

# Exploring the extrapolation limits of machine learning models for refractory complex concentrated alloys using high-throughput experiments

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Refractory complex concentrated alloys (RCCAs) are emerging as key candidates for structural applications under extreme conditions, where both strength and stability beyond 1000 °C are required. Yet, the immense compositional space of these alloys (spanning billions of possible combinations) makes their systematic exploration by conventional methods infeasible. High-throughput materials science offers a solution: combinatorial PVD synthesis enables the fabrication of thin-film materials libraries with continuous composition gradients, effectively covering binary or ternary systems within a single deposition. However, when moving to higher-order systems, the composition gradients attainable on planar substrates represent only a two-dimensional projection of a much higher-dimensional space.

In this study, we focus on a selected quaternary refractory system (A–B–C–D) and synthesize a series of combinatorial thin-film libraries covering different compositional regions. Using high-throughput mechanical characterization, we will build a large dataset for training machine learning models that predict mechanical properties across this multicomponent system. The main objective is to determine how far one can extrapolate meaningfully from a given training data cloud, quantified using the Mahalanobis distance as a metric of compositional similarity. Moreover, we will assess whether combining multiple data clouds from distinct composition regions improves the extrapolation capability of the models.

This approach will provide new insights into the limits of machine learning prediction in complex alloy systems and guide the efficient design of high-dimensional RCCAs through data-driven methods.

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