Influence of Hf on the microstructure and properties of Hf_xMoTaW medium-entropy alloys: A Multiscale AI-Integrated Approach

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Abstract

Refractory medium-entropy alloys (RMEAs) are prime candidates for high-temperature structural applications due to their inherent thermal stability [1]; however, predicting phase selection in these complex spaces remains a significant challenge. This study investigates the influence of Hf addition on the microstructural evolution of Hf_xMoTaW (x = 0, 0.5, 1) alloys using a synergistic workflow that integrates experimental metallurgy with advanced machine learning. Experimental characterization via X-ray diffraction (XRD) and high-resolution microscopy reveals that while the ternary MoTaW base forms a single BCC solid solution, the introduction of Hf triggers a transition to a multiphase microstructure. This evolution is characterized by a BCC matrix and the precipitation of a Hf-rich Laves phase (HfW_2 type) during the annealing process [2].

To unravel the atomistic driving forces behind this transition, we employed Molecular Dynamics (MD) simulations accelerated by a Machine Learning Interatomic Potential (MLIP) [3]. The MLIP, trained on high-fidelity datasets, allowed for the observation of pronounced chemical short-range ordering (CSRO) between Hf and W that traditional empirical potentials often overlook [4]. To quantitatively bridge these atomistic findings with experimental observations, we implemented a computer vision-based segmentation pipeline. This deep-learning approach enabled the automated detection and quantification of Hf-rich regions in microstructural images, providing objective metrics for phase fraction and morphology.

A key innovation of this work is the integration of CrystaLLM, a generative transformer-based model, to navigate the vast crystallographic space of refractory intermetallics [5]. Unlike traditional high-throughput screening, CrystaLLM treats crystal structures as a serialized "language" (CIF files), allowing it to generate plausible candidate structures for Hf-W-rich phases by learning underlying chemical grammar and symmetry constraints. Figure 2 represents crystal structures predicted by LLM. These AI-generated candidates were subsequently validated against experimental XRD patterns and thermodynamic predictions from Thermo-Calc, confirming the formation of the C15 Laves phase. This research demonstrates a comprehensive multiscale framework linking generative AI for structure discovery, MLIPs for atomistic stability, and computer vision for microstructural quantification establishing a new paradigm for the accelerated development of complex refractory alloy systems.

References

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Figures

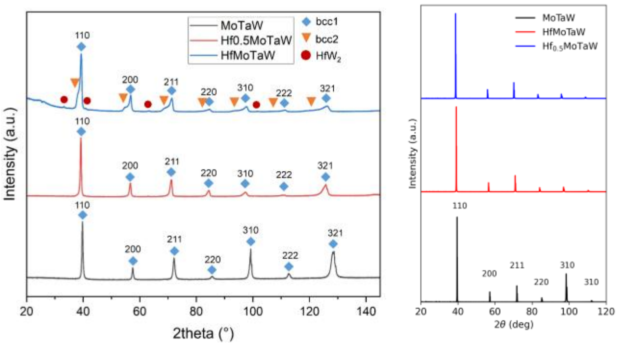

Figure 1. XRD pattern of the as-cast samples produced by arc melting (MoTaW, $Hf_{0.5}MoTaW$, HfMoTaW).

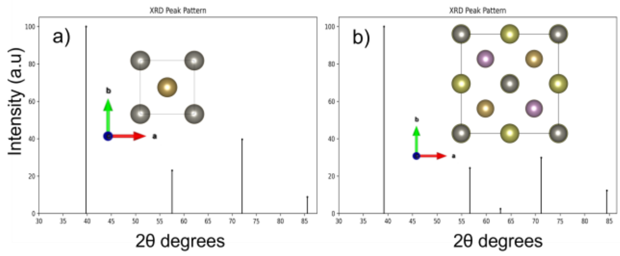

Figure 2. CrystaLLM-predicted BCC crystal structures and corresponding XRD patterns for (a) MoTaW and (b) HfMoTaW.