Explainable AI Reveals Design Rules for Multi-Principal Element Alloys

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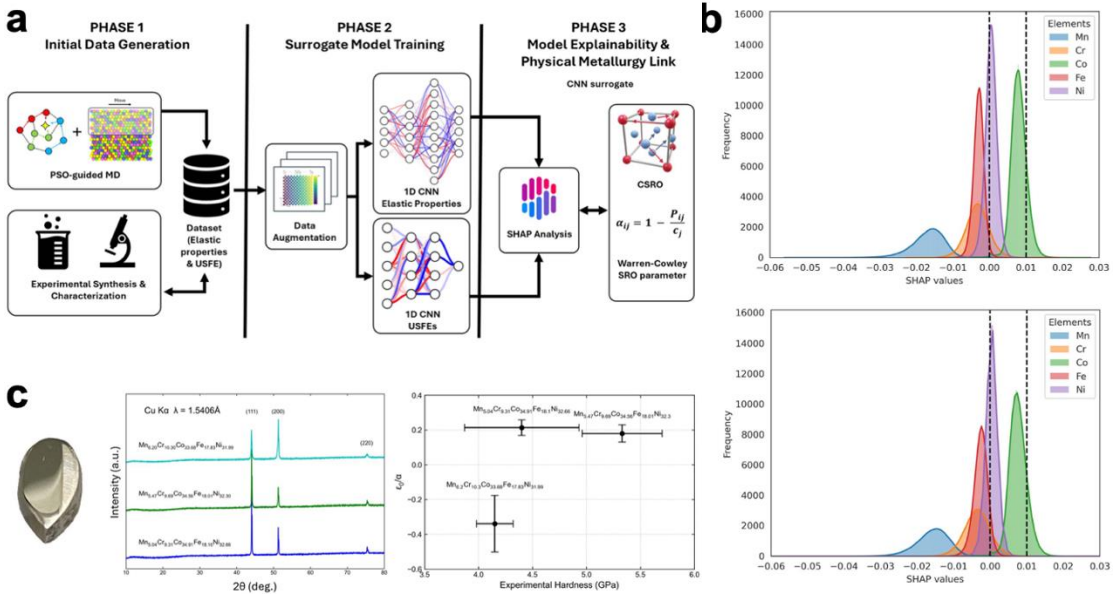
Project summary: Multi-principal element alloys (MPEAs) such as the Cantor-type FeNiCoCrMn system span a large compositional design space, but their nonlinear composition-property relationships make systematic exploration difficult. A multi-institutional team including researchers from GlycoMIP – an NSF Materials Innovation Platform and PARADIM, the Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials, combined particle-swarm-optimization-guided molecular dynamics simulations with deep-learning surrogate models and explainable-AI (Shapley) analysis to connect alloy composition and local atomic ordering to predicted mechanical behavior. The analysis showed that the bulk modulus is governed mainly by composition, lowered by manganese and raised by cobalt, while short-range-order analysis indicated that manganese and chromium tend to segregate at stacking-fault layers, where they increase the unstable stacking-fault energy. For experimental validation, the team synthesized and characterized candidate alloy compositions. The alloys formed single-phase face-centered-cubic structures whose measured hardness and Young's modulus exceeded those of the equimolar Cantor alloy, providing qualitative validation of the computationally guided alloy-selection approach. The work demonstrates how interpretable AI and physics-based modeling can produce mechanistic design rules for complex alloys.

MIP role: GlycoMIP contributed the AI-enabled computational framework used to identify MPEA candidates, while PARADIM provided synthesis and characterization capabilities for experimental validation of selected alloy compositions.



Figures. a) Computational-experimental workflow. b) SHAP analysis showing each element's contribution to the predicted bulk modulus. c) Experimental validation, including an arc-melted alloy sample, powder X-ray diffraction patterns confirming single-phase face-centered-cubic structures, and relative unstable stacking-fault energy measurements.