Computational design of high-strength, SCC-resistant aluminum alloys for aerospace applications

QuesTek Innovations LLC

Steel Research Group
Annual Meeting
March 25, 2014

Agenda

- Background – Materials Design
- Application and Problem Definition
- A computational approach to high-strength SCC resistant Al design (*Alurium*^{TM} HSCR)
- *Alurium*^{TM} HSCR alloy properties

QuesTek's ICME approach to design high-strength, SCC-resistant aluminum

Develop and apply Integrated Computational Materials Engineering (ICME) design models to design a high-strength, SCC-resistant aerospace aluminum alloy

Integrated:

- **Systems-based approach that considers all aspects of corrosion resistance, relevant microstructure, and processing steps**

Computational:

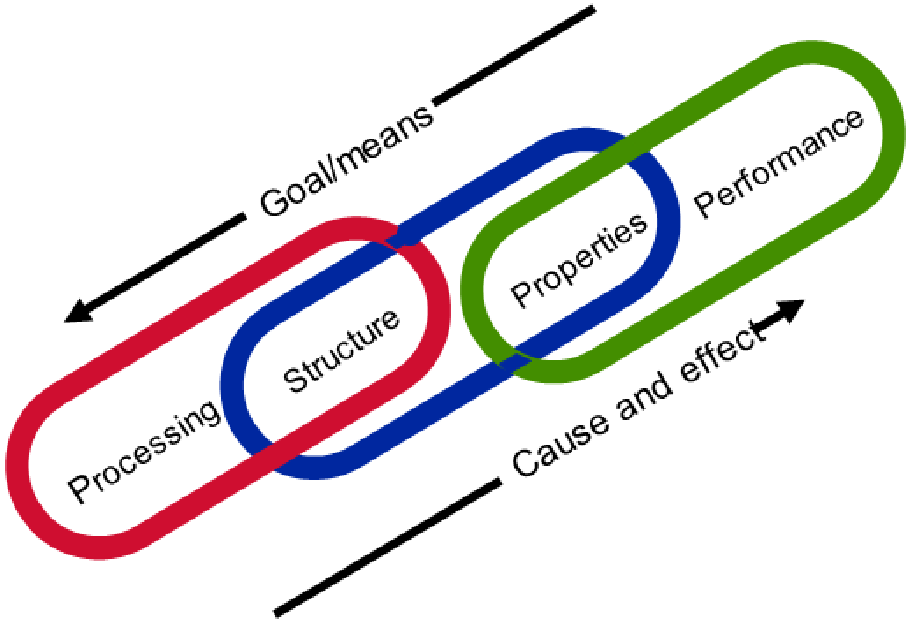
- **Mechanistic processing-structure and structure-property models that can be used in alloy design**
- **Thermodynamic models**

Materials:

- **High-strength aluminum**

Engineering

- **Solving specific problems that are relevant to aerospace applications**



QuesTek's ICME approach to design high-strength, SCC-resistant aluminum

Material Design (Structure) Tools

- Multicomponent Thermodynamics
  - Equilibrium and meta-stable phase relations and thermodynamic properties
- Multicomponent Kinetics
  - Multicomponent diffusion

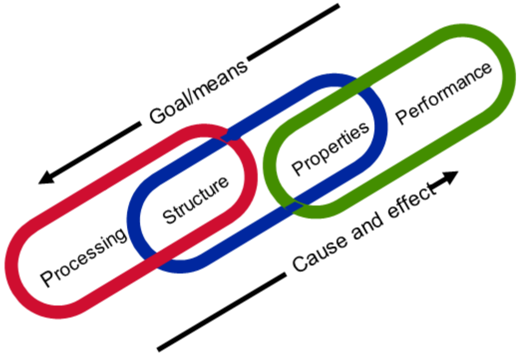
Process-Structure

- Solidification modeling
- Homogenization modeling
- Hot working simulations
- Modeling response to heat treatment (development of 2nd-phase precipitates and constituents

Structure-Property

- Quench sensitivity modeling
- Strength models
- SCC-resistance modeling
- Modeling response to heat treatment (development of 2nd-phase precipitates and constituents)

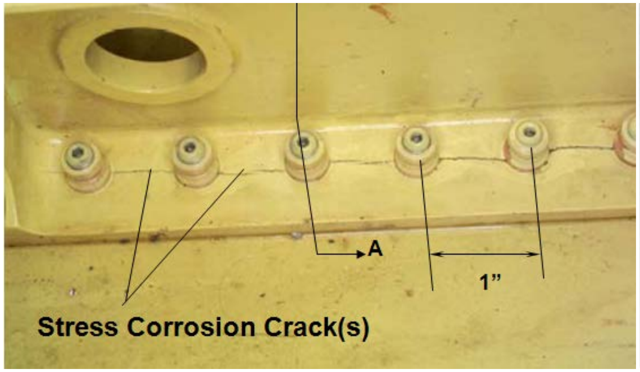
1. Develop multi-scale, mechanistic models to describe the interaction of relevant microstructural features with properties and processing steps
2. Integrate the models into a consistent software platform for computational alloy design
3. Apply the models in conjunction with thermodynamic tools and models for processing and relevant aluminum alloy properties to design a high-strength, SCC-resistant aluminum alloy for aerospace applications



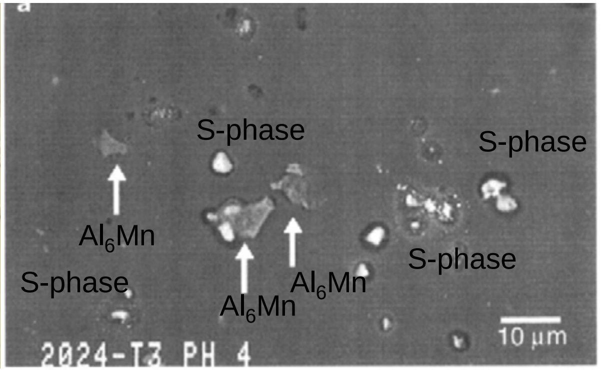
APPLICATION AND PROBLEM DEFINITION

Problem Definition – Stress Corrosion Cracking (SCC)

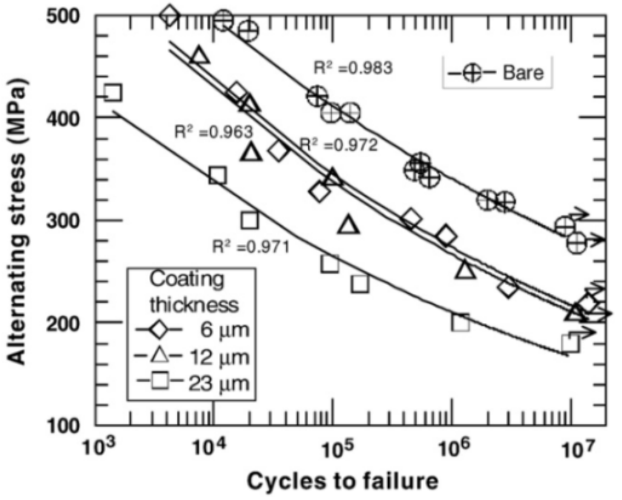
- **Light-weight, high-strength Al alloys are widely used for structural components of aircraft and ships**
- **High-strength Al alloys (such as 7050) are highly susceptible to stress corrosion cracking and general corrosion**
  - Repair and maintenance of corroded components a major cost driver
  - Heavy anodized coatings necessary for corrosion protection result in significant fatigue strength debit
- **New high-strength Al alloys are needed with microstructures optimized for SCC resistance**
  - Allows for the reduction or elimination of heavy anodized coatings, reduced fatigue debit and greater structural integrity



SCC failure in 7xxx alloy aircraft structures

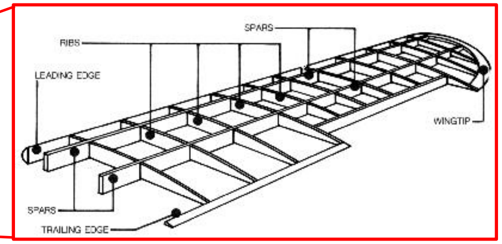


Pitting corrosion around S-phase particles in 2024-T3

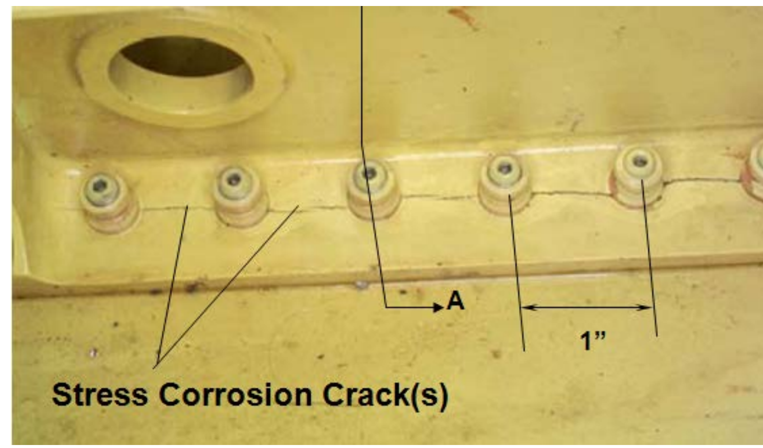


Effect of anodize coating thickness on fatigue life of 7075-T6

Application of Interest – Aircraft Wing Structures



Schematic of an aircraft wing structure



SCC failure in 7xxx alloy aircraft structure

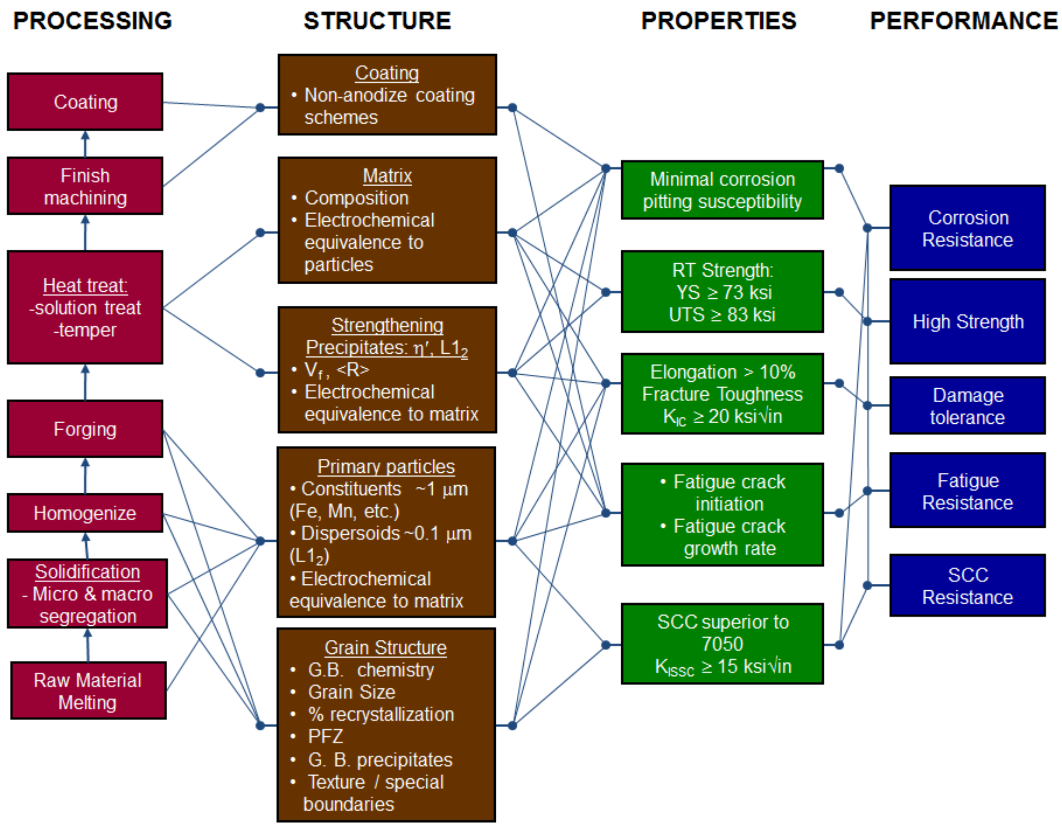
<u>Aircraft wing structural components</u>

- Currently made out of high-strength aluminum (such as 7050) and titanium
- Uncoated high-strength Al alloys are susceptible to various forms of localized corrosion in chloride environments, such as **Stress Corrosion Cracking (<u>SCC</u>)**, pitting, crevice, intergranular corrosion, and exfoliation corrosion

Alloy Design

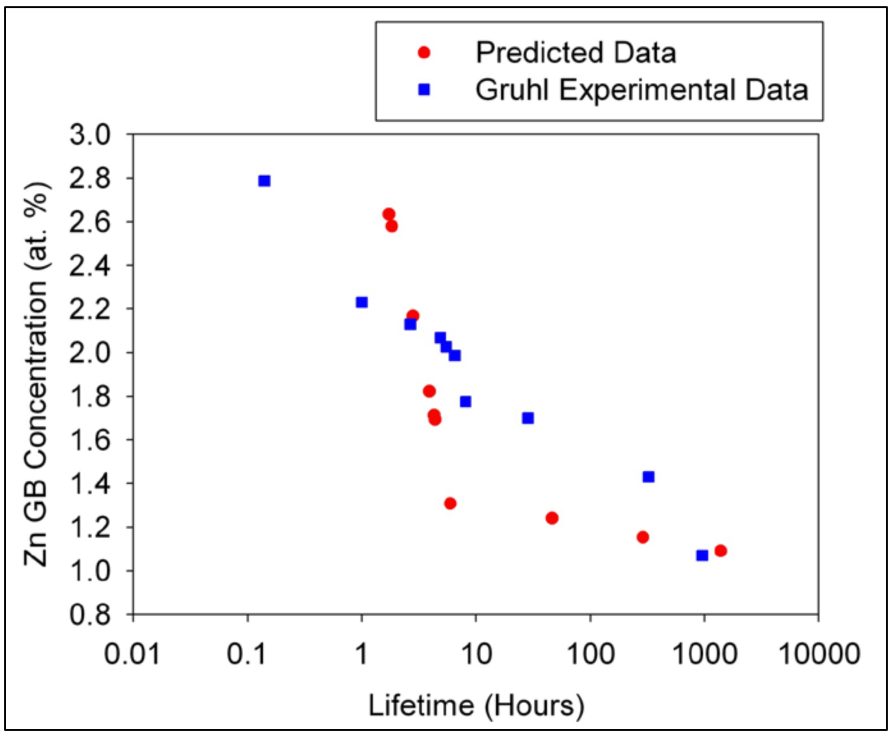
Critical Design Factors include:

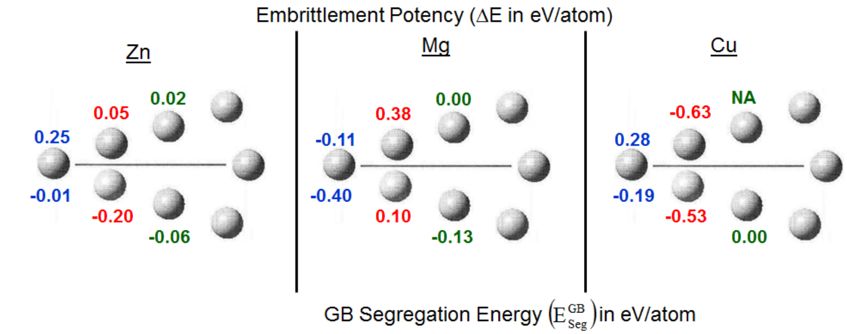
1. Tensile Strength
   - **Optimize strengthening precipitate fractions within 7xxx design space**
   - **Minimize quench sensitivity**
2. SCC resistance and toughness
   - **Grain boundary chemistry**
   - Refinement/elimination of grain boundary particles
   - **Minimize OCP difference between matrix and precipitate phases**
   - Optimal grain pinning – inhibit recrystallization
3. Fatigue
   - Maximize general corrosion resistance to minimize need for coating (reduced coating thickness)
4. Manufacturability
   - Thermal processing windows (homogenization, solution treatment)
   - Conventional alloying additions (cost)

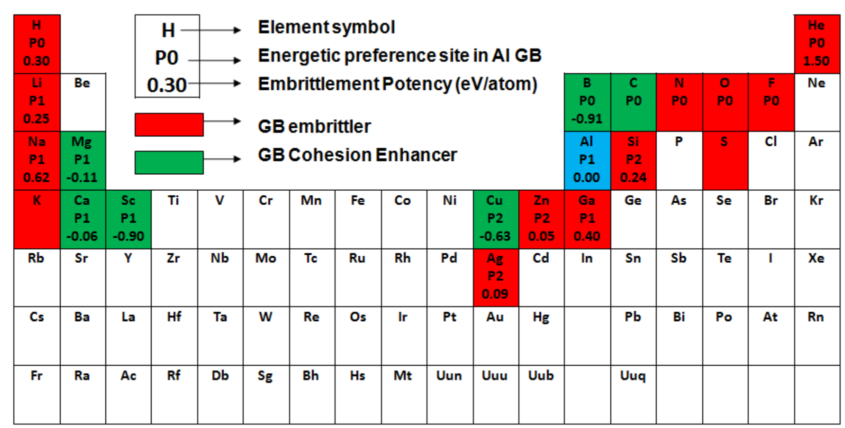


Alloy Design - Stress Corrosion Cracking

- **Grain-boundary segregation**
  - Certain alloying additions embrittle grain boundaries, others promote cohesion
  - DFT ab-initio calculations inform grain boundary segregation energy and embrittling potency of various alloying elements
  - *Design consideration - Accurate SCC lifetime predictions based on thermodynamic and DFT calculations of grain boundary character*

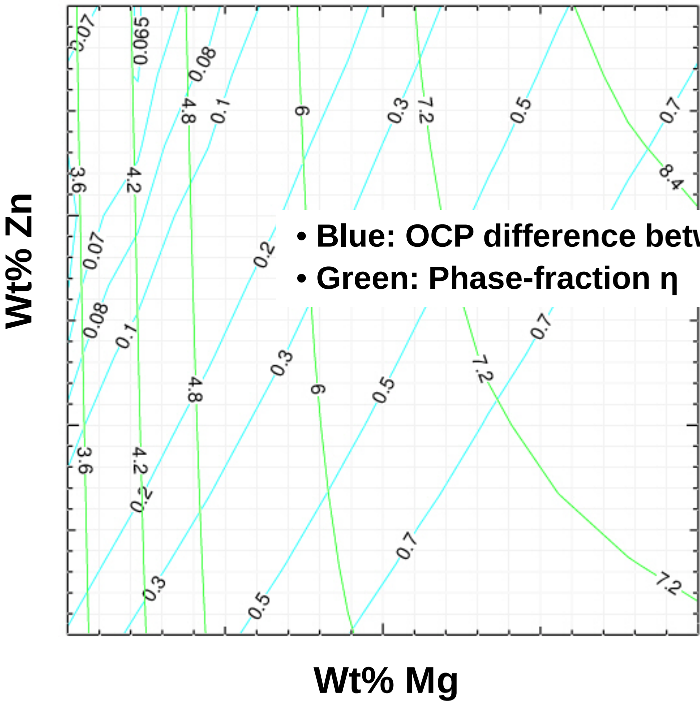






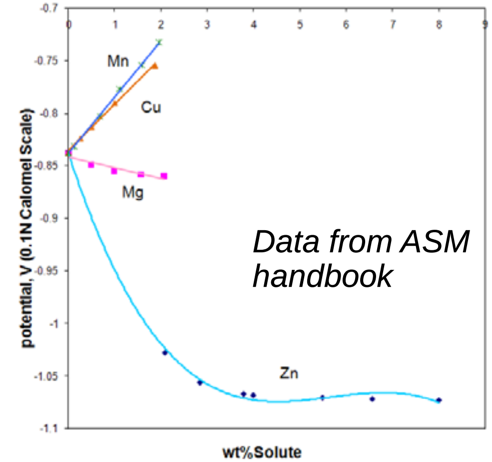
Alloy Design - Stress Corrosion Cracking

- **Corrosion potential difference between matrix and precipitates a major driver of pitting, SCC**
  - Corrosion potential of different phases predicted as a function of chemistry, integrated into computational design
  - *Design consideration - Minimize potential difference between phases to minimize anodic dissolution mechanism of SCC*

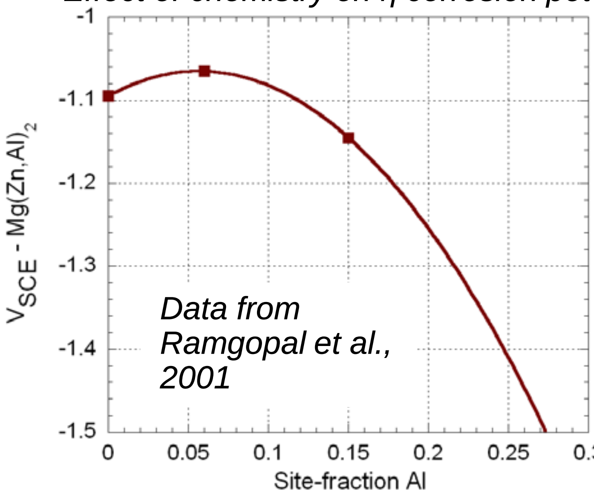


- **Blue: OCP difference between matrix and η**
- **Green: Phase-fraction η**

Effect of chemistry on matrix corrosion potential

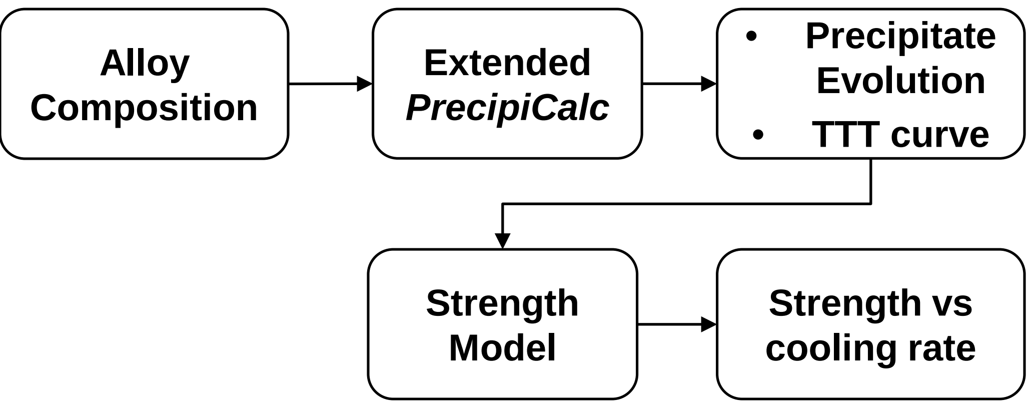


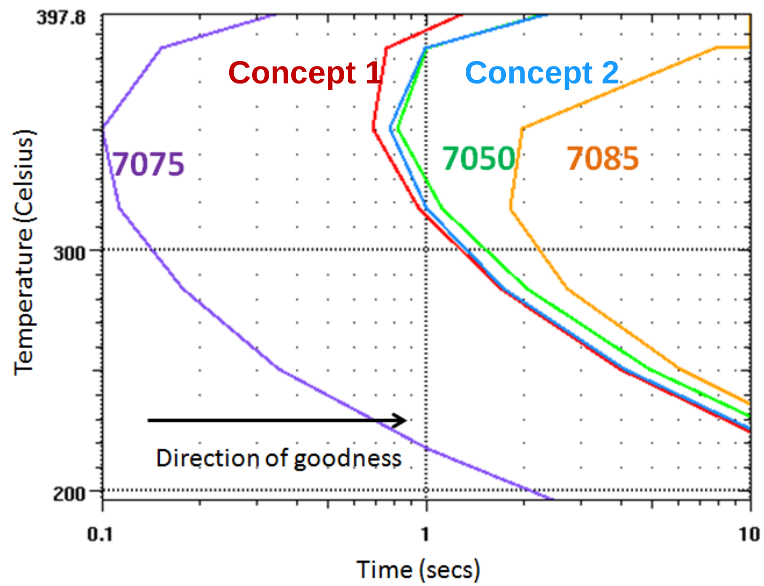
Effect of chemistry on η corrosion potential



Alloy Design – Quench Sensitivity

- PrecipiCalc extension to predict precipitation during cooling from solution treatment in 7xxx series Al
- Combine with strength models to predict critical cooling rate to avoid strength loss due to quench sensitivity
- Integrated with thermodynamic/mobility databases to predict quench sensitivity as a function of composition



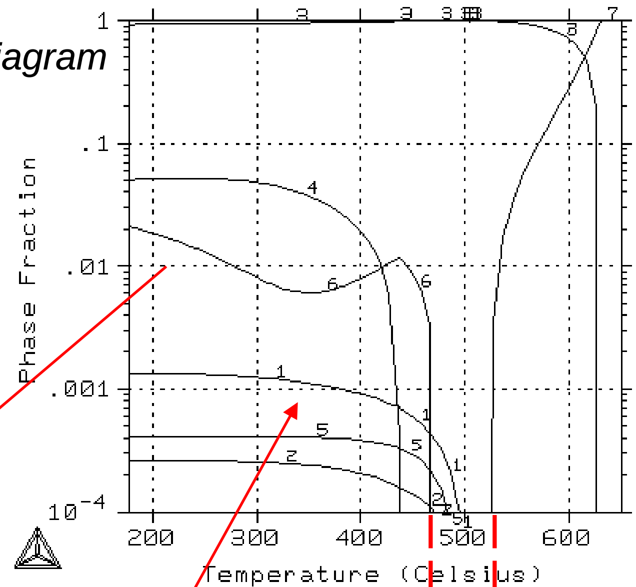


Isothermal TTT curve predictions of 1% strength loss in various 7xxx series alloys and two QuesTek concept alloys

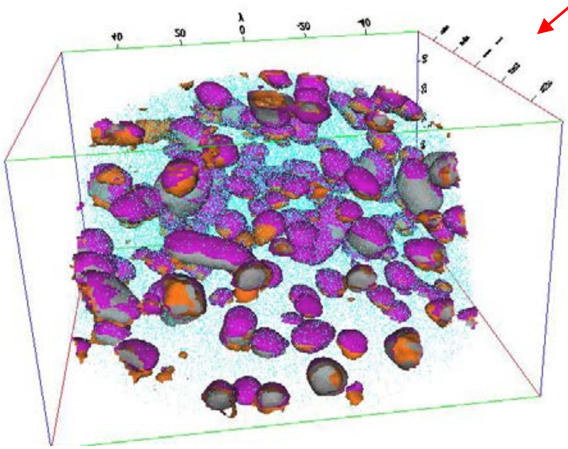
Alloy Design

- **Thermodynamic calculations inform phase stability as a function of composition for tailored microstructures and control of processing windows**
- **Solidification and homogenization modeling to identify optimal processing conditions**

Example equilibrium step diagram



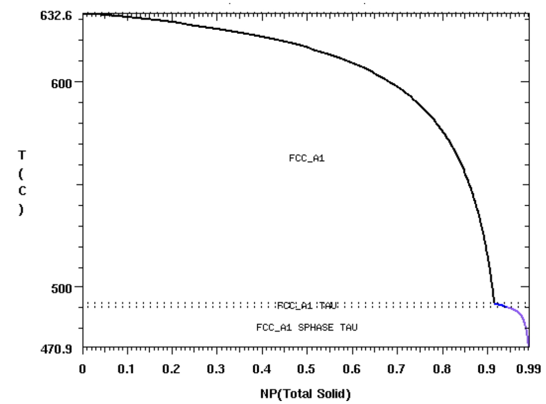
Strengthening precipitate structures (LEAP)



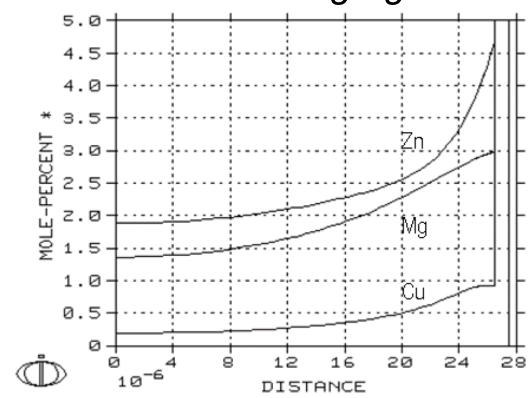
Grain pinning dispersions

Solutionizing windows

Scheil solidification

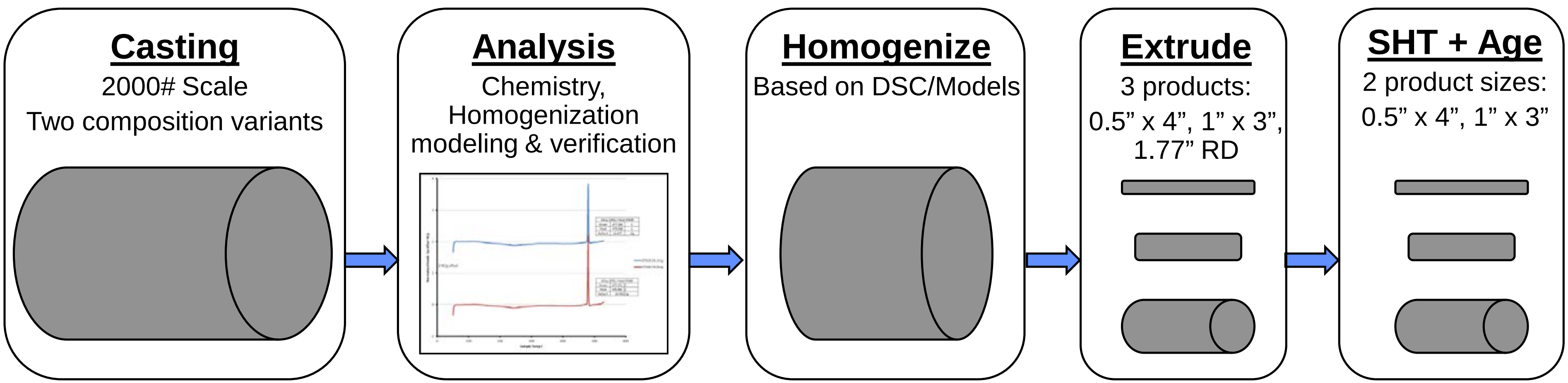


Solidification segregation

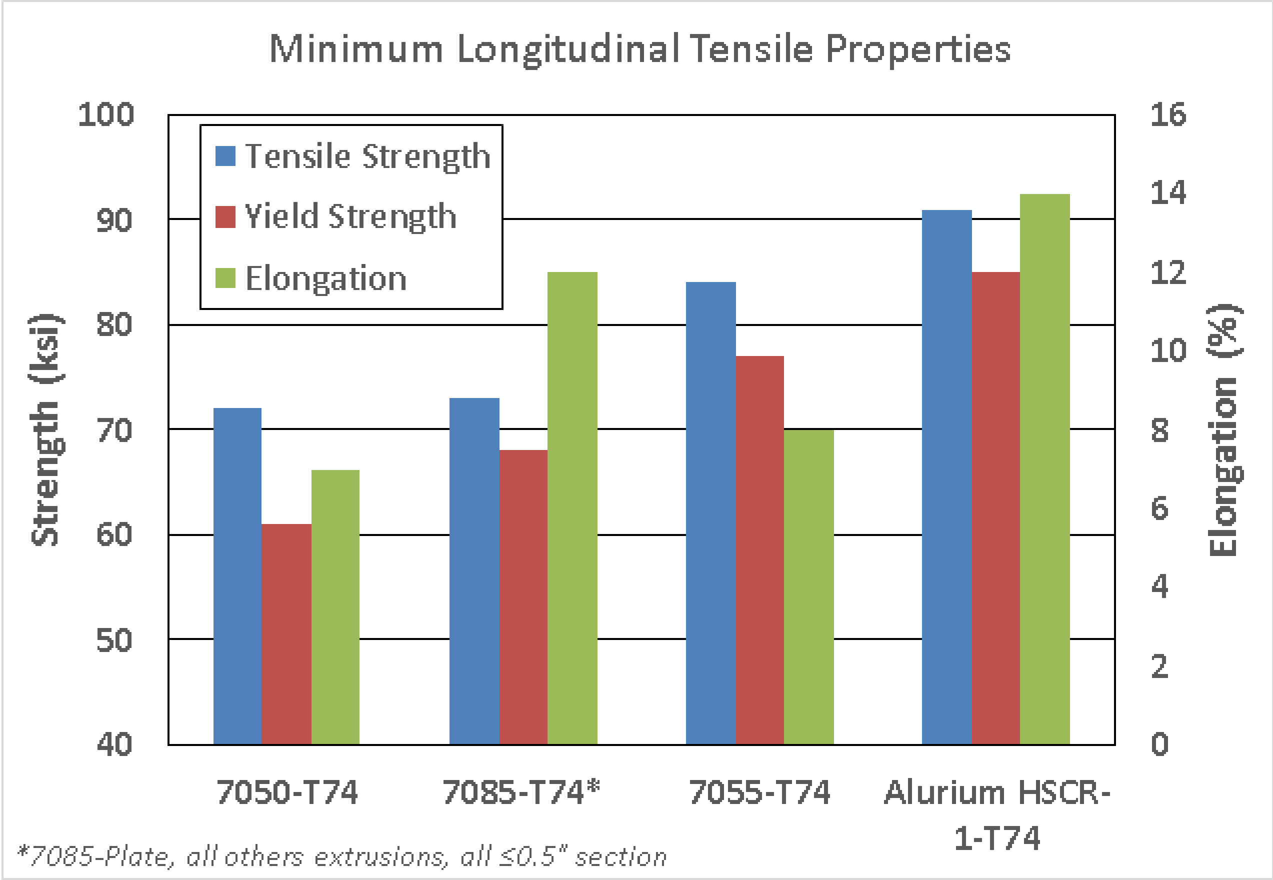


Alloy Production

- **Full-scale production of *Alurium* HSCR**
  - Melting at Universal Alloy Corp, Anaheim, CA at 2000 lb scale
  - Homogenization, extrusion to multiple product forms following production path relevant to aircraft structural components
  - Solution treated and aged to T6, T7x conditions
  - Detailed characterization in progress



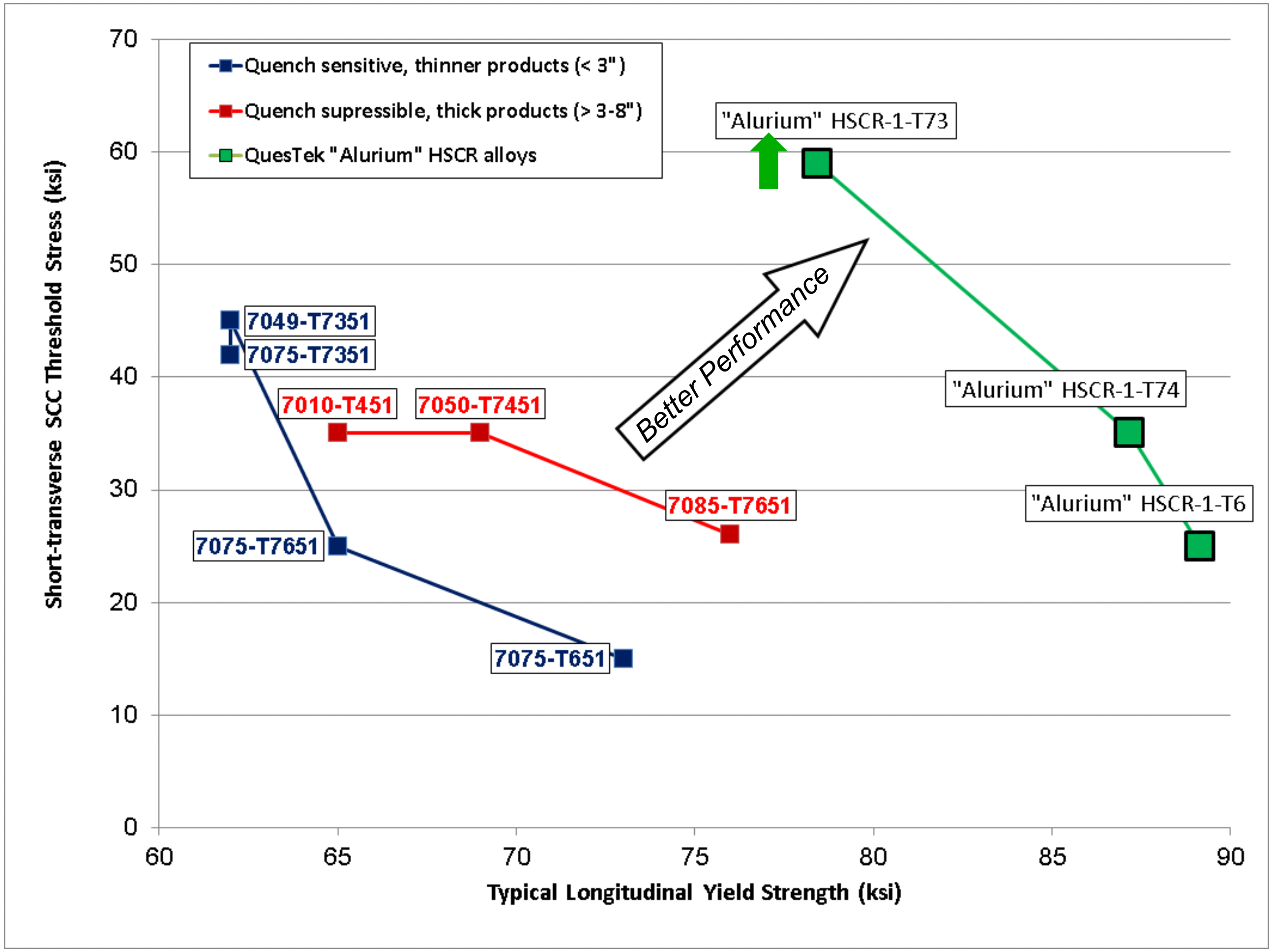
Characterization – Tensile testing



Improved strength and ductility over incumbent 7xxx alloys in equivalent temper condition

Data development in a range of temper conditions in progress

Characterization – Strength vs SCC resistance



Alurium HSCR alloy achieves a combination of strength and SCC resistance that is significantly better than incumbent aluminum alloys

Data development on various heat treatment conditions in progress

Alloy Characterization

- **Complete - Tensile testing, SCC threshold stress testing (ASTM G47)**
- **In process – Additional G47 testing, fracture toughness (K_{IC}, K_{ISCC}), fatigue crack growth, axial fatigue, ASTM B117 salt fog and exfoliation corrosion testing, coating evaluations**

Summary

- QuesTek's computationally designed *Alurium* HSCR alloy achieves a combination of strength and SCC resistance not achieved by commercial alloys, including:
  - **15-25% higher strength than 7050-T74 in the longitudinal direction**
  - **G47 threshold stress > 75% of longitudinal yield strength in T73 condition**

Acknowledgements and References

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