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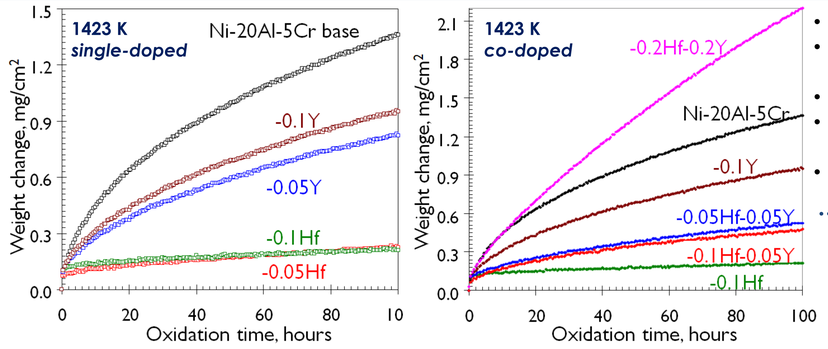
PHASES PSU

Computational Design and Discovery of Ni-base Alloys and Coatings: Al-Cr-Ni + Hf

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**)

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 (HfO_2)
- There is a practical need to predict and validate *critical* Hf content in the alloy

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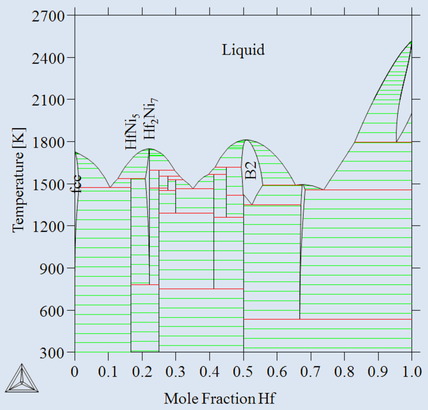
Methodology

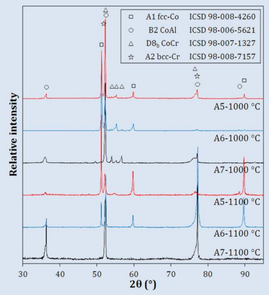
***ab initio* DFT – Predict thermodynamic properties**

CALPHAD thermodynamic modeling – constituent binaries and ternaries



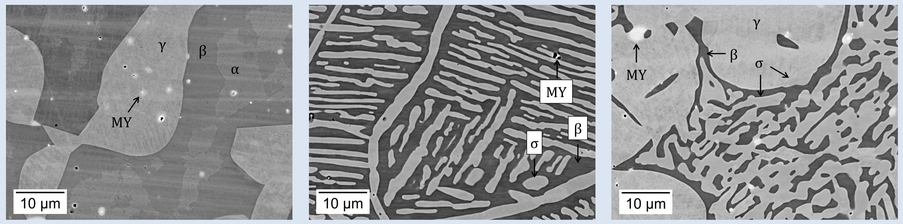
Remodeling of the important Hf-Ni binary using DFT predictions

X-Ray Diffraction – Phase identification



Coating Database

Electron Probe Micro-Analysis – Accurate compositional measurements



Liu et al. (2015) PLOS ONE 10(4) doi: 10.1371/journal.pone.0121386.

Thermochemical data: enthalpy, entropy, heat capacity, activity…

Scarce experimental data, supplemented by first-principles

Phase equilibria data: liquidus, solidus, phase boundary/composition

Experimental data from present work and literature

Gibbs energy (parameterized)

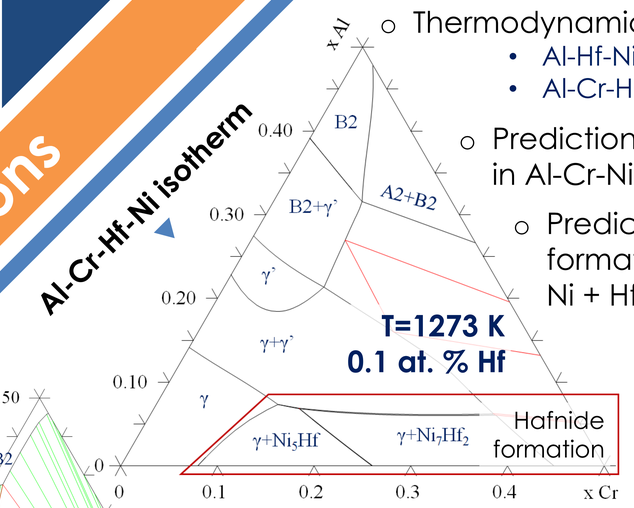
http://www.calphad.org

Phase diagrams, direct applications

Practical applications, alloy design, T, P, n_i conditions

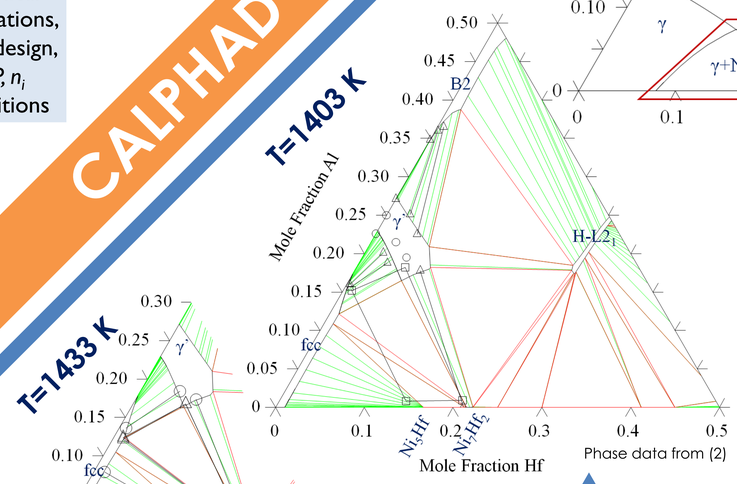
CALPHAD Predictions

Al-Cr-Hf-Ni isotherm



T=1273 K
0.1 at. % Hf

Al-Hf-Ni isotherms



(1) Nagarajan et al. (1997) *Z. Metall.* 88 p. 87-90
(2) Zhang et al. (2008) *Intermetallics* 16 p. 139-147

Results & Discussion

- Thermodynamic modeling
  - Al-Hf-Ni ternary
  - Al-Cr-Hf-Ni quaternary
- Prediction of Hafnides in Al-Cr-Ni alloys
- Prediction of HfO_2 formation in Al-Cr-Ni + Hf

Predicted HfO_2 formation