SCIENCE OF ENTROPY-STABILIZED ULTRA-HIGH TEMPERATURE MATERIALS: PREDICTIVE AND MULTI-PHYSICS MODELING

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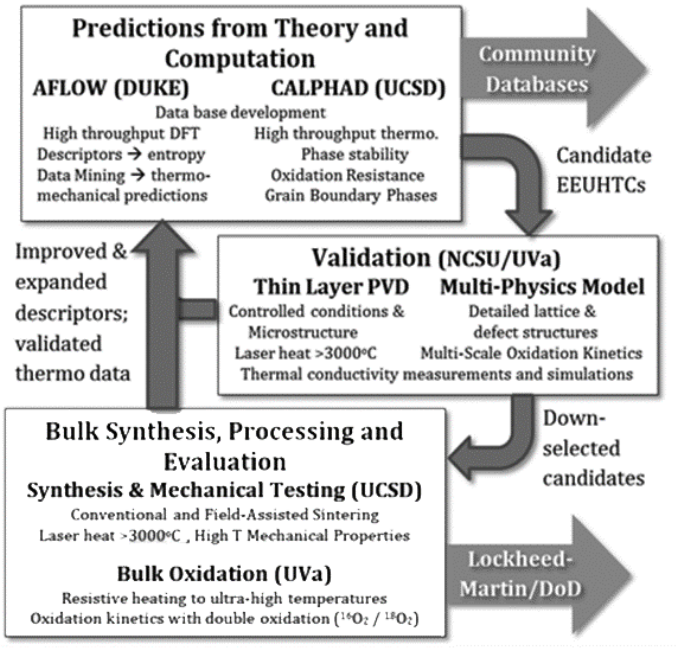
Our team is exploring a new concept in the development of ultra-high temperature materials - engineering the configurational entropy contribution to the free energy. We are doing this by using compositions with multiple refractory elements in near equi-molar concentrations. The work has focused primarily on unique refractory alloys that combine multi- and single-component sublattices; these are di-borides with layered sublattices, as well as nitrides, carbides, and carbo-nitrides with interpenetrating multi-and single-component face-centered-cubic sublattices.



Critical to this design concept is using predictive computation for the efficient identification of stable compositions without competing phases at ultra-high temperatures from a large number of possibilities, and the systematic down-selection of these compositions through prototyping, multi-physics modeling ,and advanced bulk processing and characterization. This is illustrated in the figure. The effort has also been developed to provide feedback from experiment back to the theory and modeling, hence iteratively improving all aspects of this integrated effort.

After a brief overview, this presentation will focus on the predictive and multi-physics modeling aspects of the program, and their integration within the experimental efforts. Topics will include property descriptors for searching first-principles data bases, high-throughput CALPHAD for identifying competing phases, theory and simulations of thermal transport, and first principles studies of the structure and bonding in these new classes of entropic materials. The experimental aspects of this effort will be discussed in a separate companion presentation.

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