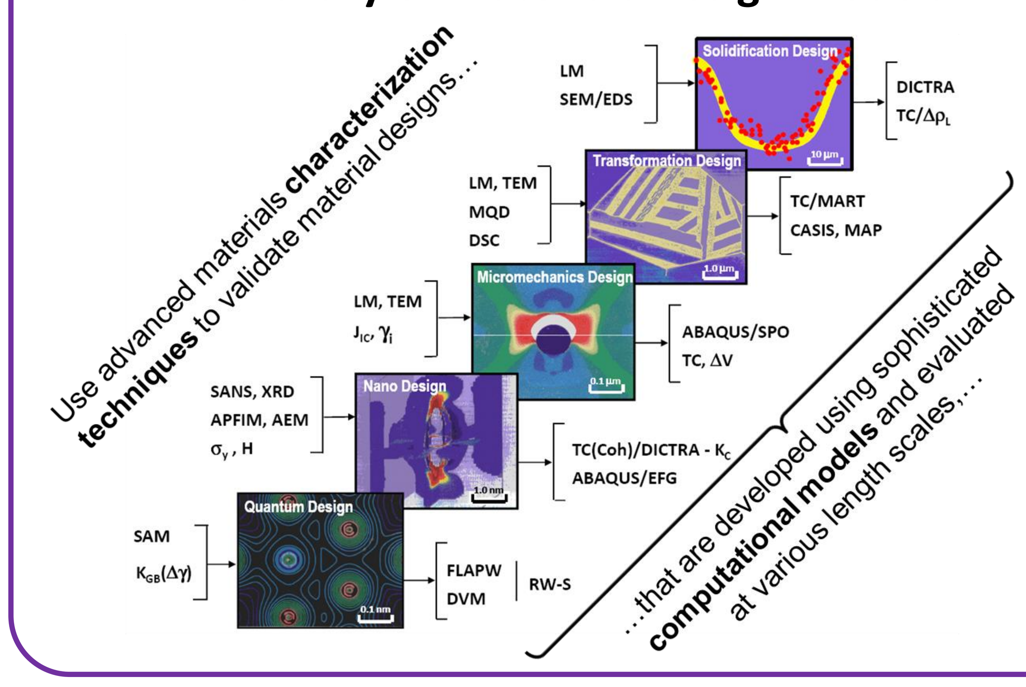
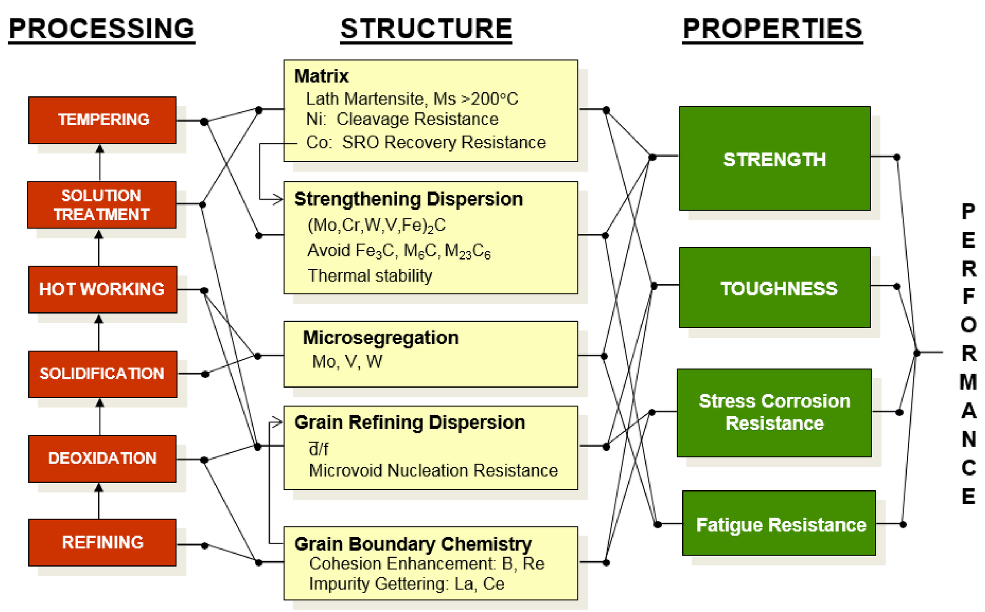
Computationally Designed Alloys for Turbine Applications
QuesTek Innovations LLC, Evanston, IL

Integrated Computational Materials Engineering (ICME) Approach to Materials Design

Hierarchy of Materials Design Models



Systems Design Chart



NIST-Funded Materials Genome Success Story

Materials Innovation Case Study:
QuesTek's Ferrium® M54® Steel for Hook Shank Application

- **Public validation of success of QuesTek's ICME-based approach**
- *Ferrium* M54 Steel qualified for U.S. Navy T-45 hook shanks with >2x life vs. incumbent alloy, providing $3 Million cost savings to the fleet
- From design to commercialization in 4 years with flight qualification within 3 more
- Accomplishment of MGI goal of new materials innovation in less than 10 years

QuesTek's Commercially Available *Ferrium* Steel Application Successes

Ferrium C61™ rotor shaft for Boeing Chinook helicopter 20% increase in power density (power to weight ratio) versus incumbent steel

Ferrium S53® roll pin for C-5 aircraft In flight service on U.S. Air Force platforms A-10, C-5, KC-135, and T-38 to replace existing corrosion-prone steels

Cost-Effective, Castable Single Crystal Superalloy for Turbine Blade Applications

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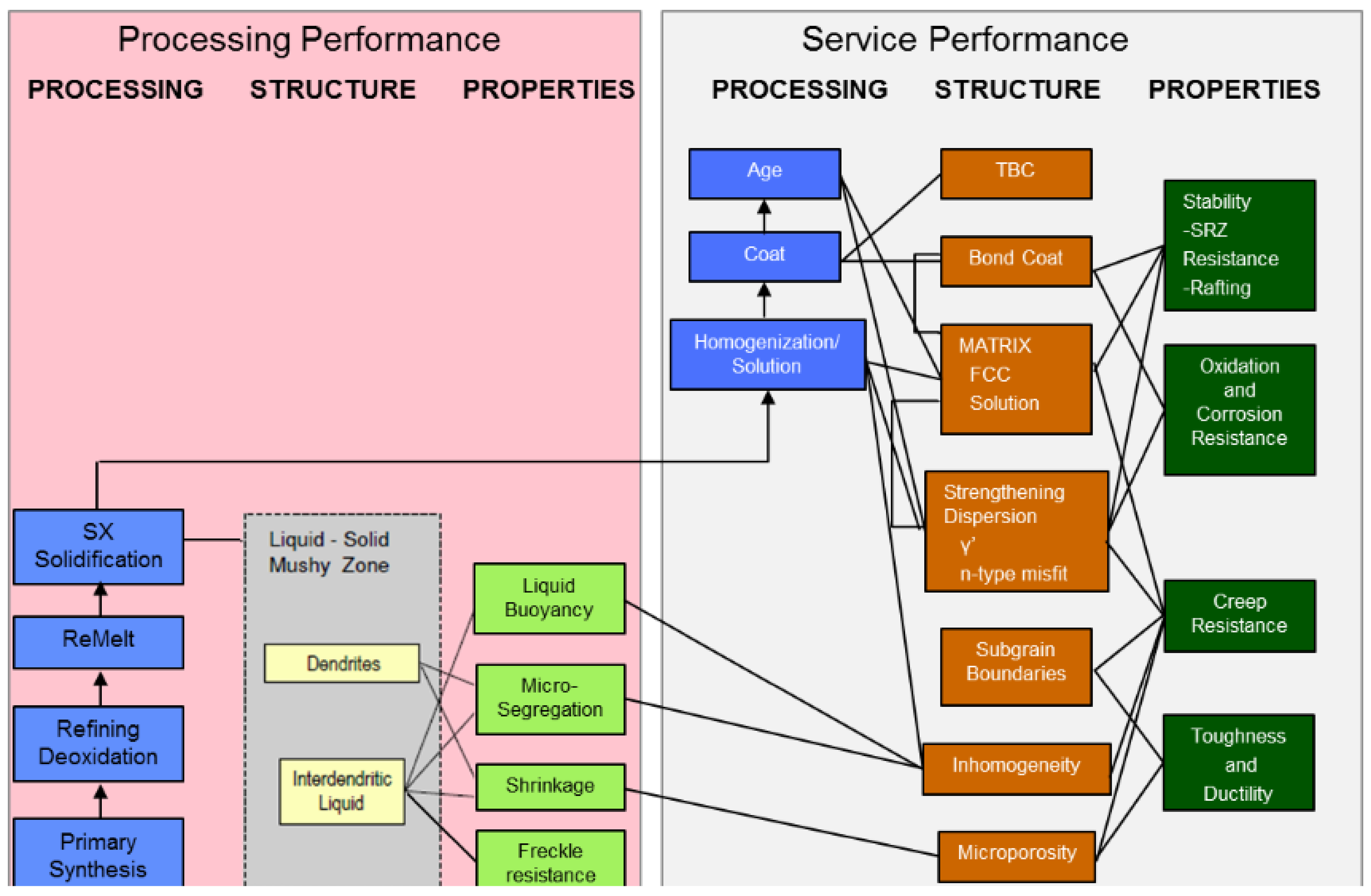
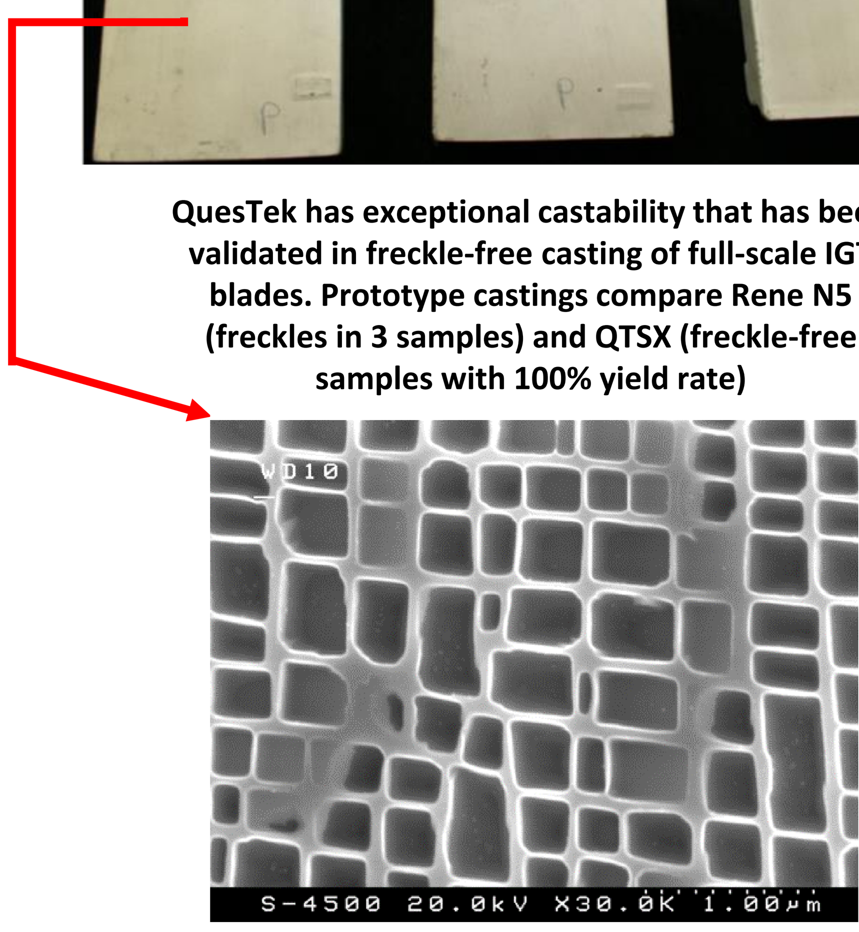
QuesTek's QTSX™ Alloy Design



ID	Re	Al	Co	Cr	Hf	Mo	Ta	Ti	W	other	
PWA1480	-	5	5	10	-	-	12	1.5	4		*Re-free alloys*
PWA1483	-	3.6	9	12.2	-	1.9	5	4.1	3.8	0.07C	
GTD444	-	4.2	7.5	9.8	0.15	1.5	4.8	3.5	6	0.08C	
CMSX7	-	5.7	10	6	0.2	0.6	9	0.8	9		*Recently-developed*
CMSX8	1.5	5.7	10	5.4	0.2	0.6	8	0.7	8		
PWA1484	3	5.6	10	5	0.1	2	9	-	6		*2nd Gen alloys*
CMSX4	3	5.6	9	6.5	0.1	0.6	6.5	1	6		
Rene N5	3	6.2	7.5	7	0.15	1.5	6.5	-	5	0.01Y	
CMSX10	6	5.7	3	2	0.03	0.4	8	0.2	5	0.1Nb	*High-Re alloys*
TMS238	6.4	5.9	6.5	4.6	0.1	1.1	7.6	-	4	5.0Ru	

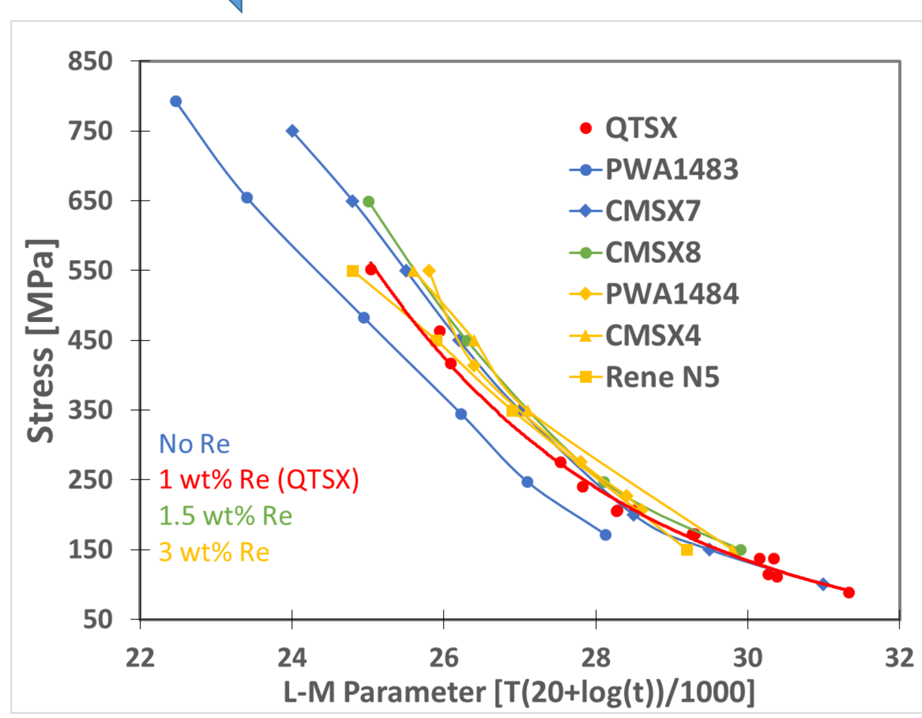
QuesTek's QTSX alloy design contains these same elemental constituents, but with 1 wt. % Re

QuesTek has exceptional castability that has been validated in freckle-free casting of full-scale IGT blades. Prototype castings compare Rene N5 (freckles in 3 samples) and QTSX (freckle-free samples with 100% yield rate)



Characterization and microstructure confirm the achievement of the design goal of γ' phase fraction and lattice misfit

Properties



QTSX shows comparable creep properties with lower Re content

Exploration of High-Entropy Alloys (HEAs) for Turbine Applications

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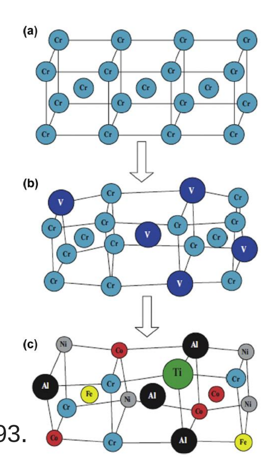
High Entropy Alloys (HEAs)

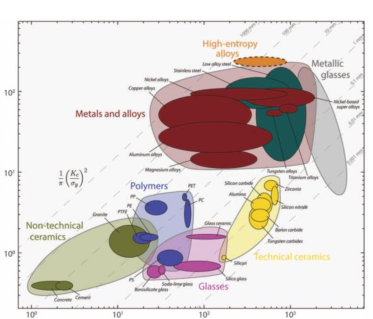
HEAs are **stable** single phase FCC, BCC, or HCP disordered solid solutions at or near equiatomic compositions in multicomponent systems (n>=5)

- BCC or FCC: AlCoCrCuFeNi and its derivatives (add Ti,Mo,V,Mn,Nb etc.)
- Refractory BCC (MoNbTaTiVW)
- HCP (AlLiMgScTi, DyGdHoTbY)



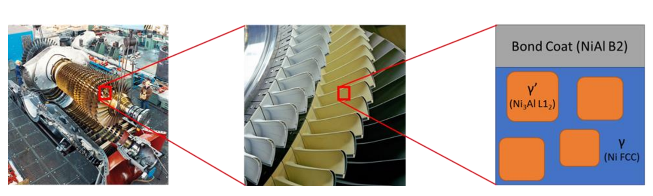
Zhang, et al. *Progress in Materials Science* 61 (2014): 1-93.

HEA Potential as IGT Blade Alloy

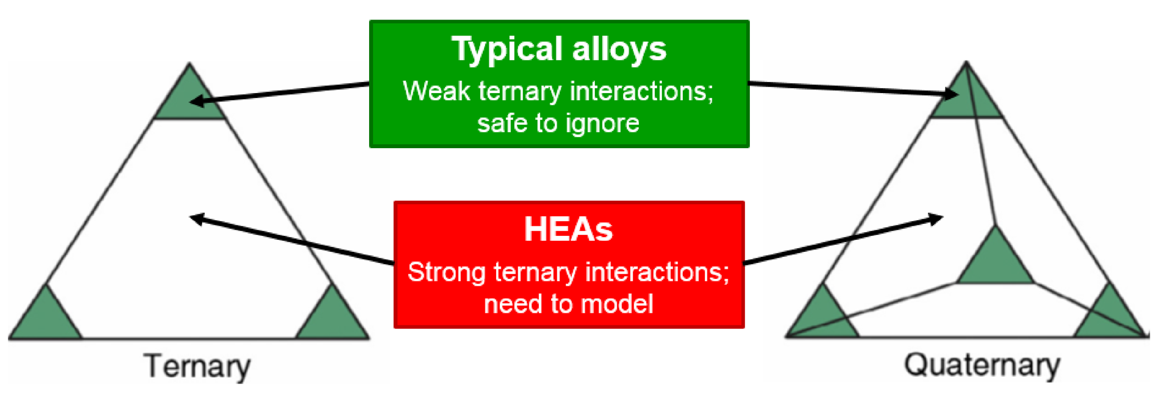


Gludovatz et al. *Science* 345.6201 (2014): 1153-1158.

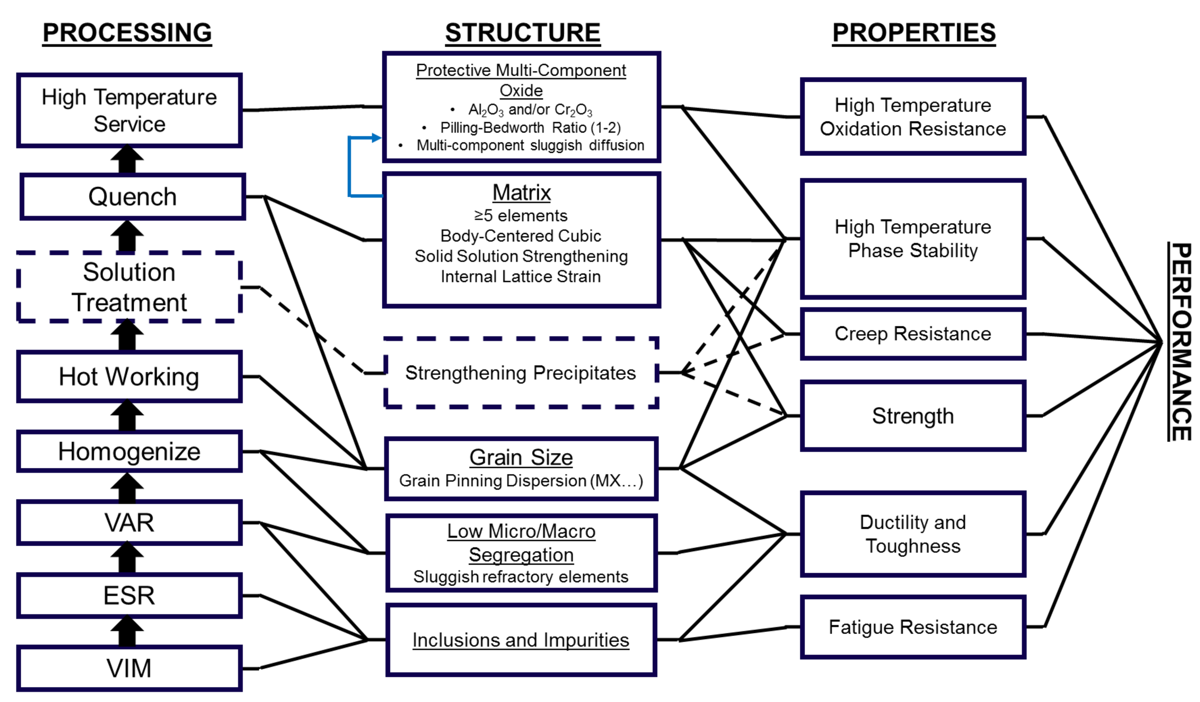
- Stability at higher temperatures than Ni/Ni_3Al
- Higher strength
- Better thermodynamic compatibility with bond coat



Primary Design Challenge: Limited CALPHAD Databases

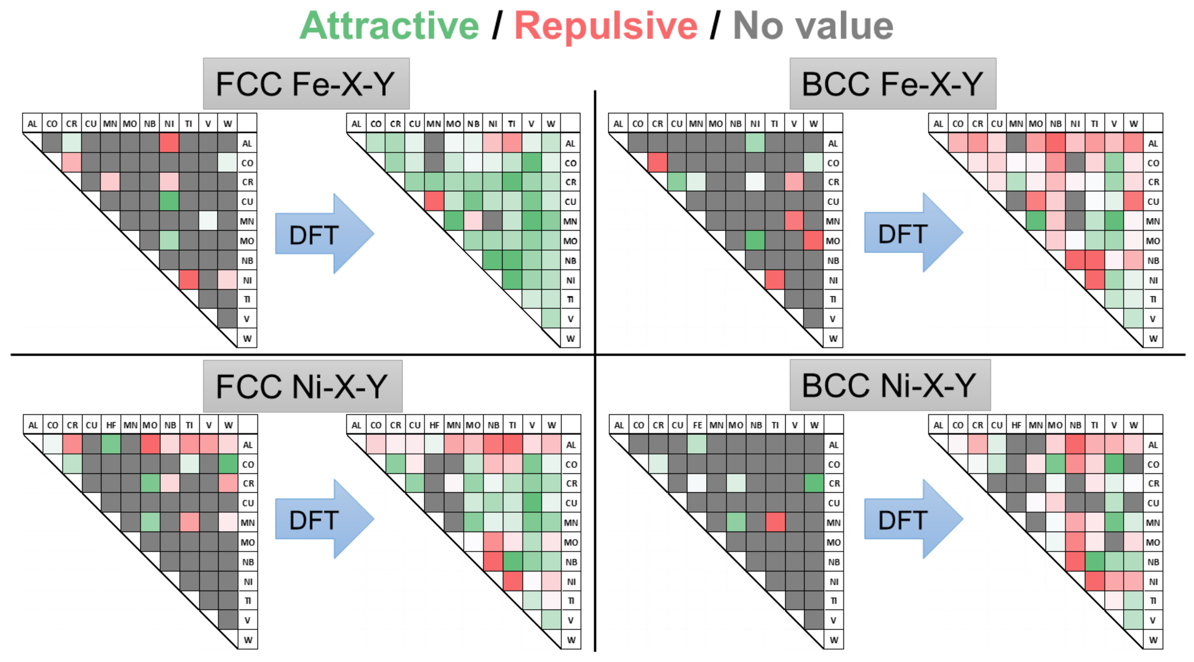


HEA Design



Phase I – Extending CALPHAD with High-Throughput DFT

Attractive / Repulsive / No value



Significant improvement in ability to predict stable HEA compositions (QT-HEA) vs. legacy CALPHAD databases (TCFE6 and TTNI7).

Database	Agreement with Exp.
TCFE6	24%
TTNI7	24%
QT-HEA	55%

Phase II Plan

- Extend HEA CALPHAD database with additional elements
- Develop HEA structure-property models
  - **Strength**: Solid solution, grain size, precipitate strengthening
  - **Oxidation**: Alumina and chromia formation
  - **Creep**: Vacancy diffusivity
- Lab-scale validation and model calibration
- Alloy design and prototype scale-up
- Collaborate with Peter Liaw at the University of Tennessee for creep and performance characterization