tests are typically conducted in induction, arc, and electron beam furnaces. High-temperature/high-vacuum testing apparatuses have a variety of operations [29]. The apparatus used for thermogravimetry, X-ray, and optical measurements (including liquid or vapor production) provided more in-depth research into phase stability than the other apparatus.

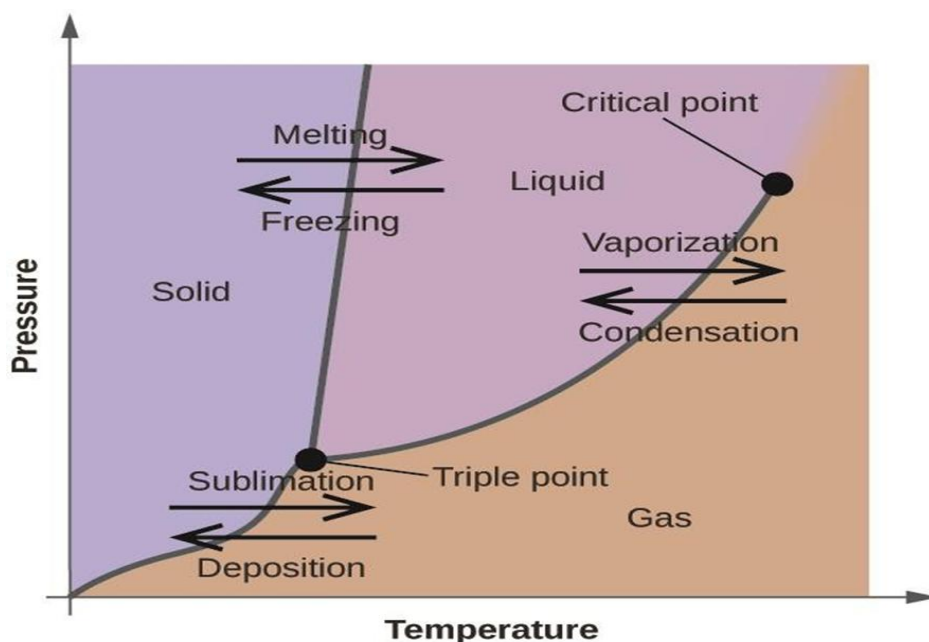


Figure 5. Phase Stability Diagram [30].

8. COMPUTATIONAL METHODS FOR PHASE STABILITY PREDICTIONS

Various computational techniques exist concerning different theoretical grounds for the prediction of phase stability. Phase diagram simulations are generally divided into two main groups: ab initio density functional theory (DFT) or quantum mechanics (QM) simulations and classical atomistic simulations [31]. The principle of computational modeling based on quantum mechanics lies in solving the Schrödinger equation for N electronic degrees of freedom at a given time instant t , expressed in terms of atomic coordinates $\{R_i(t), P_i(t)\}$. Classical atomistic methods rely on a quantum mechanical equation to predict the energy and forces of all N particles of a system based on the positions of electrons and nuclei [32].

In practice, direct solutions of the many-body Schrödinger equation for engineering-scale systems are computationally prohibitive. Therefore, density functional theory (DFT) is commonly employed as an approximation framework that enables efficient prediction of phase stability, formation enthalpy, electronic structure, and defect behavior in UHTCs while maintaining acceptable computational cost [33].

Table (2 b). Strategically in UHTC Research

System	Database maturity	Experimental validation	Current limitation
Zr-C	Excellent	High	Minor
Hf-C	Good	Moderate	Missing high-T data
Zr-B	Good	High	Oxidation uncertainty
Ta-C	Moderate	Limited	Sparse experimental data
Multicomponent UHTCs	Weak	Very limited	Database incomplete

There are several types of atomistic simulations that can be distinguished based on the type of particles and their dynamics. Simulations used to determine the atomic structures of solids, isolated surfaces, and nanostructures of interest are mainly molecular dynamics (MD), Monte Carlo, and mesoscale methods. As mentioned in Section 8.2, both types of simulations have been successfully employed to predict the phase stability of various nitrides, oxides, and carbides of IV and V group metals, where they are frequently used together with experimental information and data. This hybrid computational and experimental approach, the CALPHAD method, is the most popular modeling tool employed in developing and advancing engineering materials. Its main asset consists of estimating parameters required in the thermodynamic assessment of the materials of interest [34]. Another important limitation is the insufficient availability of validated thermodynamic databases for complex UHTC systems. This issue becomes particularly critical for emerging high-entropy carbides and borides, where experimental phase-equilibrium data remain limited, reducing the predictive capability of current CALPHAD assessments [35].

Despite significant progress, several challenges remain in thermodynamic modeling of UHTCs. For example, CALPHAD assessments of multicomponent Zr-Hf-Ta-C systems are often limited by the scarcity of reliable experimental thermodynamic data. Similarly, oxidation modeling of HfB₂-SiC composites at

temperatures above 2200°C remains difficult because evaporation of B_2O_3 and non-equilibrium oxide growth mechanisms are not fully captured by equilibrium thermodynamic calculations. Furthermore, DFT predictions may show discrepancies when modeling highly defective or non-stoichiometric carbide phases due to computational limitations and uncertainties in exchange-correlation functionals.

9. CHALLENGES AND LIMITATIONS IN THERMODYNAMIC MODELING

Challenges and standard modeling tools used in phase stability in UHTCs. Phase-related equilibria, reactions, or stability in plasma can be understood to carry out such simulations. Despite the numerous computational methods applied to solve those problems, certain aspects still need to be addressed [36]. This paper mainly discusses the challenges and limitations of integrating thermodynamic modeling and experimental observations and will be presented based on the following components. Those challenges include data accuracy from experiments, which is a challenge in flow-through plasma and during equilibration studies [37]. Also, features short discharge times, sheath formation, and non-ideal experimental procedures, which could make it difficult to reproduce all conditions quantitatively with simulations. The accuracy of plasma composition calculations is another challenge. A detailed outline from [38] from DFT will follow. Extrapolation from thermodynamics to practice is left out of the discussion because it needs to consider the chemical activity of impurities.

Table 3 (a). Database limitations

Technique	Validates	Advantages	Application	Experimental validation	Technology readiness	Limitations
XRD	Phase	Accurate	TPS	High	Mature	No oxidation kinetics
SEM	Microstructure	Excellent	Leading edges	Moderate	Prototype	Surface only
DSC	Transformation	Quantitative	Nuclear propulsion	Low	Conceptual	Limited temperature
TGA	Oxidation	Excellent	Deep-space reactors	Very Low	Future	No phase identification

Table 3 (b). Comparison of Experimental Characterization Techniques and Computational Modeling Methods for Materials Research.

Technique	Validates	Advantages	Limitations
XRD	Phase	Accurate	No oxidation kinetics
SEM	Microstructure	Excellent	Surface only
DSC	Transformation	Quantitative	Limited temperature
Method	Length scale	Output	Best application
DFT	Atomic	Formation energy	Stable phases
MD	Atomic/time	Diffusion	High-temperature behavior
CALPHAD	Thermodynamic	Phase diagrams	Equilibrium
Phase-field	Microstructure	Grain evolution	Phase evolution

Thermodynamic modeling is a powerful tool for predicting phase stability and chemical equilibrium in ultra-high-temperature ceramics (UHTCs), and different computational programs can generate standard models and databases. In this context, large and coherently evaluated thermodynamic databases are available [39]. However, phase stability prediction involving UHTCs represents a great challenge mainly due to the slice of accessible experimental data, computational effort, and degree of covalency that should be considered in terms of existing models and databases. UHTCs have been proposed for several challenging applications, including the leading edges of space vehicles (small debris shielding) and atmospheric re-entry vehicles [40]. In addition, UHTCs may be employed as plasma-facing materials in the upcoming fusion reactors due to their extraordinary physicochemical properties in extreme conditions like high temperature, thermal shock resistance, and material purity.

10. ULTRA-HIGH-TEMPERATURE CERAMICS (UHTCs) IN SPACE EXPLORATION

Ultra-high-temperature ceramics (UHTCs) are a family of materials known to retain their physical properties and mechanical behavior at temperatures over 3000°C [41]. They are highly resistant to oxidation and have several peculiar properties that make them an ideal choice of material for application in space exploration. Although such ceramics were initially considered as materials for re-entry vehicles, they are currently being investigated for a wide range of applications, including in nuclear thermal rockets, solid rocket motors, leading edges, air-breathing vehicles, and re-usable heatshield materials for future missions to planets with atmospheres. Their exceptional physical and mechanical properties have also been found to be valuable in non-aerospace applications, such as in extreme environments [42].

For example, ZrB₂-SiC composites have demonstrated operational capability at temperatures exceeding 2000–2200°C, while HfB₂-SiC systems can withstand temperatures approaching 2500°C under oxidizing conditions. The formation of protective SiO₂-rich surface layers significantly reduces oxidation rates and limits mass loss during prolonged exposure. Similarly, TaC exhibits one of the highest known melting temperatures (~3880°C), making it attractive for rocket nozzle applications where severe thermal loads and erosion conditions are encountered. The development and application of these ceramics for space exploration have presented many new experimental and computational challenges, especially with respect to their phase stability and behavior in ablation environments. Every material that is considered for use in space environments requires careful experimentation and validation for structural integrity, longer life, and enhanced future capabilities [43]. The thermal environment in space drives scientists to look for materials that differ in physical, thermal, mechanical, and high-temperature properties. The intense heating that occurs during aerocapture and entry for re-entry spacecraft also requires extremely high-temperature materials. Proposed missions to the surface of Venus and for high-speed crewed return are particularly challenging because of the higher rate of heat transfer (and higher temperatures) on entry and the requirement for load-bearing capability over long mission durations [44].

Table 4 (a). Specific Example: ZrB₂-SiC in Hypersonic Vehicle Leading Edges

Application	Hypersonic Vehicle Leading Edges
Material System	Zirconium Diboride-Silicon Carbide (ZrB ₂ -SiC) Composite
Thermodynamic Modeling Role	- Used to simulate oxidation kinetics at >2000°C

Models predict protective SiO₂-rich glass layer formation Determines stability range of ZrO₂ and B₂O phases in high-temperature oxygen-rich environments (Phase Stability Importance) - Maintains solid structure during high-speed atmospheric flight SiC component oxidizes to form SiO₂, which creates a protective glass layer ZrB₂ oxidizes to ZrO₂, which remains solid and stable at high temperature (Resulting Benefits) - Low oxidation rate and high structural integrity Resistance to thermal shock from rapid heating/cooling [45]. Extended lifespan of vehicle edges under extreme reentry conditions. (Real-World Use) Used in advanced research for materials in NASA's Hypersonic Inflatable Aerodynamic Decelerator (HIAD) and reentry vehicle nose cones [46].

10.1. More Examples Like This (e.g., for TaC, HfC, etc.)

Table 4 (b). Tantalum Carbide (TaC) in Rocket Nozzles

Application	Rocket Nozzle Throat Liners in Solid Rocket Motors
Material System	Tantalum Carbide (TaC)
Thermodynamic Modeling Role	- Predicts sublimation temperatures (~3900°C)

- Evaluates formation of Ta₂O₅ layer at elevated oxygen partial pressure
- Assesses phase decomposition in low-oxygen or vacuum conditions Phase Stability Importance - TaC resists decomposition under low-oxygen and vacuum
- Oxidation-resistant up to ~2400°C in controlled environments
- Prevents rapid material loss during combustion cycles Resulting Benefits - Superior thermal resistance and erosion protection
- Maintains structural integrity in aggressive, high-temperature exhaust flow Real-World Use Considered for high-performance rocket nozzles and solid propellant exhaust cones in advanced launch systems

Table 4 (c). Hafnium Carbide (HfC) in Atmospheric Reentry

Application	Leading Edges in Hypersonic Transport
Material System	Hafnium Diboride-Silicon Carbide (HfB ₂ -SiC) Composite
Thermodynamic Modeling Role	- Predicts oxidation rates of SiC and HfB ₂

- Simulates viscous SiO₂ layer formation
- Models' evaporation of B₂O₃ under low-pressure flight conditions Phase Stability Importance - HfB₂ forms stable HfO₂ phase
- SiC forms SiO₂ protective coating

- Avoids liquid phase formation that can damage TPS Resulting Benefits - Exceptional thermal and oxidative protection
- Smooth, self-healing glass surface from SiO₂ prevents material loss Real-World Use Proposed for next-gen hypersonic gliders and orbital reentry vehicles with reusable TPS materials

Table 4 (d). ZrC–HfC–TaC Ternary Alloys in Space Reactors

Application	Heat Shields and Cladding in Nuclear Spacecraft
Material System	Ternary Carbide Alloys (ZrC–HfC–TaC)
Thermodynamic Modeling Role	- Simulates solid solution behavior and eutectics [47]

- Evaluates thermal conductivity and phase segregation
- Predicts stability under radiation and thermal cycling Phase Stability Importance - Maintains integrity under high neutron flux
- Avoids radiation-induced amorphization
- Stable phases prevent cracking or expansion Resulting Benefits - Improved longevity in deep-space environments
- Stable cladding and shielding for radioisotope power systems (RPS) [48] Real-World Use Considered in materials research for NASA's Kilopower reactor and space fission power systems [49]

NASA has investigated UHTC materials for thermal protection systems, leading edges, and atmospheric re-entry vehicles through several research programs, including the Hypersonic Inflatable Aerodynamic Decelerator (HIAD) project and advanced thermal protection system developments [50].

$T_0 = \Delta A / \Delta H_v$, where T_0 is the equilibrium transition temperature, ΔH_v denotes the enthalpy change associated with the phase transformation, and ΔA represents the Gibbs free energy difference between the parent and transformed phases. The equation indicates that phase stability is governed by the balance between energetic and thermodynamic driving forces.

11. FUTURE DIRECTIONS AND EMERGING TRENDS

The field of ultra-high-temperature ceramics (UHTCs) has rapidly developed over the last two decades primarily due to the resurging interest in space exploration, where the demands of exposed atmospheric re-entry can place significant requirements on the materials used in various space vehicles and systems. The proposed review is an extensive introduction to the materials design for next-generation space vehicles and an analysis of the potential opportunities for predictive thermodynamic modeling and phase stability for UHTCs and their composites. Challenges in the use of predictive modeling are also discussed in the background interplay of thermodynamics and materials science. Finally, essential databases for characterizing UHTCs and enabling computational approaches are presented.

We anticipate that the interdisciplinary approach stemming from combinatorial nanoscience, computational phase stability, and oxidation prediction will define future developments in UHTC research. Considering that nanoscale dispersions have paved the way for improving oxidation resistance by orders of magnitude, one pathway of high-impact research may be to apply these advanced concepts to develop enhanced materials that display further superior oxidation resistance in more complex thermomechanical and thermochemical environments. The generation of thermodynamic databases is an often-underappreciated frontier in ceramics research. In recent years, important strides have been made in measuring divalent-rich materials. Future challenges include measuring the solubilities of rare earths, the effect of the addition of metal impurities to UHTCs, and the validation and correction of water pressure measurements across multiphase systems.

Table 5. Strategies

Strategy	Objective	Result / Outcome	Example Material/System
Use of CALPHAD for multi-component phase prediction	Predict equilibrium phases and temperature ranges for stability	Accurate phase diagrams for UHTC systems (e.g., ZrB ₂ –SiC), guiding composite design	ZrB ₂ –SiC, HfB ₂ –SiC
DFT-based computation of formation energies	Understand atomic-level bonding and phase stability	Identification of stable phases and prediction of oxidation-resistant compositions	HfC, TaC, ZrC
Oxidation testing under simulated reentry environments	Validate material behavior in high-temperature oxidative atmosphere	Confirmed formation of protective oxide layers (e.g., SiO ₂ , HfO ₂) that reduce mass loss	HfB ₂ –SiC, ZrB ₂ –SiC
Addition of SiC to diboride matrices	Improve oxidation resistance and thermal shock resistance	Formation of viscous SiO ₂ layer that seals surface cracks and slows oxygen diffusion	ZrB ₂ –SiC, HfB ₂ –SiC composites

Thermogravimetric analysis (TGA) and ablation rate testing	Quantify material degradation under heat loads	Determined oxidation onset temperatures, mass change kinetics, and suitable operation windows	HfC, TaC
Designing ternary UHTC systems (e.g., ZrC-TaC-HfC)	Enhance thermal conductivity, phase stability, and mechanical strength	Discovery of solid solutions with increased melting point and reduced thermal expansion mismatch	ZrC-TaC-HfC alloy
Plasma wind tunnel testing of fabricated components	Simulate reentry/hypersonic flight to observe real-time behavior	Demonstrated low erosion rates and thermal stability under simulated Mach 8–10 reentry conditions	HfB ₂ -SiC (nose tips), TaC (nozzles)
Modeling microstructural evolution under heat stress	Predict grain coarsening, oxide growth, and internal stress evolution	Informed material processing techniques to maintain phase homogeneity and structural integrity	HfC, ZrB ₂
Development of UHTC coatings on substrates (e.g., C/C)	Extend lifetime of structural materials with a protective surface layer	Enabled reuse of carbon-carbon (C/C) components by preventing oxidation at high temperatures	HfB ₂ -SiC on C/C

12. CONCLUSION AND SUMMARY

This paper has broadly reviewed the modeling of thermodynamic properties and phase stabilities in UHTCs. A significant number of studies concentrate on microstructural characterization, and only a few reports have been made on thermodynamic treatment. To the best of my knowledge, no previous review in the open literature addresses the importance of thermodynamic studies dealing with phase stabilities for material development. Thanks to the availability of thermodynamic databases, an accurate description of multiple-phase interactions and the relevant thermodynamic properties can now be provided, considering the individual arrangements of different species in multiple-point defects, enabling consistent phase diagrams. The next steps for researchers are also suggested, such as further studies focusing on assessing the materials' thermodynamic parameters and closer collaboration between experimentalists and computer modelers to provide a better basis for future material development.

The review has systematically summarized both the atomistic and phase-field modeling using various approaches and tools, focusing on the considerations of multiphase stabilities based on the grand canonical potential or fugacity. The modeling of Frenkel pair defects on phase stabilities has also been emphasized, as they are directly linked to material irradiation in a fusion reactor environment. All the reviewed issues, like interface energies, the kinetics of reactions, and reaction pathways, are inherently included within the phase field when equilibrium thermodynamic modeling on individual systems, including metastability, is impossible. These tools are believed to directly and inevitably contribute to adjusting potential phase compositions and microstructures for space use of carbides. They will benefit from ultra-high-temperature ceramics and other crystalline materials under different pressures. Ultra-high-temperature ceramics (UHTCs) are critical to the advancement of space exploration technologies, particularly in hypersonic flight, re-entry vehicles, and propulsion systems. This review highlights how thermodynamic modeling has become an indispensable tool for understanding and optimizing the phase stability, oxidation resistance, and mechanical integrity of UHTCs under extreme conditions. By leveraging computational techniques such as CALPHAD (CALculation of PHase Diagrams), ab initio methods, and molecular dynamics simulations, researchers can predict phase transformations, design novel compositions, and guide experimental efforts more efficiently. These insights are crucial for developing UHTCs that maintain stability above 2000°C and withstand harsh oxidative and thermal shock environments encountered in space missions. Despite significant progress, challenges remain in bridging modeling with experimental validation and in scaling laboratory results to mission-ready applications. Continued interdisciplinary collaboration between materials scientists, thermodynamic modelers, and aerospace engineers is essential for translating UHTC research into reliable aerospace components.

Different experimental techniques provide complementary information regarding phase stability. Thermogravimetric analysis (TGA) is particularly effective for quantifying oxidation kinetics and mass changes during high-temperature exposure, whereas differential scanning calorimetry (DSC) accurately determines phase transition temperatures and transformation enthalpies. X-ray diffraction (XRD) is preferred for phase identification, while scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM/EDS) enables detailed characterization of microstructural evolution and elemental redistribution. Consequently, a combination of these techniques is generally required to obtain a comprehensive understanding of UHTC phase stability.

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