MATERIALS ENGINEERING
SEMINAR

"High-throughput Calculations and Experimentation for the Discovery of Refractory Complex Concentrated Alloys"

By

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ABSTRACT

In the present era of high temperature materials, Ni-based superalloys continue to exert themselves as the industry standards in high stress and highly corrosive/oxidizing environments, such as are present in a gas turbine engine, due to their excellent high temperature strength, thermal and microstructural stability, and oxidation and creep resistance. Gas turbine engines are essential components of energy generation and propulsion in the modern age. However, Ni-based superalloys are reaching their limits in the operating conditions of these engines due to their melting onset temperatures, which are approximately 1300 °C. Therefore, a new class of materials must be formulated to surpass the barriers posed by Ni-based superalloys, as increasing the operating temperature leads to increased efficiency and reductions in fuel consumption and greenhouse gas emissions. One of the proposed classes of materials is termed refractory complex concentrated alloys, or RCCAs, which consist of 4 or more refractory elements (in this study, selected from: Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and W) in equimolar or near-equimolar proportions. So far, there have been highly promising results with these alloys, including far higher melting points than Ni-based superalloys and outstanding high-temperature strength in non-oxidizing environments. However, improvements in the room temperature ductility and high-temperature oxidation resistance of RCCAs are still needed. Also, given the millions of possible alloy compositions spanning various combinations and concentrations of refractory elements, more efficient methods than just serial experimental trials are needed for identifying RCCAs with desired properties. A coupled computational and experimental approach for exploring a wide range of alloy systems and compositions is crucial for accelerating the discovery of RCCAs that may be capable of replacing Ni-based superalloys.

In this thesis, the CALPHAD method is utilized to generate basic thermodynamic properties of approximately 67,000 Al-bearing RCCAs. The alloys are then down-selected on the basis of certain criteria, including solidus temperature, volume percent BCC phase, and aluminum activity. Machine learning models with physics-based descriptors are used to select several BCC-based alloys for fabrication and characterization, and an active learning loop is employed to aid in rapid alloy discovery for high hardness and strength. This method resulted in rapid identification of 15 BCC-based, four component, Al-bearing RCCAs exhibiting room-temperature Vickers hardness from 1% to 35% above existing literature alloys. This work exemplifies the advantages of utilizing Integrated Computational Materials Engineering- and Materials Genome Initiative-driven approaches for discovery and design of new materials with novel properties.

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