CALPHAD Modelling and Integrated Computational Materials Engineering (ICME) for Materials Design

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Agenda

- Introduction to QuesTek
- CALPHAD for practical alloy design problem solving
  - *Ferrium*® M54® scale-up and qualification
  - *Ferrium* C64® composition optimization
  - QT-SX Ni-superalloy single-crystal design

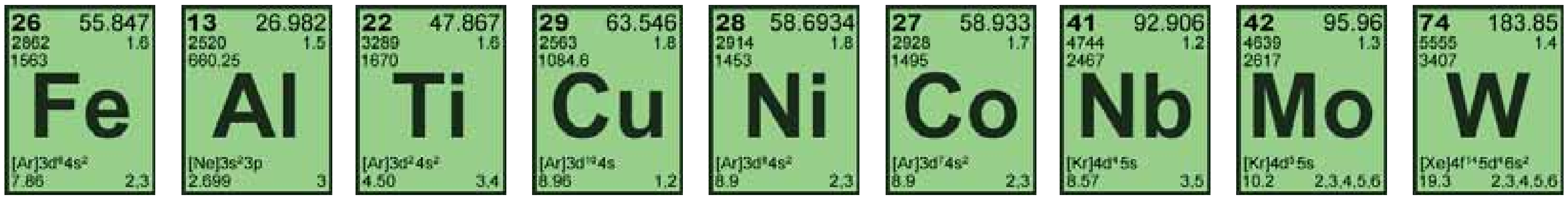
Introduction to QuesTek

Background—QuesTek Innovations LLC

- Founded 1997 (Prof. Greg Olson, cofounder)
- 23 employees (13 with PhD, 6 with MS, 4 with BS)
- 12 US patents awarded (and 18 US patents pending)
    - 25 foreign (and 21 foreign pending)
- Create IP and license it to producers, processors, OEMs, end-users
- 4 commercially available steels

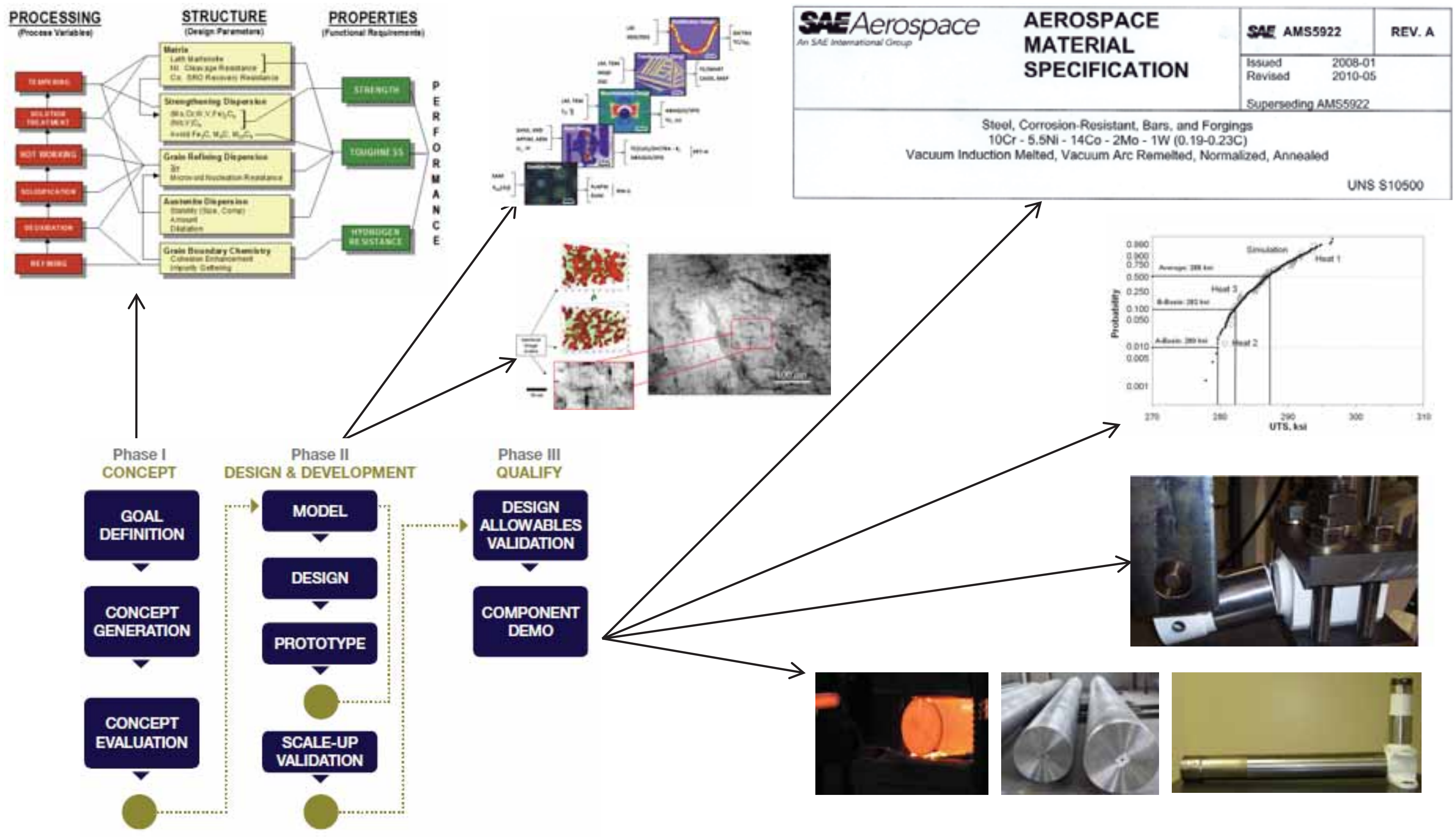
Background—QuesTek Innovations LLC

- A global leader in computational materials design:
  - Our ***Materials by Design***® expertise applies the ***Integrated Computational Materials Engineering*** **(ICME)** technologies and ***Accelerated Insertion of Materials*** (AIM) methodologies to design an deploy innovative, novel materials faster and at less cost than traditional methods
  - Aligned with the US ***Materials Genome Initiative***
- Designing novel alloys for government and industrial sectors



QuesTek's *Integrated Computational Materials Engineering* approach

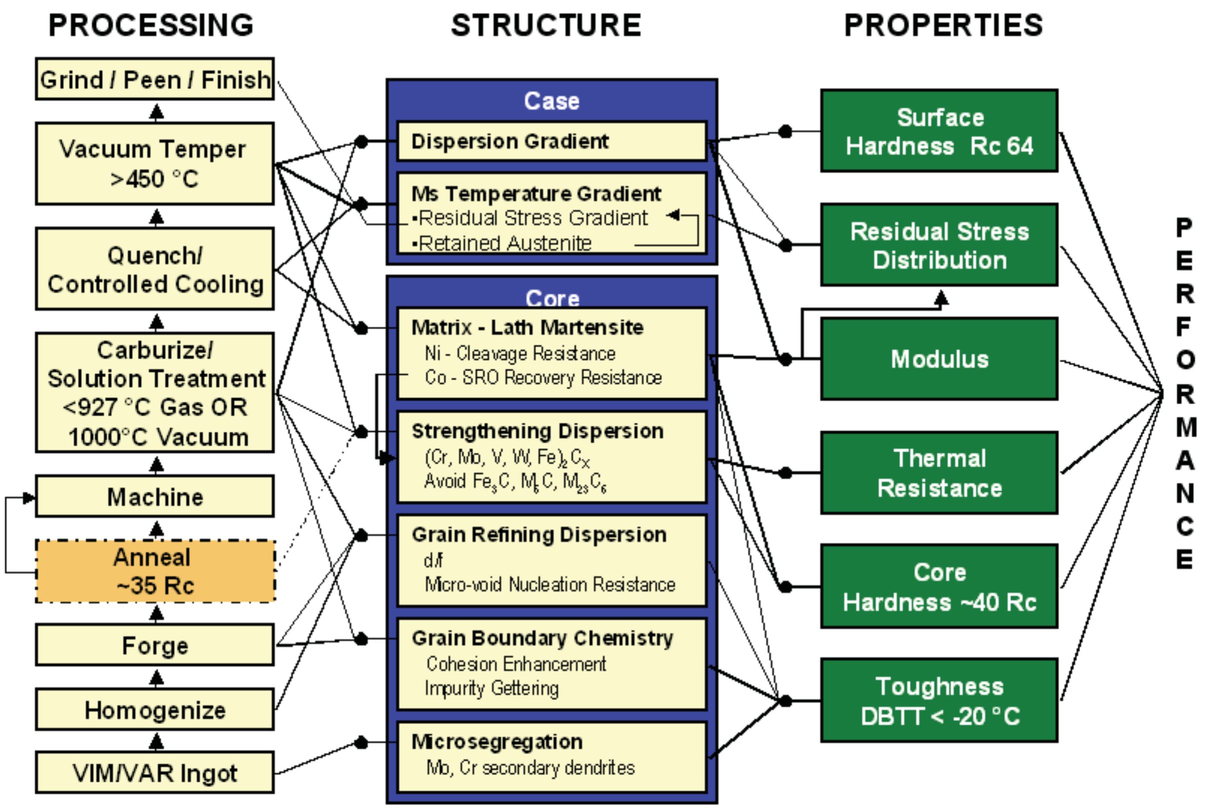
"Integrated Computational Materials Engineering (ICME) methods involve the holistic application of different computational models across various length scales to the design, development, and rapid qualification of advanced materials."



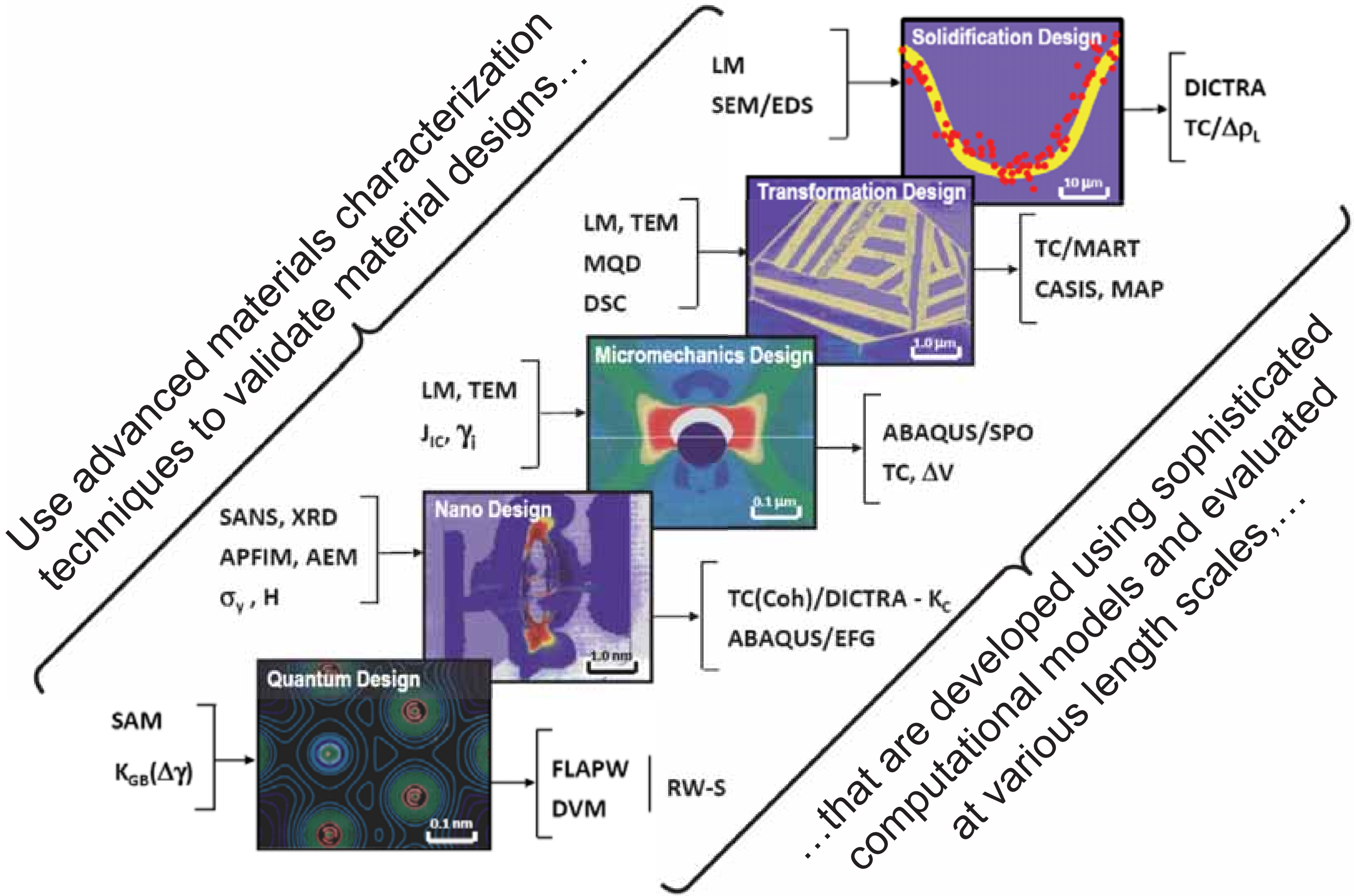
Computational materials design overview:
Systems design charts

Design material as a system to meet customer-defined performance goals

e.g. this "Design Chart" for *Ferrium* C64 was developed under a contract resulting from U.S. Navy Solicitation Topic #N05-T006.



Computational materials design overview:
Computational modeling and experimental tools



QuesTek's ICME-designed *Ferrium*® steels

- *Ferrium* M54® (AMS 6516; MMPDS) structural steel
  - Greater strength, toughness, fatigue resistance over 300M / 4340; excellent resistance to stress corrosion cracking (SCC).
- *Ferrium* S53® (AMS 5922; MMPDS) structural steel
  - Corrosion-resistant upgrade from 300M / 4340.
- *Ferrium* C64 ® (AMS 6509), carburizing
  - Greater strength, surface hardness, toughness, temperature and fatigue resistance vs. AISI 9310 and Alloy X53.

Commercially available from Carpenter Technology

CARPENTER®

Increasing number of applications across commercial and military aerospace

Ferrium M54 scale-up and qualification

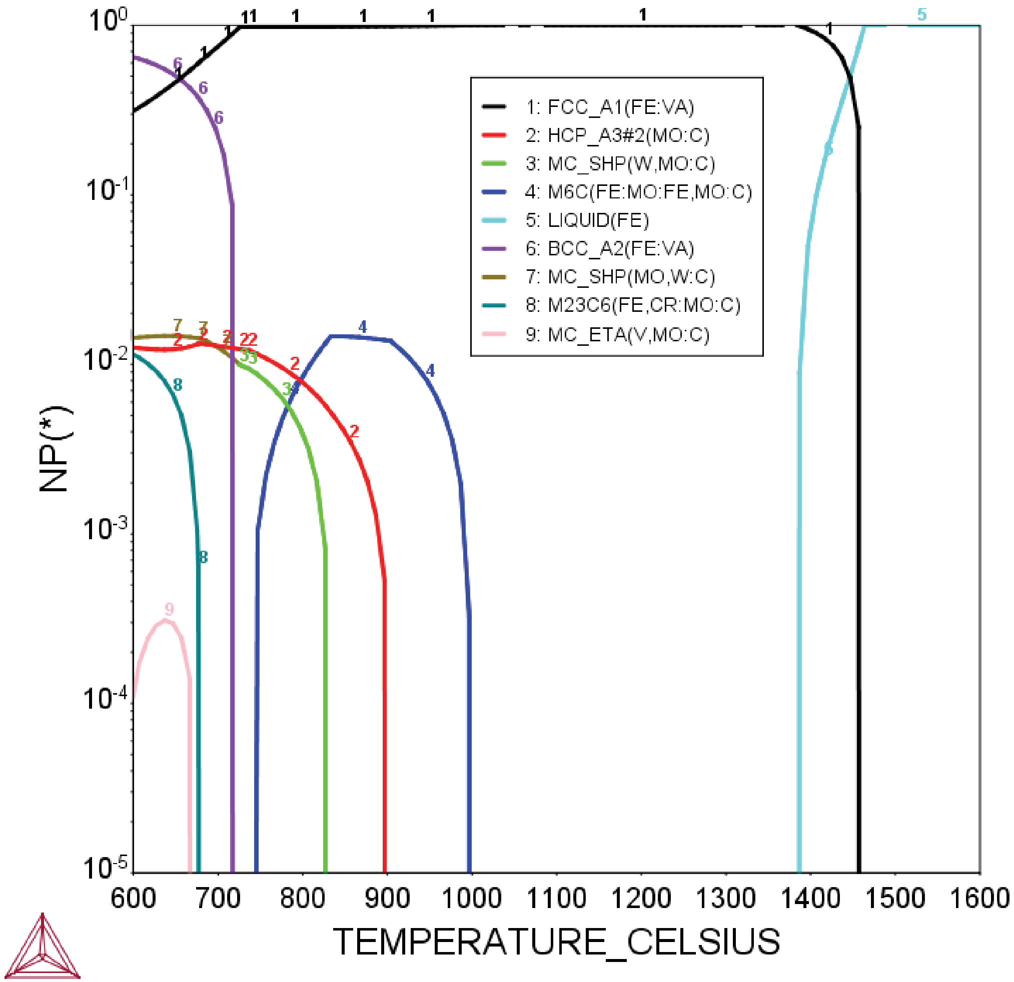
M54: Improved Minimum Properties vs. Other VIM/VAR Steels

	4340 (AMS 6414)	300M (AMS 6419)	*AerMet*100 (AMS 6532)	*Ferrium* M54 (AMS 6516)
S-basis Minimum Ultimate Tensile Strength (MPa)	1792	1930	1931	1965
S-basis Minimum 0.2% Yield Strength (MPa)	1496	1585	1620	1655
Minimum K_{IC} Fracture Toughness (MPa-√m)	~49*	~44*	110	110
Reported Minimum K_{ISCC} (MPa-√m)	~11	~11	~24	~96

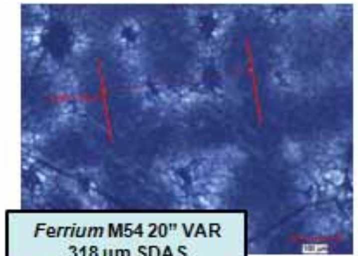
* No procurement minimum

M54 has higher S-basis minimums, 4x the SCC resistance, and a lower raw material cost than AerMet 100

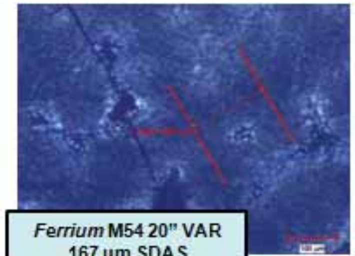
CALPHAD Thermodynamic Foundation: M54 1-D Phase Diagram, “step diagram”



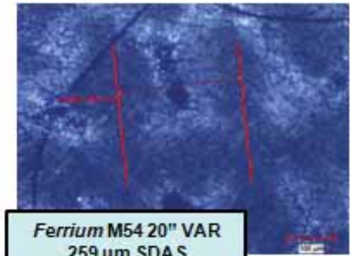
Scale up of M54:
Predict segregation and ensure homogenization



Ferrium M54 20" VAR
318 µm SDAS

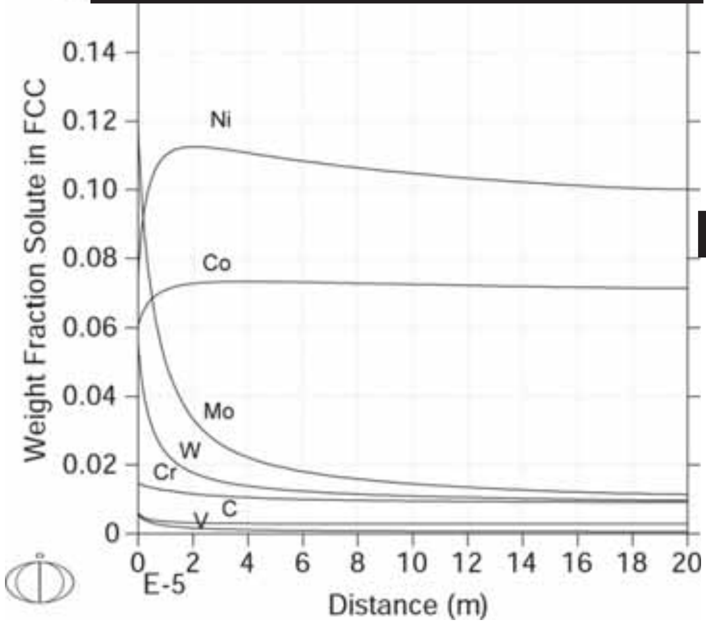


Ferrium M54 20" VAR
167 µm SDAS

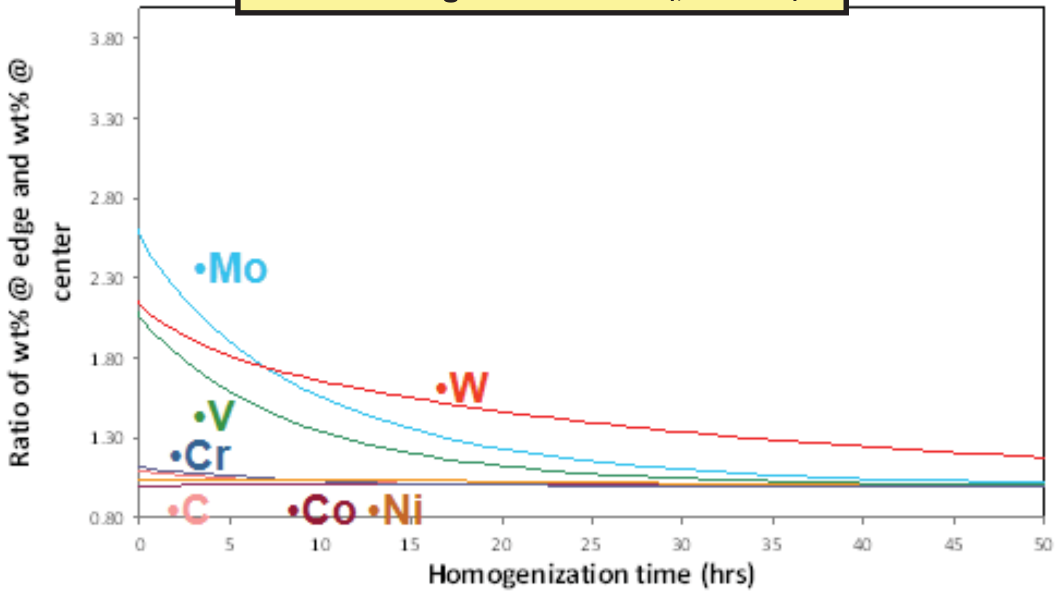


Ferrium M54 20" VAR
259 µm SDAS

M54 solidification simulation

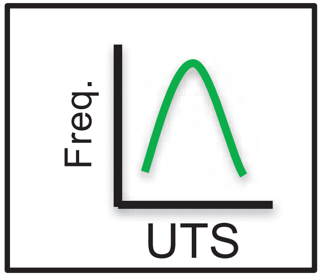


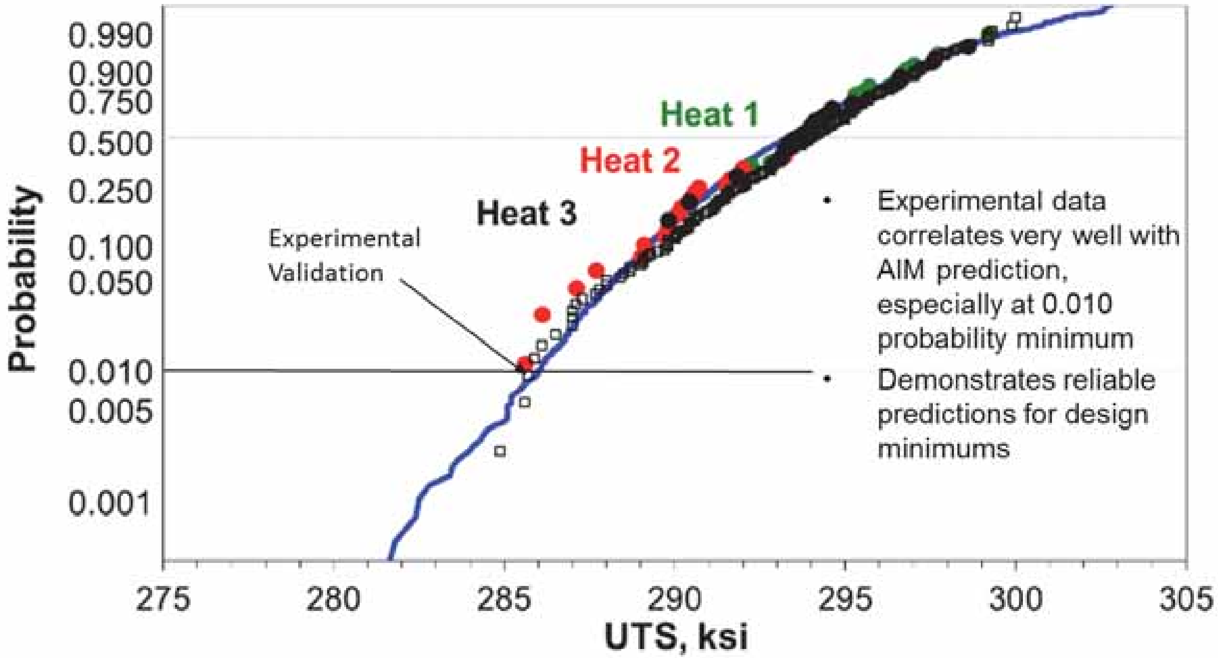
M54 homogenization at T_1, $SDAS_1$



"Accelerated Insertion of Materials" (AIM): Uncertainty analysis for alloy qualification

Monte Carlo distribution of processing parameters (T_i, x_i) → Thermo-Calc, Dictra, Prisma → Structure-Property Model (e.g., UTS) →





- Experimental data correlates very well with AIM prediction, especially at 0.010 probability minimum
- Demonstrates reliable predictions for design minimums

From CALPHAD to Flight:

Accelerated Component Qualification

- T-45 M54 hook shanks U.S. Navy-qualified with **>2x life** vs. incumbent:
- The U.S. Navy estimates **$3 Million saved** by implementing M54 steel
- QuesTek serving as prime contractor to deliver 60 hook shanks (first 8 delivered in Jan, 2016)
- M54 approved to replace 300M on F/A-18 for landing gear components due to **greater strength, toughness, fatigue and SCC resistance**

From clean sheet alloy design to flight in **7 years**, this ICME-based program demonstrates the goals set by Materials Genome Initiative

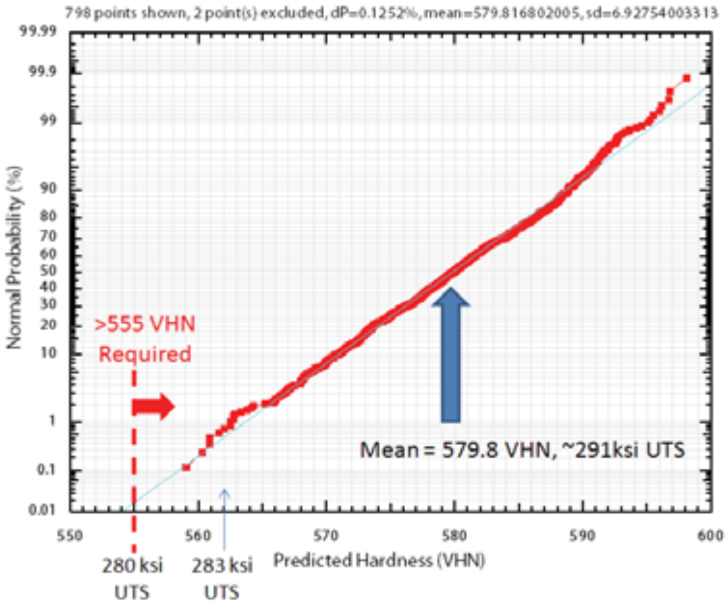
Ferrium M54 hook shank forging

Completed Ferrium M54 steel T-45 hook shank

Other leading applications of M54:
Commercial landing gear
Oil and gas case running tools (C-160 type)
High performance fasteners

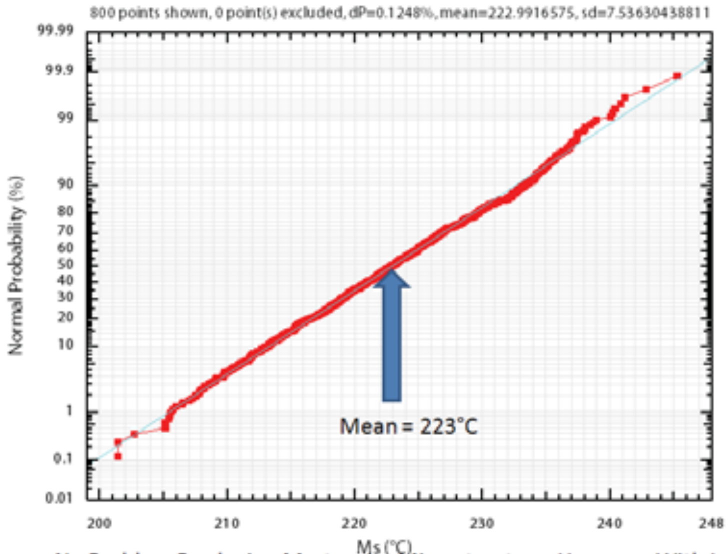
Further AIM M54 examples

Hardness



According to Pure Model Prediction Based on Quantifiable Variations, It Is Possible To Meet the Strength Requirement. The Predicted 1% Minimum Strength is 562VHN, Which Corresponds to 283ksi in UTS.

Martensite Start Temperature



No Problem Producing Martensite Microstructure. However, With Lower Ms, The Cryo Treatment Would Be More Important

Ferrium C64 composition optimization

Ferrium C64 High Performance Carburizing Steel Upgrade from 9310 or Alloy X53

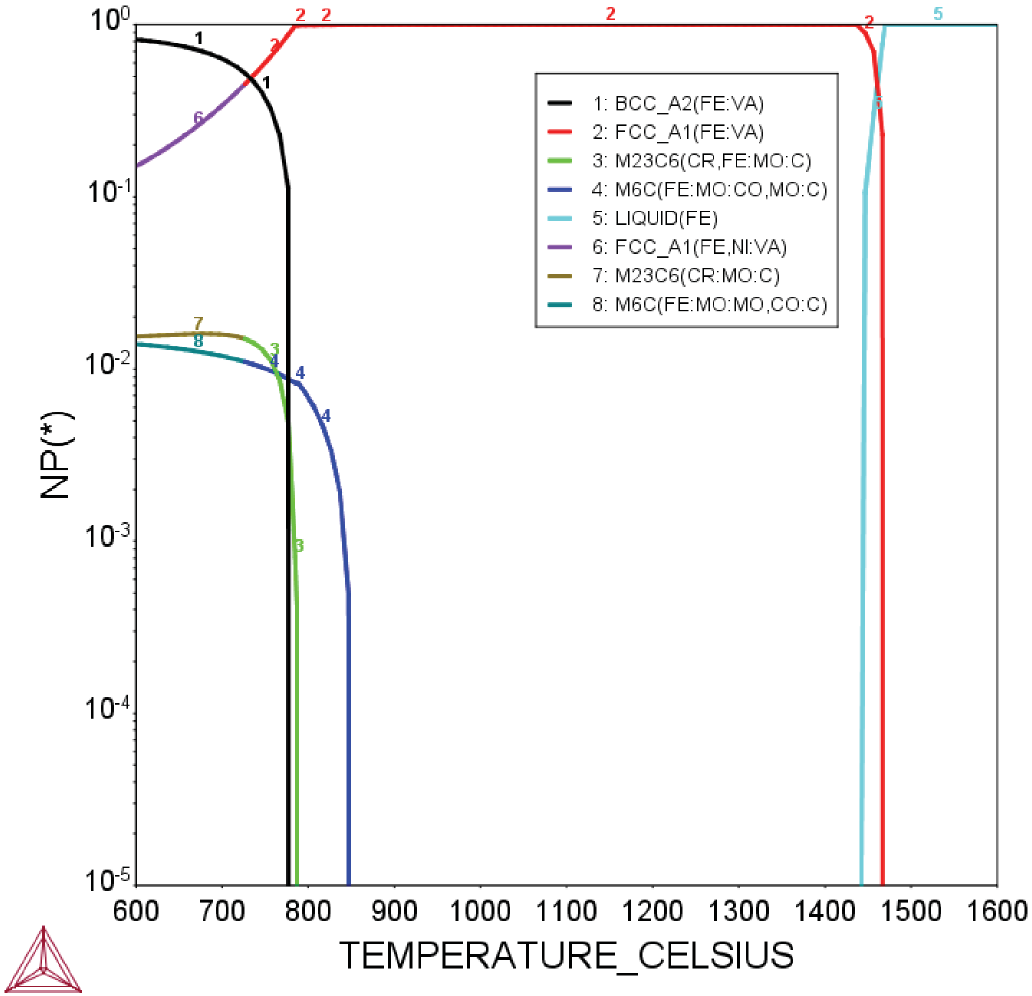
62-64 HRC case, high-strength core

- For gears, shafts, integrally-geared shafts, pins, ball screws, etc.
- Designed for vacuum carburization
- High tempering temperature →greater temperature resistance
- Greater corrosion resistance than incumbent alloys

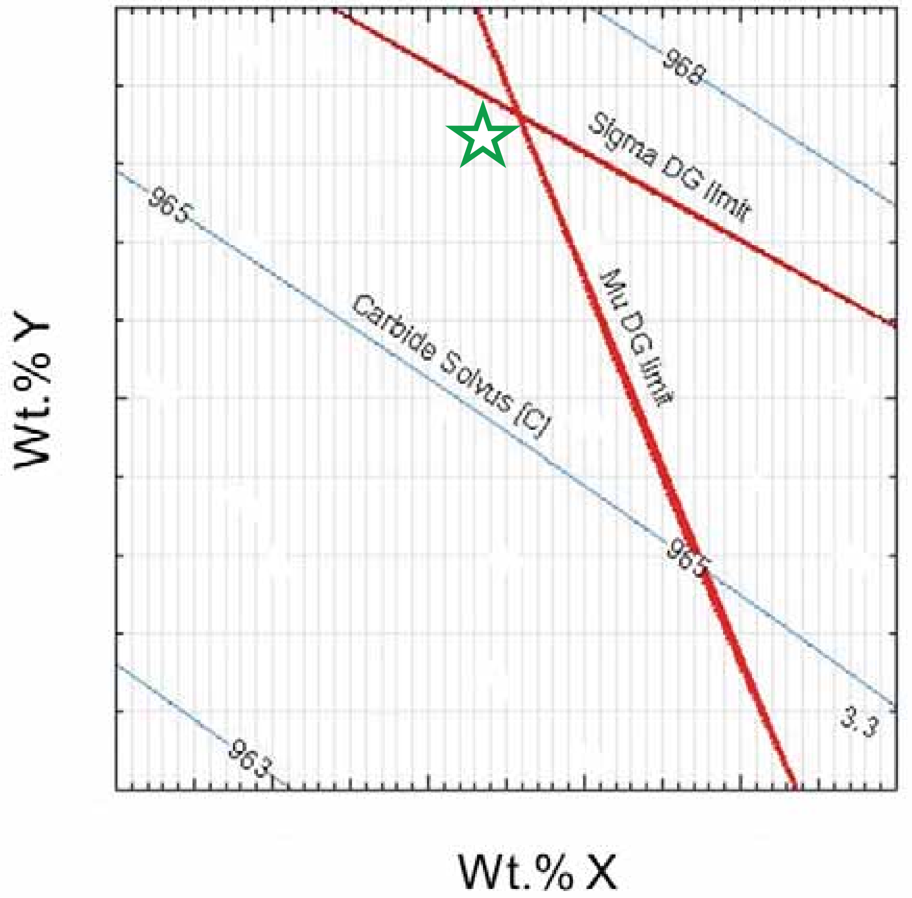
Typical Alloy Properties	YS (MPa)	UTS (MPa)	Core Hardness (HRC)	El (%)	RA %	Fracture Toughness (MPa √m)	Achievable Surface Hardness (HRC)	Tempering Temperature (°C)
AISI 9310	1068	1206	34-42	16	53	93	58-62	149
Alloy X53	965	1172	36-44	16	67	126	59-63	204
***Ferrium* C64**	**1372**	**1578**	**48-50**	**18**	**75**	**93**	**62-64**	**496**

Commercially Available LATROBE SPECIALTY METALS A Carpenter Company

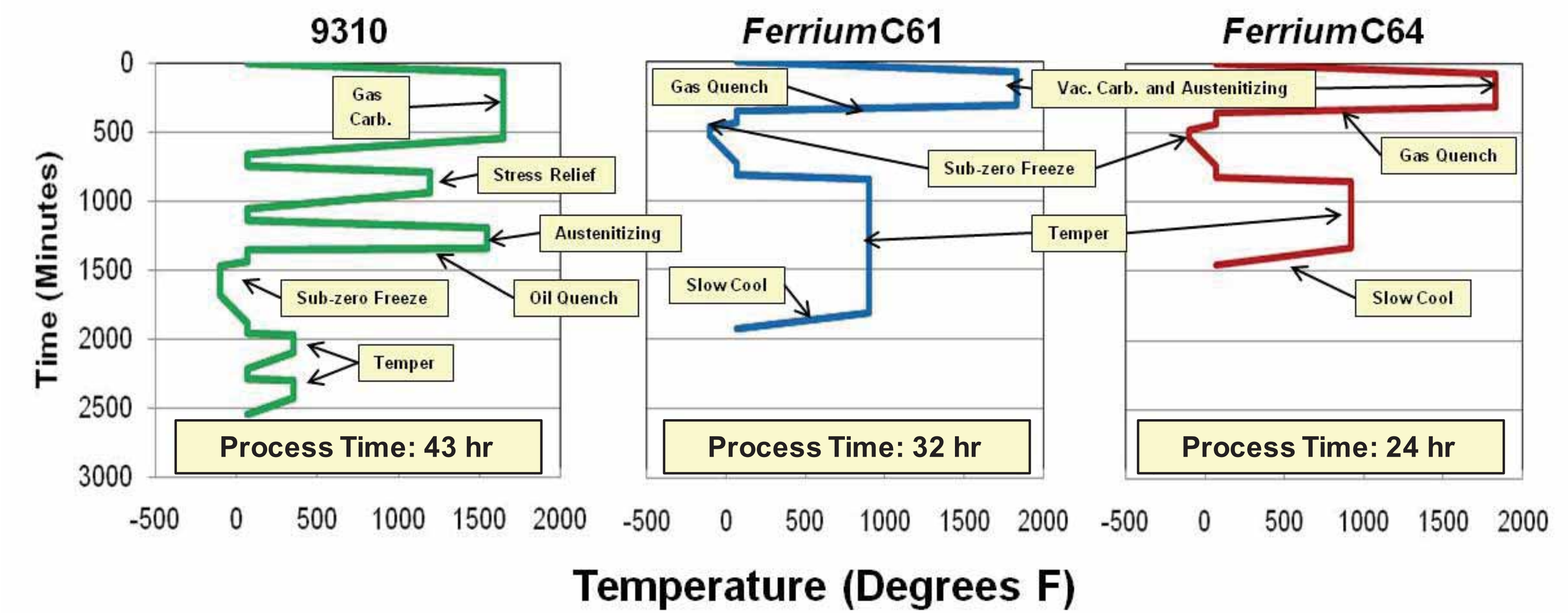
C64 Step Diagram



Ferrium C64 – design for avoidance of topologically closed-packed (TCP) phase stability



Ferrium C61 and C64 - Designed for vacuum carburization to reduce manufacturing costs



9310 processing from: "Effect of Shot Peening on Surface Fatigue Life of Carburized and Hardened AISI 9310 Spur Gears", The Shot Peener, Fall 2002

- Higher temperatures, shorter process times for *Ferrium* steels
- Austenitizing occurs during carburization of *Ferrium* steels
- Eliminate three thermal steps and associated plating/stripping

Ferrium C64 steel
Leading applications examples

Next Generation Helicopter Gear Steel

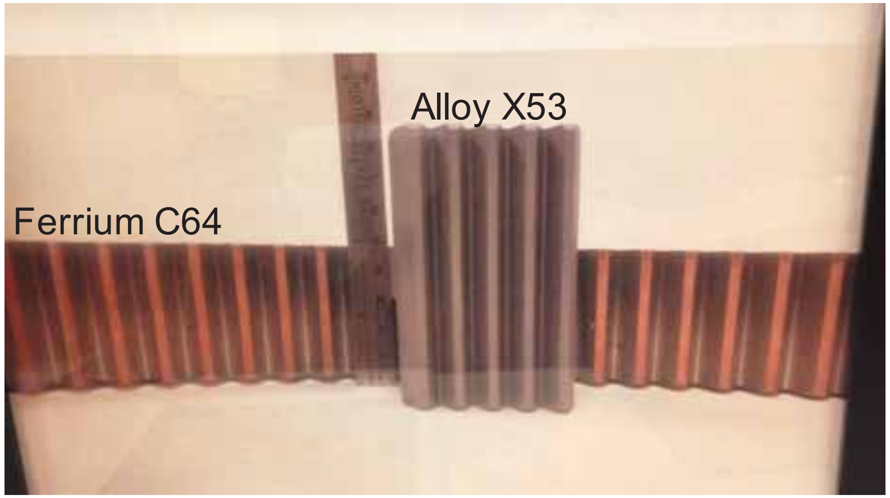
"..over 30% increase in power to weight ratio achieved with C64 …"

"C64..allows gears to run at high load levels without failure and carry more loads through the gearbox.." (Army Technology Magazine, March 2015)

U.S.ARMY

Sikorsky
A United Technologies Company

Bell Helicopter
A Textron Company



Multi-year programs with Bell Helicopter and Sikorsky for qualification of next gen transmission gears

Power density improvements at helicopter company: ">30% increase in power to weight ratio achieved with C64"

Adopted by the auto racing sector (Formula-1)
Considered for Wind Turbine gear-boxes

QT-SX Ni-superalloy single-crystal design

Single Crystal (SX) Ni Superalloy Design for IGT

- **DOE SBIR Phase I, Phase II, and Phase IIA awards**
- **SX castings – High Temperature Performance**
  - Desirable for better creep resistance – no grain boundaries
- **IGT blade castings are large > 8 inches**
  - Slower solidification / cooling rates exacerbate processing issues
- **Primary casting (processing) constraints:**
  - **Freckle formation**
  - High angle boundaries (HAB) and low-angle boundaries (LAB)
  - Hot-tearing
  - Shrinkage porosity
- **3rd generation blade alloys are especially difficult to cast as SX due to their high refractory content**
  - Increased tendency for hot tearing
  - Increased tendency for **freckle formation**

QuesTek's approach: ICME-based design of a new processable, high-performance single crystal alloy for IGT applications

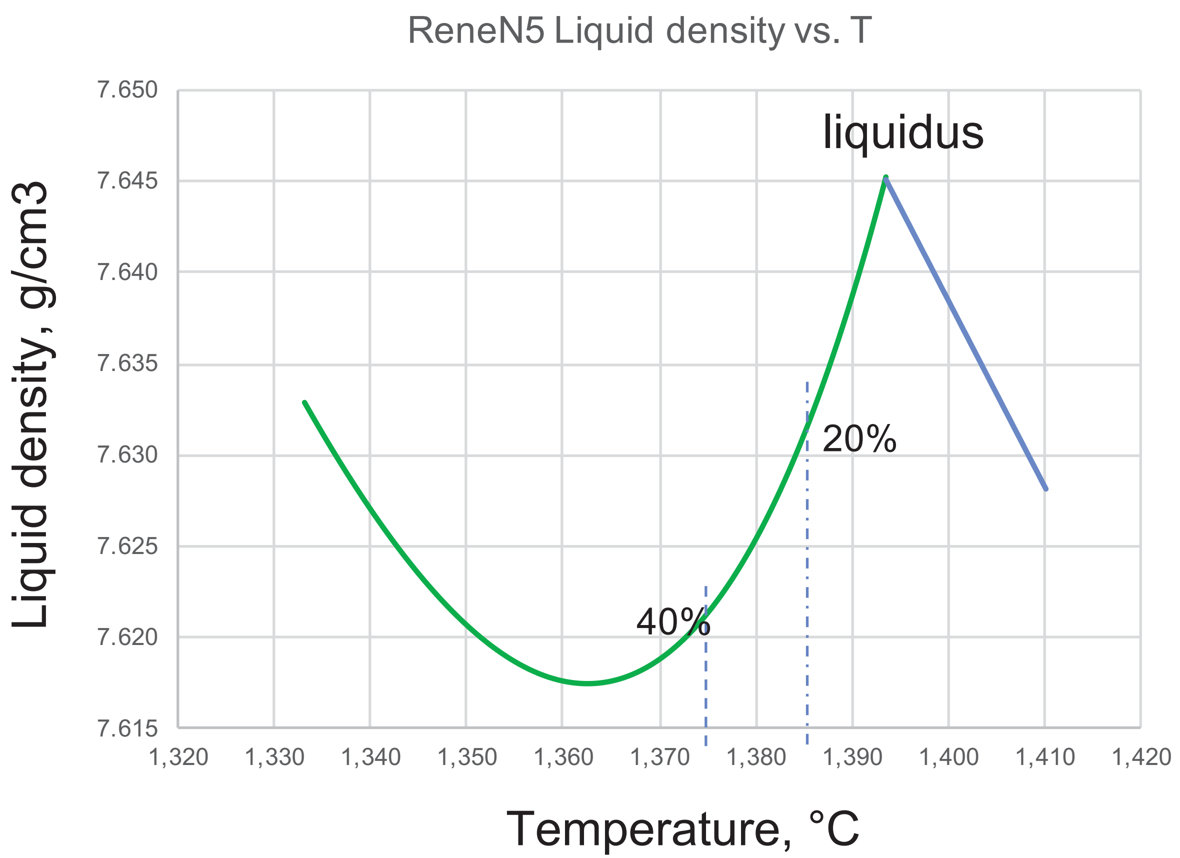
Creep Metric: Coarsening Rate Constant

- Coarsening rate constant, K, describes average particle size ($\bar{R}$) evolution with time (t) in LSW theory
  - $\bar{R}^3 - \bar{R}_0^3 = K(t - t_0)$
- Kuehmann/Voorhees model for coarsening rate predicts K from equilibrium partitioning of solute to precipitates and diffusivities
  - $K_{KV} = \frac{8}{9}\sigma V_m^\beta \left[\left[X_i^\beta - X_i^\alpha \right]^T \left[\frac{\delta^2 G^\alpha}{\delta X_i \delta X_j} \right] \left[D_{jk}^\alpha \right]^{-1} \left[X_k^\beta - X_k^\alpha \right] \right]^{-1}$
  - σ =surface energy, V=molar volume, X=mole fraction, D=diagonal diffusivity, T=temperature, G=Gibbs energy
  - We use normalized rate: $\frac{K}{\sigma V_m^\beta}$
- Slower coarsening rate constant is correlated to improved creep performance
- Diffusivities and Gibbs energy from CALPHAD

Freckling Metric: Liquid density during solidification

Freckle-resistance is related to the modeling of the liquid density during solidification base on a critical Rayleigh number:

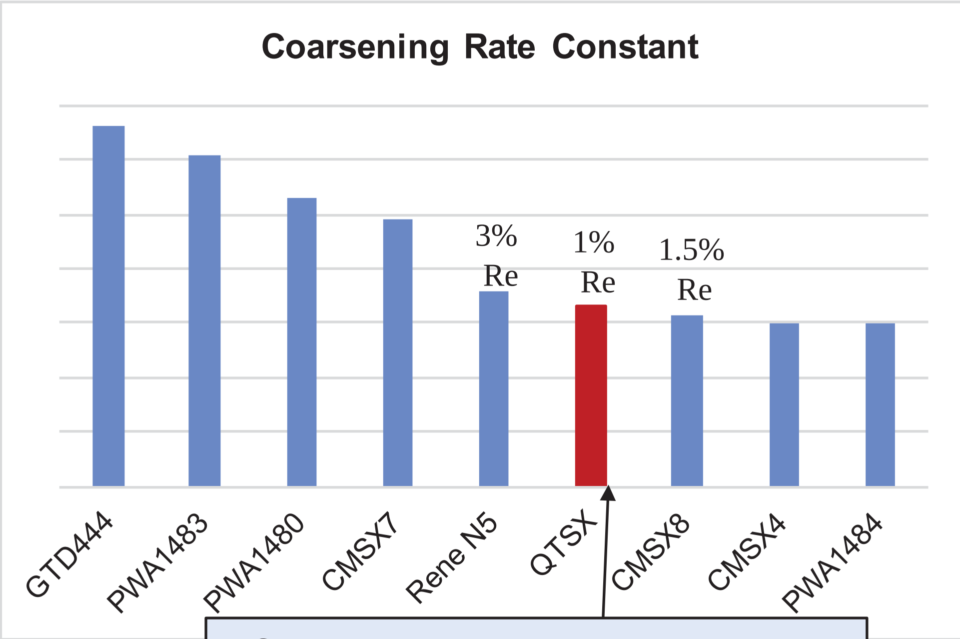
$$\overline{Ra} = C\Delta\rho^{0.4}\Delta T^{0.4}\frac{\lambda_1^2(G,R)}{G}$$



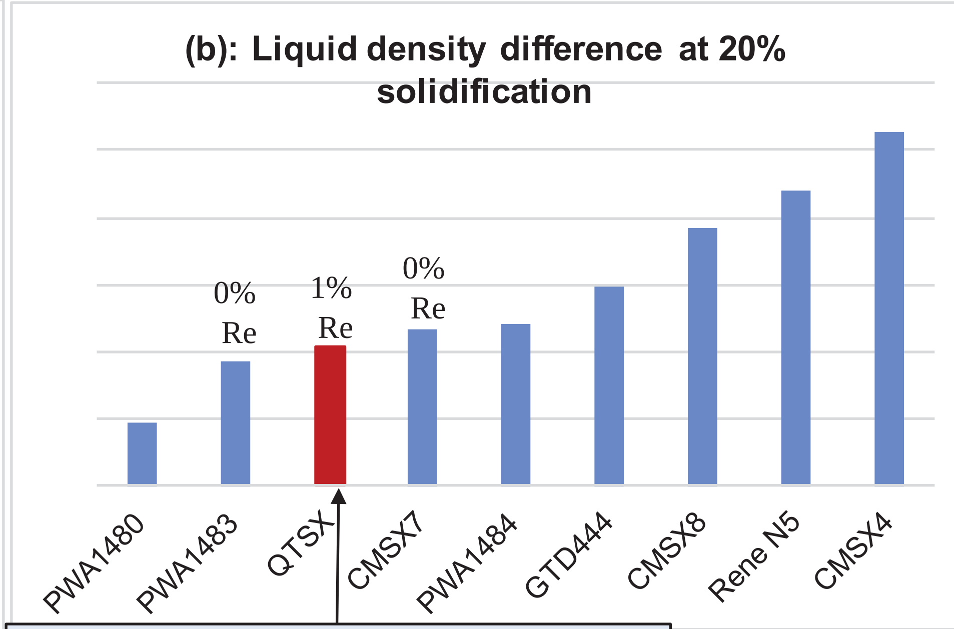
Actual modeling output is a combined use of various databases and software

Optimize alloy composition to balance critical properties, as predicted from CALPHAD modeling

Creep Metric (lower is better) Freckling Metric



Comparable coarsening rate to CMSX-8 (1.5% Re) alloy

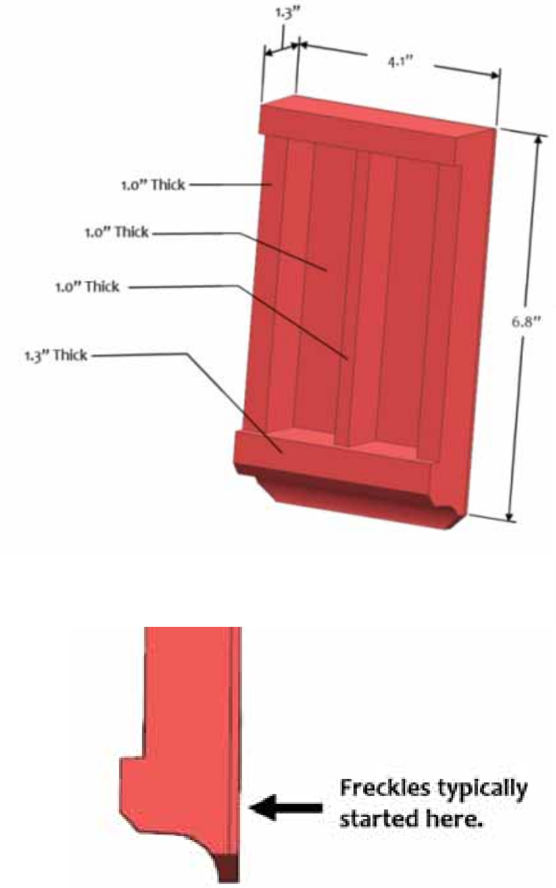


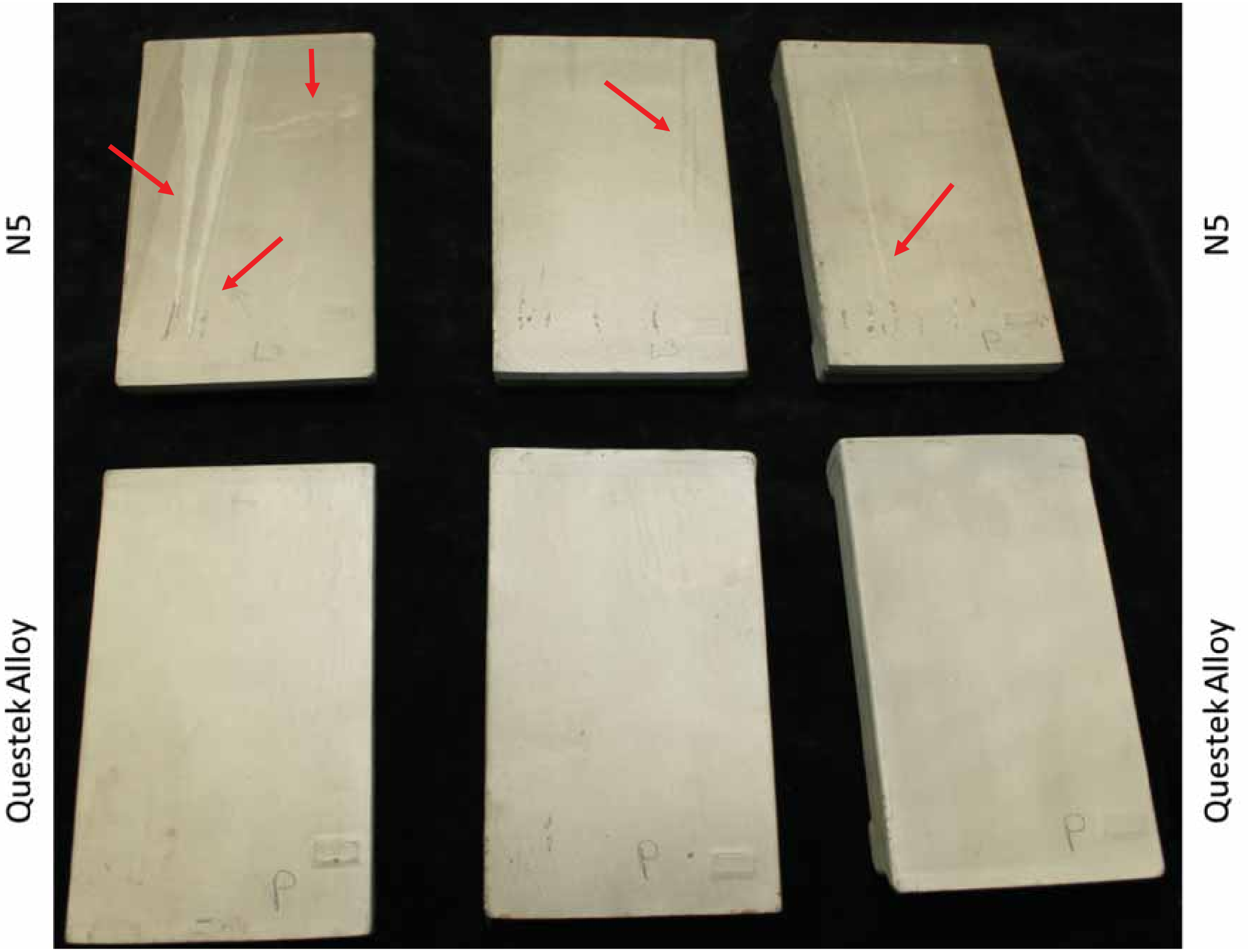
Reduced buoyancy differences (less than non-Re CMSX-7)

Coarsening rate model primarily a function of effective vacancy diffusivity in γ matrix.

Model liquid composition and volume evolution during solidification.

No freckling observed in prototype castings





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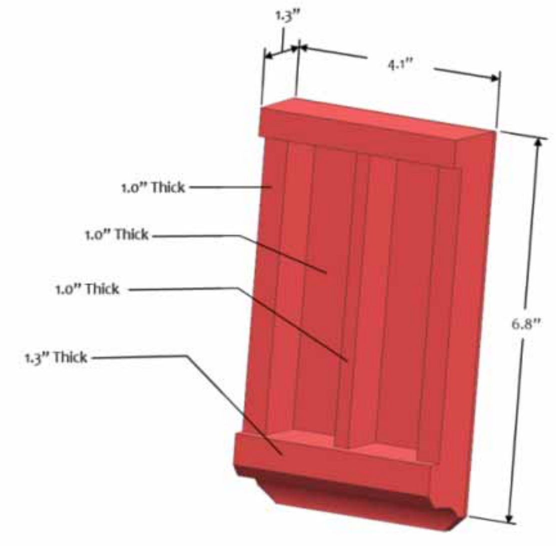
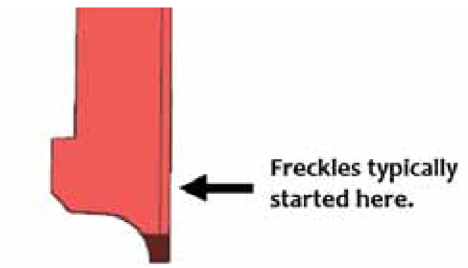
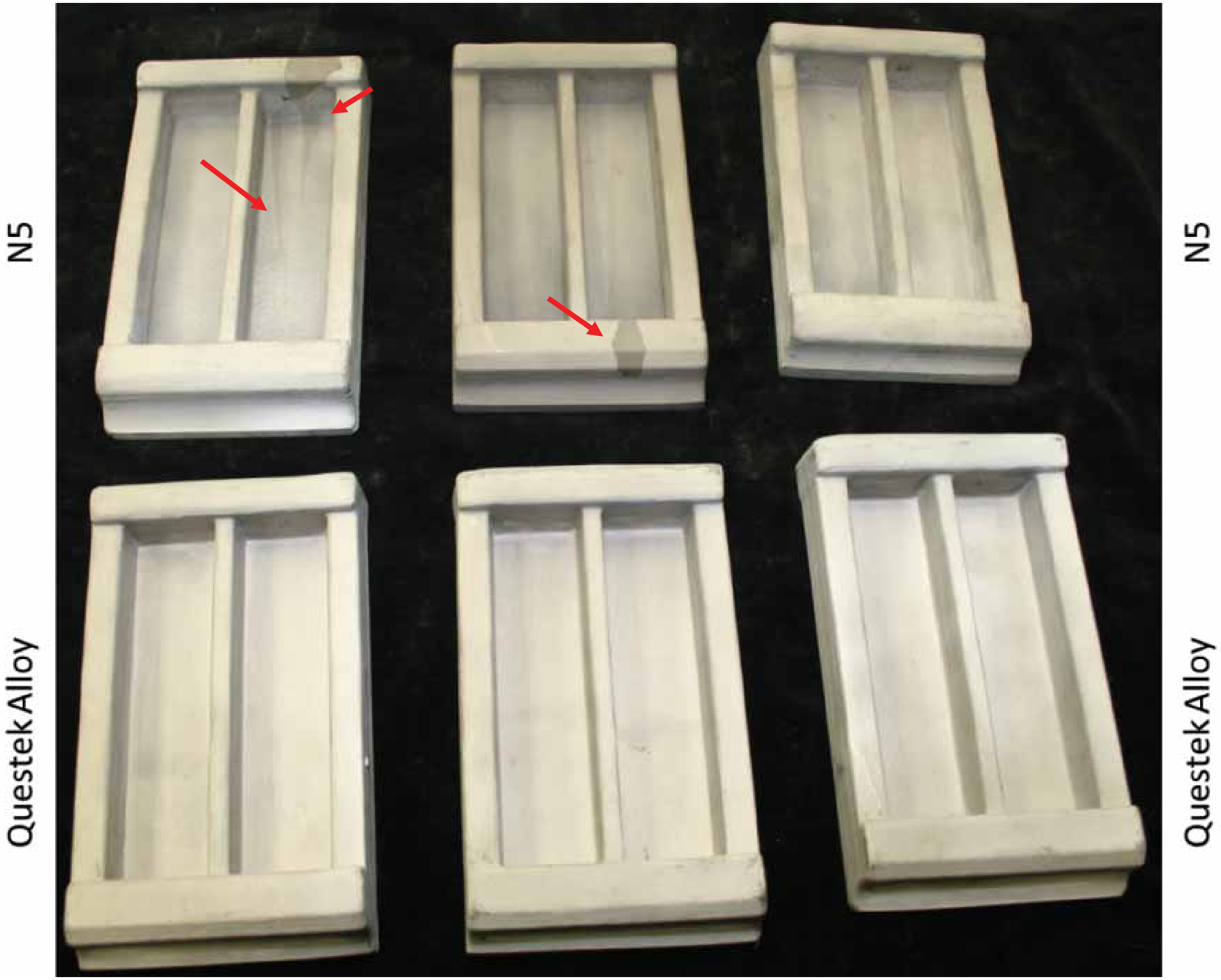


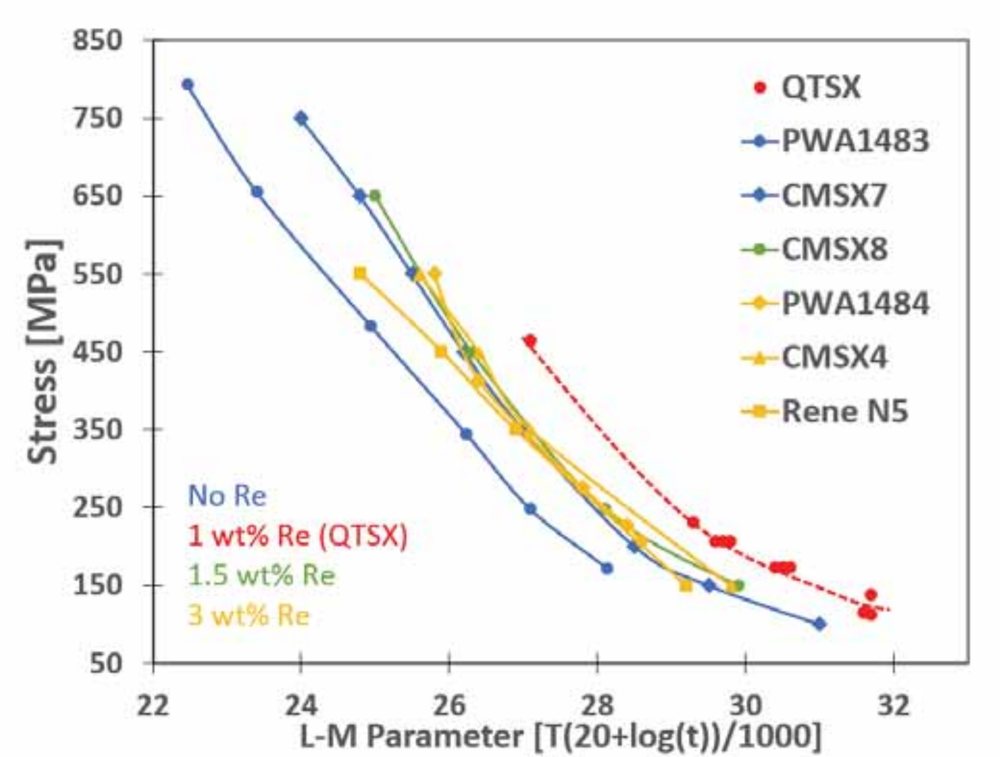




QTSX is as creep resistant as legacy alloys but with less Re

*Creep Comparison to Select Incumbent SX alloys**

**Baseline data taken from respective patent filings, literature*



Higher L-M parameter is better at a given stress.

Thank You

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