ICCES, 2026, vol.36, no.1

Tech Science Press

DOI: 10.32604/icces.2026.014055

PROCEEDINGS

Data-Driven Intelligent Design of ZrC–TaC–SiC Coating Compositions and Their Ablation Behavior

Yujia Zhang[1], Zhixiang Zhang[1], and Jia Sun[1,*]

[1]Northwestern Polytechnical University, Xi'an, 710072, China

[*]Corresponding Author: Jia Sun. Email: j.sun@nwpu.edu.cn

ABSTRACT

Ultra-high-temperature ceramic (UHTC) coatings are critical materials in thermal protection systems for hypersonic vehicles. However, conventional development approaches, which rely on empirical accumulation and trial-and-error optimization, are inefficient, time-consuming, and associated with high experimental costs and material waste, severely limiting rapid screening and performance breakthroughs for novel coating compositions. To overcome this bottleneck, this study focuses on the ZrC–TaC–SiC ternary system (denoted as Z*n*T*m*S*t*, *n*, *m*, *t* = 0–100) and proposes a machine-learning-based design strategy to enhance the ablation resistance of these coatings.

We compiled 170 sets of experimental data from multiple literature sources to develop a random forest regression model, capable of predicting three key performance metrics—surface ablation temperature, mass ablation rate, and linear ablation rate—across the entire compositional space of the ZrC–TaC–SiC system. The model effectively captures the nonlinear relationships between composition and ablation behavior, enabling rapid and accurate estimation of performance for unexplored compositions. High-throughput virtual screening of the full compositional space identified four promising formulations: Z60T30S10, Z60T10S30, Z80T15S5, and Z80T5S15. Model predictions show their mass and linear ablation rates are consistently on the order of 10^{-4} g/s and 10^{-4} mm/s, respectively.

Subsequently, experimental samples of the selected compositions were successfully fabricated via supersonic atmospheric plasma spraying and validated using oxy-acetylene ablation tests (60 s). The experimental results showed excellent agreement with model predictions, with ablation rate prediction errors on the order of 10^{-5}. Microstructural analysis revealed that high TaC content (15–30%) promotes excessive formation of $Zr_6Ta_2O_{17}$ during ablation, weakening the thermal stability of the oxide layer and resulting in structural discontinuities; non-uniform sintering further increases porosity. In contrast, the Z80T5S15 composition with low TaC content (5%) achieves a dense and continuous oxide layer by regulating the Zr/Ta oxide phase ratio, exhibiting superior ablation resistance.

The integrated "machine learning–experimental validation" strategy developed in this study significantly reduces the development cycle and cost for high-performance UHTC coatings, providing a new paradigm for intelligent design and performance prediction of ultra-high-temperature ceramic coatings.

KEYWORDS

Ultra-high-temperature ceramics; ZrC–TaC–SiC ternary coatings; machine learning; performance prediction; ablation behavior

Funding Statement: This work was supported by National Defense Basic Scientific Research Program of China (JCKY2022607C007), National Natural Science Foundation of China (52472107, 22581260172), National Key R&D Program of China (2021YFA0715802).

Copyright © 2026 The Author(s). Published by Tech Science Press.
This work is licensed under a Creative Commons Attribution 4.0 International License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Conflicts of Interest: The authors declare no conflicts of interest to report regarding the present study.