DREXEL UNIVERSITY
Materials Science and Engineering
College of Engineering

Department of Materials Science and Engineering

Defense of Dissertation

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3100 Market Street

Computational Design of Refractory High Entropy Alloys with Optimized Mechanical Properties

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Abstract

Refractory high-entropy alloys (RHEAs) are promising candidates for structural applications in extreme environments such as turbines in aircraft engines and power plants, due to their exceptional strength retention and thermal stability. However, their vast compositional design space creates significant challenges for traditional trial-and-error development. This dissertation presents a computational framework that leverages *ab-initio* calculations and physics-informed machine learning to efficiently explore the RHEA composition space and predict key properties linked to mechanical performance. First, a bond-based model is developed to predict lattice parameters by accounting for charge transfer effects through DFT-calculated bond lengths from binary intermetallics. This model outperforms Vegard's law and enables rapid estimation of atomic volumes for strengthening and misfit analysis. Second, a statistical model of lattice distortion is introduced, using bond-length and electronic-structure descriptors to predict the root-mean-squared atomic displacement, which correlates with solid-solution strengthening in multicomponent alloys. Third, a machine-learning surrogate model is constructed to predict unstable stacking fault energies (γ_{USF}) on {112} and {123} slip systems to estimate dislocation motion on those planes. By comparing γ_{USF} , values across planes, a new descriptor—the H-parameter—is proposed to quantify slip-plane competition, which correlates with experimentally observed work-hardening behavior. Together, these tools provide an efficient and interpretable approach for linking alloy chemistry to macroscale properties, offering practical guidance for the design of next-generation RHEAs with balanced, tunable properties.