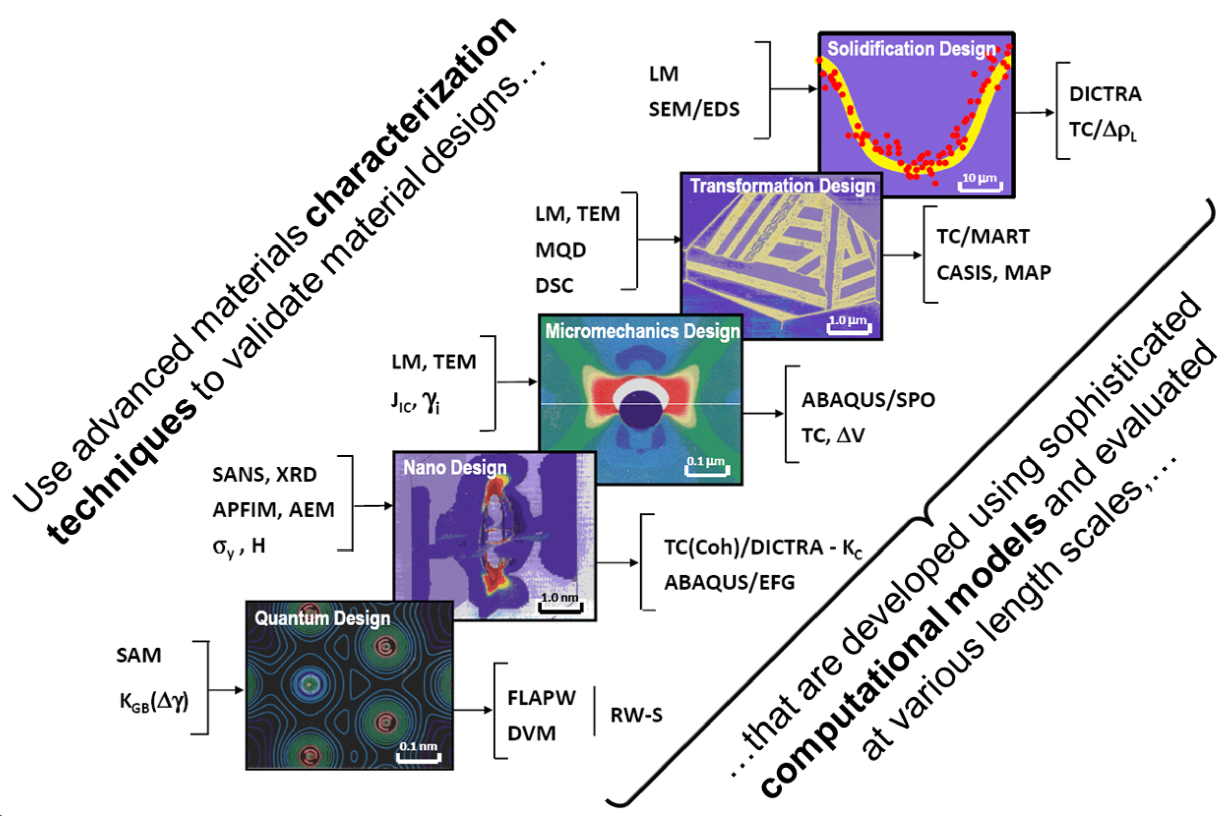
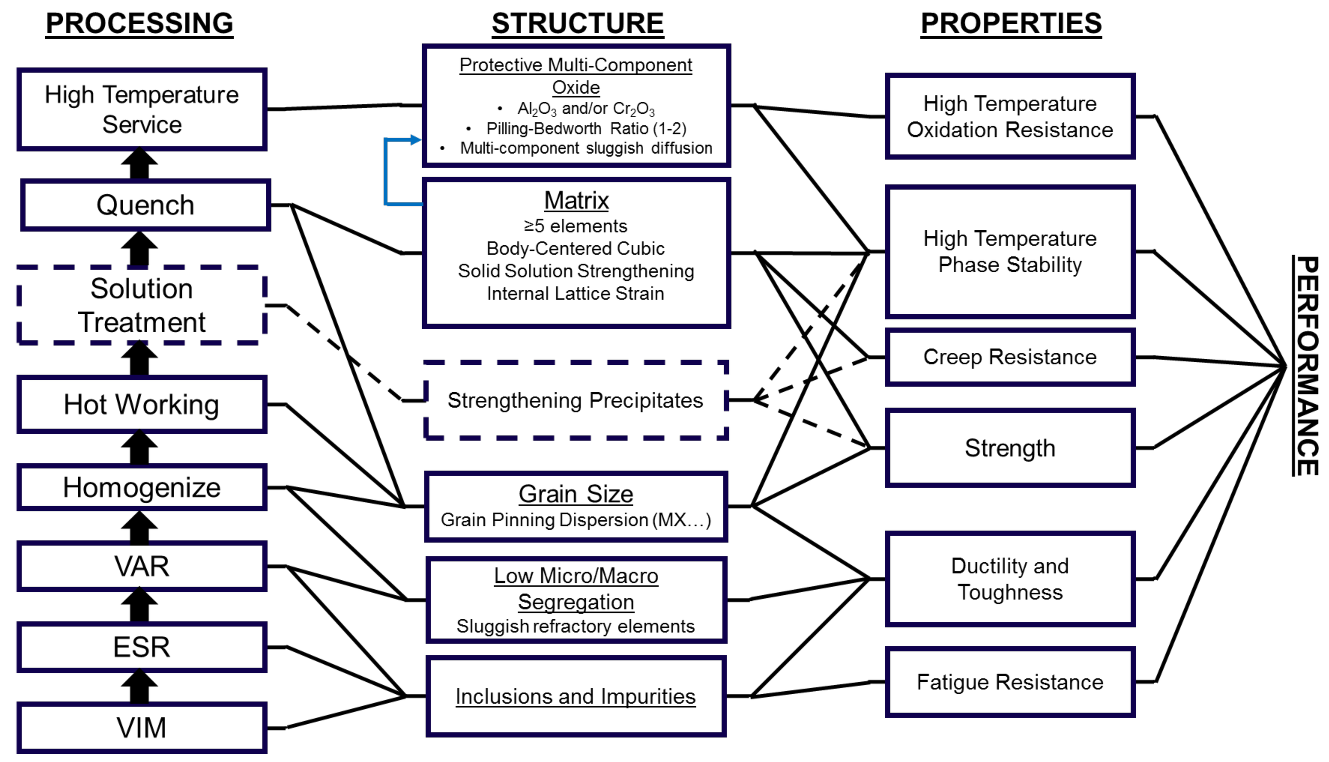
ICME Design of High-Temperature Turbine Materials
QuesTek Innovations LLC, Evanston, IL

Integrated Computational Materials Engineering (ICME) Approach to Materials Design

Hierarchy of Materials Design Models



Systems Design Chart



NIST-Funded Materials Genome Case Study

- **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 offers 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

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

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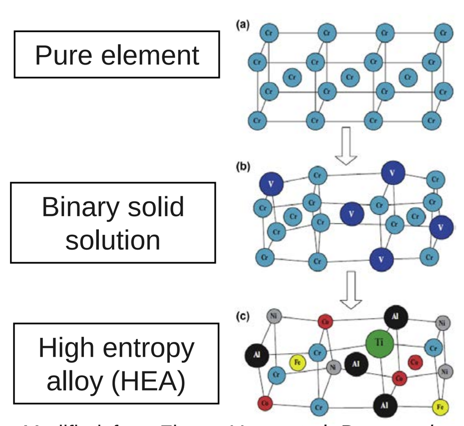
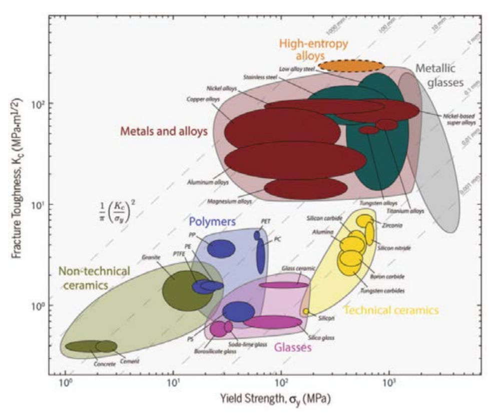
Phase II DOE NETL SBIR Program, TPOC Mark Freeman

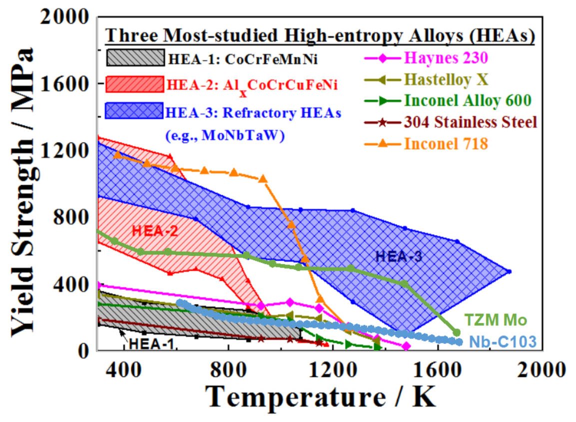
HEA Potential as IGT Blade Alloy



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

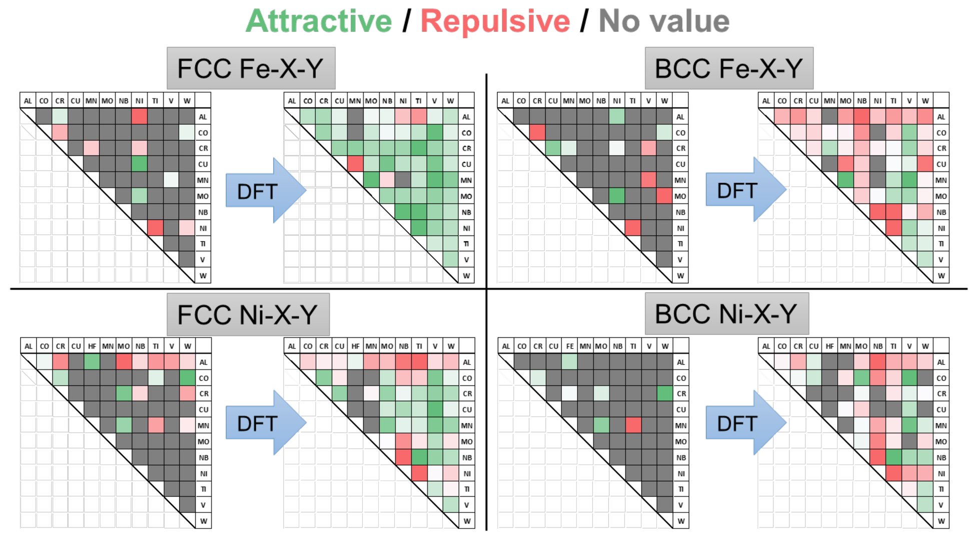


Gludovatz et al. *Science* 345.6201 (2014): 1153-1158.



Modified, from Diao et al., Curr. Opin. Solid State Mater.Sci. (2017), http://dx.doi.org/10.1016/j.cossms.2017.08.003

Phase I – Improving Design Tools with High-Throughput DFT



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

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

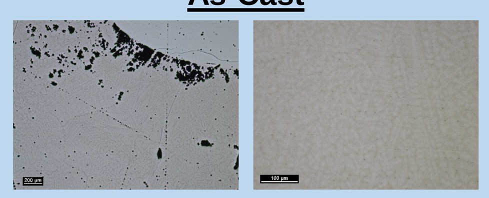
Phase II – Prototyping and Characterizing Designs

CALPHAD Design Approach

- Identify systems with acceptable freezing ranges, and solution windows
- Identify systems that should have the least amount of secondary phase formation
- Identify systems that can alloy possible oxidation protection elements (Cr, Al, etc)

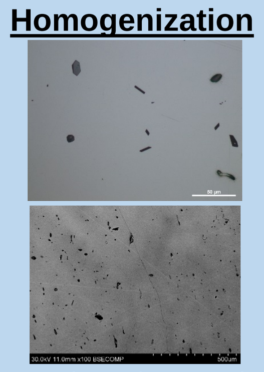
Arc Melting

As-Cast



NbMo-containing HEA, as-cast condition with unincorporated inclusions, pores and material segregation

Homogenization



AlCrMoTiV, as-homogenized, single phase with minor Al oxides

Goals:
- Produce HEAs by conventional processes (arc melting, VIM, etc.)
- Machinable, formable, and/or weldable
- Compatibility with coatings

Challenges:
- Large ΔT_m between components leads to defects
- Inherent brittleness
- Higher temperature materials have higher temperature detrimental phases (laves, sigma, etc.)
- As-cast inhomogeneity and producing numerous defects

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

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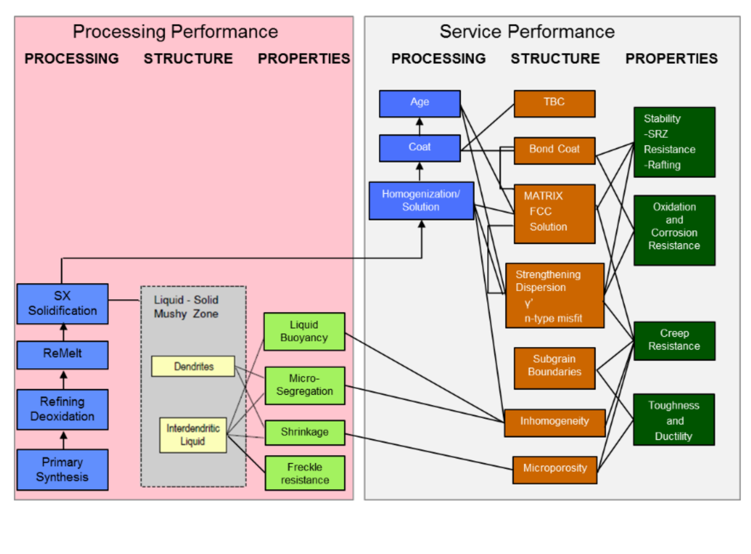
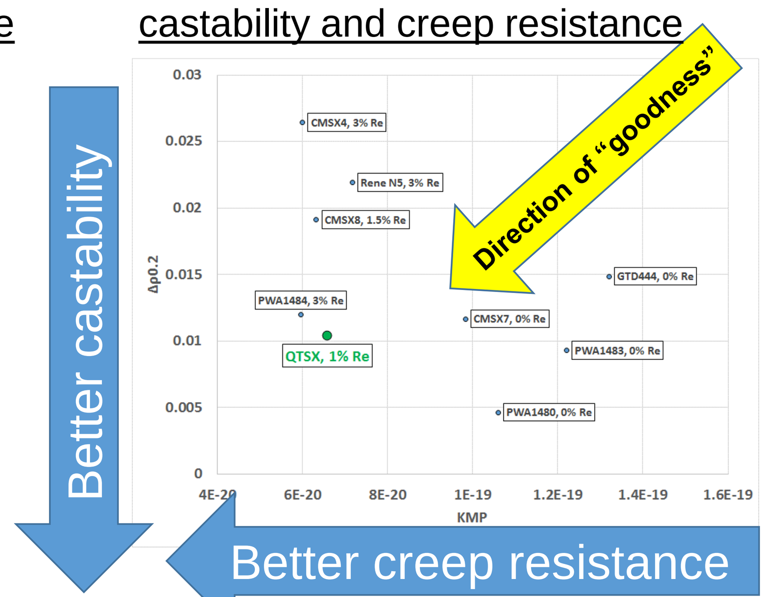
Design Challenge: Single crystal Ni superalloy with low Re, good castability, yet similar creep resistance to current alloys

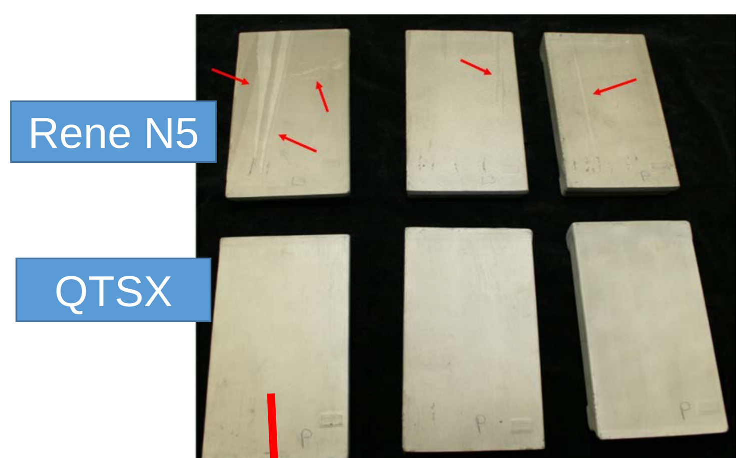
Systems-level approach to design for microstructure of crystal growth and service

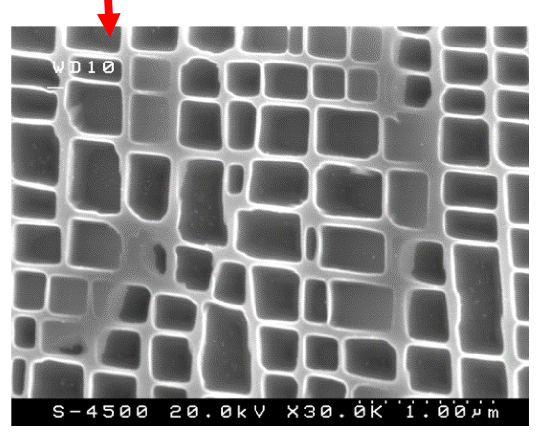


Developed models for castability and creep resistance



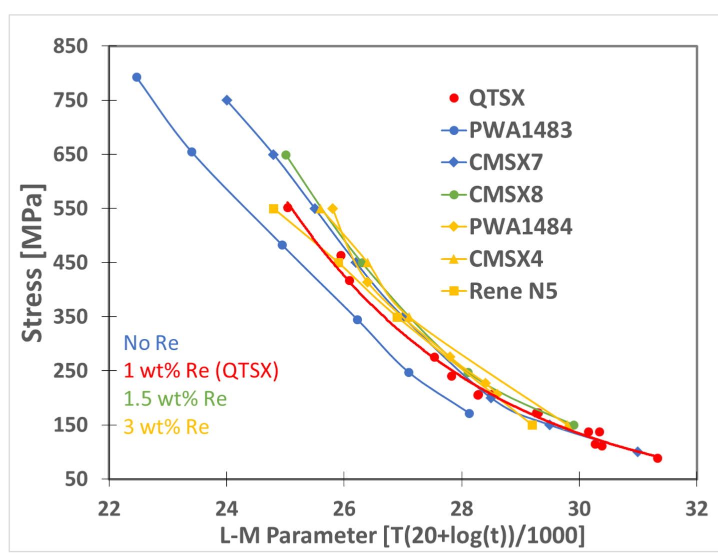
QTSX design performs well in component-level prototypes





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

QTSX 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)



QTSX shows comparable creep properties with lower Re content

Improved Models of Long Term Creep Behavior for Fossil Energy Power Plants

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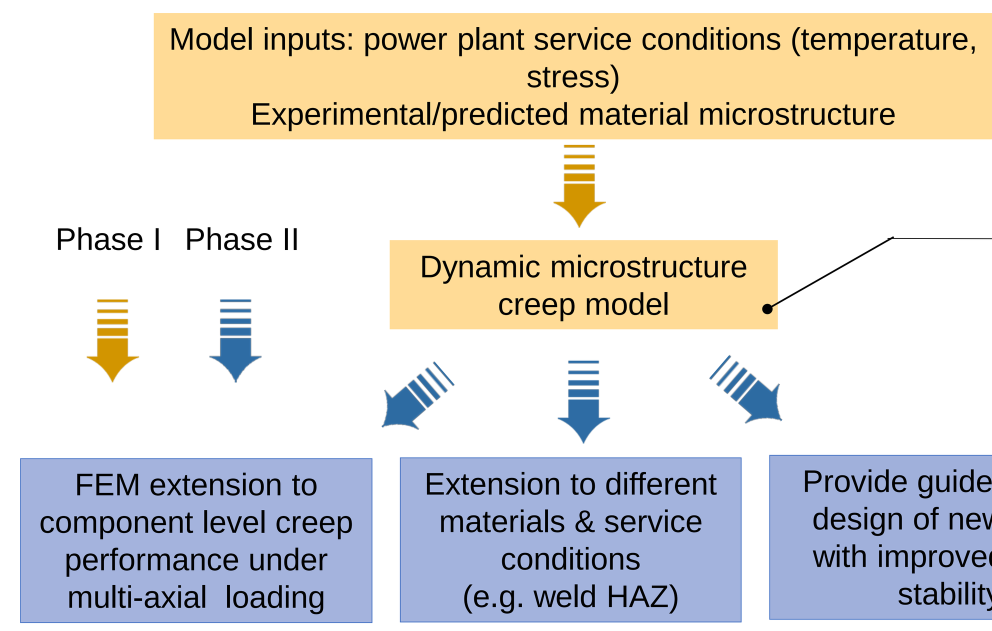
Objective: Develop a physics-based creep model that is capable of predicting long term behaviors (~300,000 hrs).



- Fundamental creep mechanisms.
- Microstructure dynamics.
- Long term creep rate as a function of (Temp, stress, microstructure).
- Validated with existing creep data (>100,000h).
- Extendable to describe creep behavior to greater than 300,000 h (~30 years).

Model Prediction with Microstructure Evolution