Project Objectives
- Develop a thermodynamic foundation for accelerated design of Ni-base alloys and coatings:
  - Ni-Co-Cr-Al + Si, Hf, Y (MCrAlX)
- Study effects of major and minor alloying elements on the phase stability: Hf and Y additions to Ni-systems
- Experimental validation
- Assist in the development of the automated thermodynamic modeling tool (ESPEI)

Methodology
- CALPHAD thermodynamic modeling – constituent binaries and ternaries
- ab initio DFT – Predict thermodynamic properties
- X-Ray Diffraction – Phase identification
- CALPHAD database
- Electron Probe Micro-Analysis – Accurate compositional measurements
- Remodeling of the important Hf-Ni binary using DFT predictions

Benefits of Reactive Element (RE) Additions
- Doping with Hf, Si, Y improves oxidation resistance
- Co-doping can further improve resistance, particularly under thermal cycling conditions
- Alloys are sensitive to RE overdoping
- Overdoping can manifest as formation of hafnium intermetallics and/or hafnium oxide (HfO₂)
- There is a practical need to predict and validate critical Hf content in the alloy

Results & Discussion
- Thermodynamic modeling
  - Al-Hf-Ni ternary
  - Al-Cr-Hf-Ni quaternary
- Prediction of HfO₂ formation in Al-Cr-Ni alloys
- Prediction of Hafnides in Al-Cr-Ni alloys

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