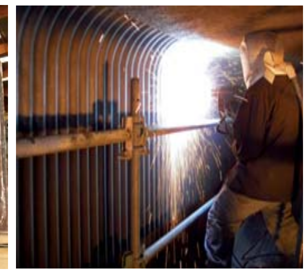
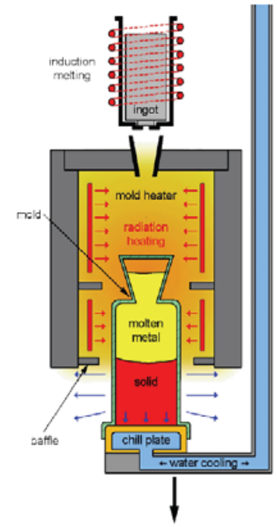
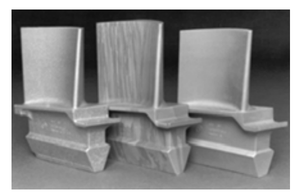
Computational Design of Weldable High-Cr Ferritic Steel

***NETL* 2016 CCR Project Review Meeting**


David Snyder,
Jason Sebastian,
Jiadong Gong,
Gregory B. Olson

QuesTek Innovations LLC




Siemens SGT5-8000H 375MW Gas Turbine

QuesTek INNOVATIONS LLC
Materials By Design®

Overview

- SBIR project case studies
    1. **Computational Design of Weldable, High-Cr Ferritic Steel**
    2. Design of Castable SX Ni-based Superalloys for IGT Blade
    3. Computational High Entropy Alloy Design
- Closing

Case Study #1

Computational Design of Weldable, High-Cr Ferritic Steel

Acknowledgment: "This material is based upon work supported by the Department of Energy under Award Number DE-SC0006222"

SBIR Program PHASE II, DOE PM: Sydni Credle

Project Goal

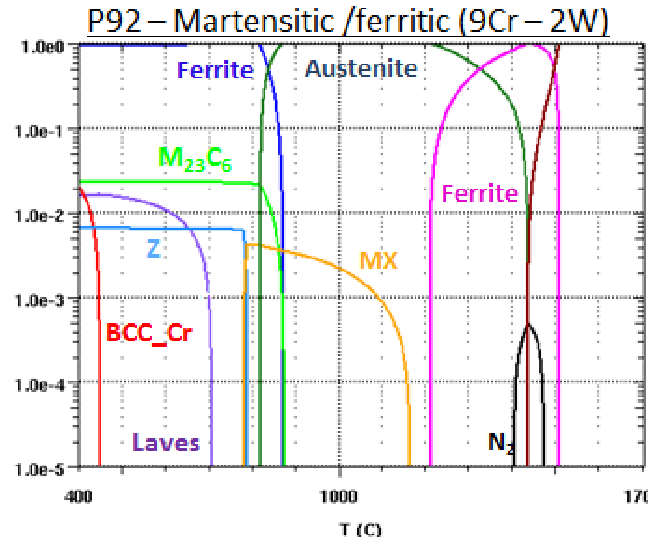
- New material development to enable AUSC and future steam power plant technologies
  - Pushing low-cost ferritic steels closer to the 760°C/35 MPa goals
- Target: lower-temperature sections of boiler, such as boiler tubes and headers (~600-700°C)
  - Incumbent alloys: FM stainless steels (SAVE12, P92) - operation ≤ ~620°C
  - Excellent parent material mechanical properties, largely limited by post-weld performance (Type-IV cracking susceptibility)
  - **New higher-temperature, easier-to-weld alloy is an enabling technology for future boiler tube upgrades**

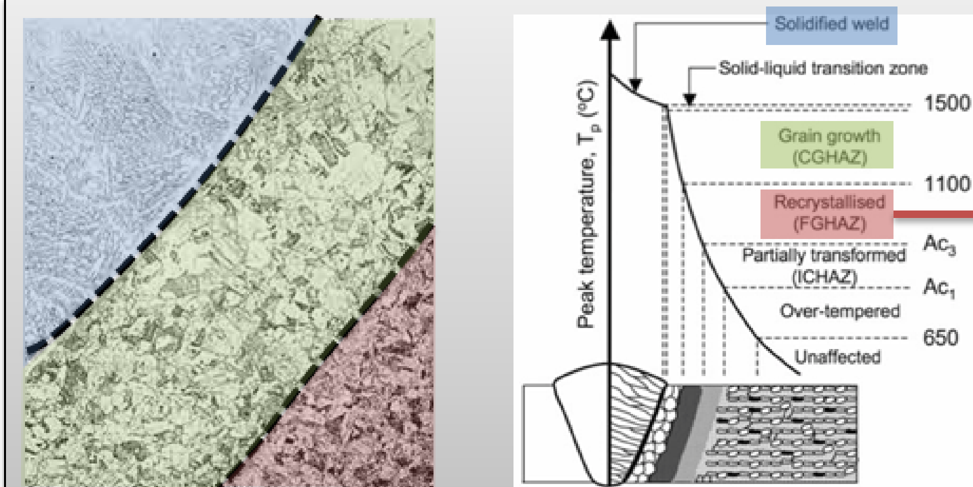
Alloy	Cr	Ni	Mo	W	V	Nb	Mn	Ta	Co	Si	C	N
SAVE12	11	0.6	--	3	0.2	0.07	0.2	0.07	3.0	0.3	0.01	0.04
P92	8.75	0.3	0.45	1.9	0.2	0.06	0.5	--	--	<0.5	0.09	0.06

Current Issues with Incumbent Materials

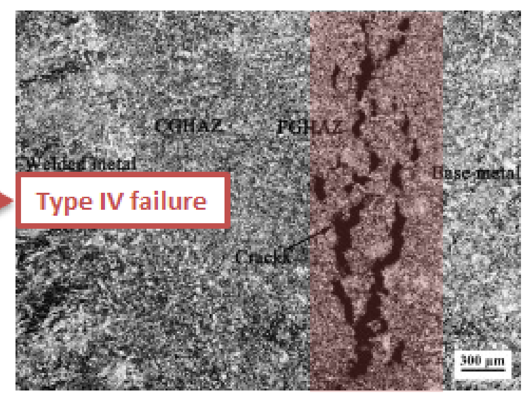
1. Phase transformation during welding
- Incomplete martensitic transformation → requires PWHT
- Recrystallization leads to fine-grain HAZ → grain boundary sliding failure

2. Thermodynamic stability during service
- Equilibrium Laves, Z phases at service temperatures (transient structure)





Both austenite and martensitic form after welding leads to high residual stress, prone to cracking

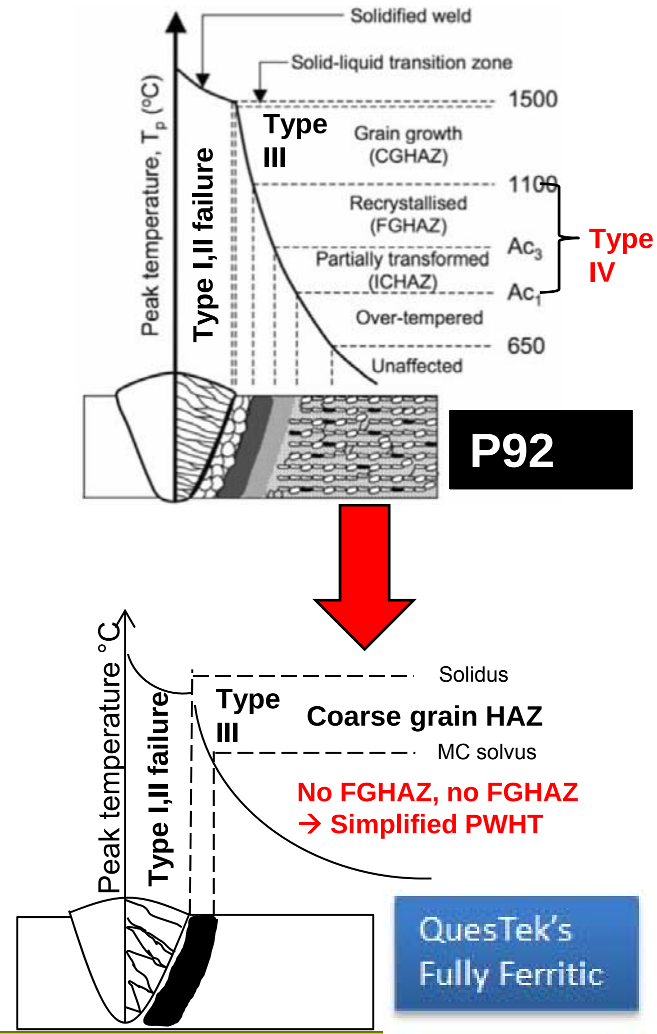


Small grains in FGHAZ/ICHAZ are susceptible to grain boundary sliding (Type IV failure)

Lei Zhao, Engineering Failure Analysis, Volume 19, January 2012, Pages 22-31

QuesTek's Strategy:
Fully-ferritic microstructure to reduce Type IV Cracking

- Avoid high temperature austenite
  - No transformation in HAZ during welding to eliminate recrystallization effects
  - ***Sacrifice martensite strength for uniform weld microstructure, reduced susceptibility to Type IV cracking***
- Compensate for creep strength with ordered precipitates (next slide)
  - Precipitation on cooling – *simplified PWHT*
- Design for efficient grain pinning for toughness
  - Optimize grain size for ductility vs Type IV crack resistance
- Simplify PWHT and minimize weld factor

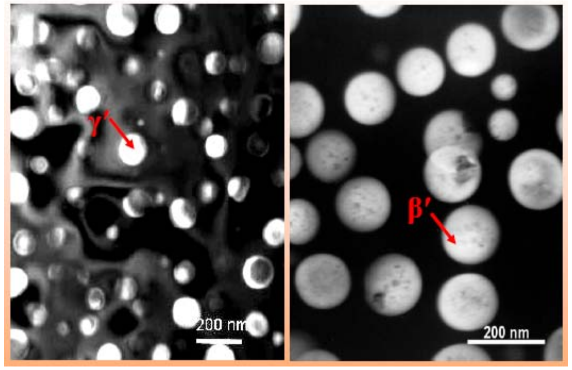


QuesTek's Fully Ferritic

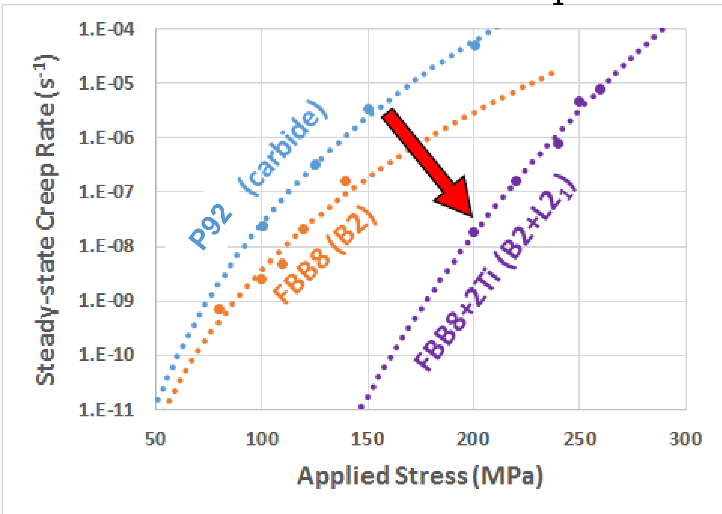
Intermetallic precipitate strengthening

- Ordered phase (B2, $L2_1$) strengthened BCC Fe – *analogous to γ/γ' Ni*
  - Enhanced strengthening efficiency
  - Demonstrated improvements in creep resistance over legacy grades
  - Precipitates on cooling for simplified PWHT

- Critical factors of design:
  - Creep Strength
    - Optimal Vf, <R>
    - Lattice misfit, coarsening resistance
  - **Low-temperature Toughness** (DBTT)
  - Oxidation Resistance (Cr_2O_3 vs Al_2O_3)
  - Fabricability (e.g. forgeability)



Ni – $L1_2$ BCC Fe – B2 and $L2_1$



Intermetallic strengthened BCC-Fe shows suppressed creep rates vs legacy carbide-strengthened alloys

P. Liaw (2008), Sun (2015), Rawlings (2016),

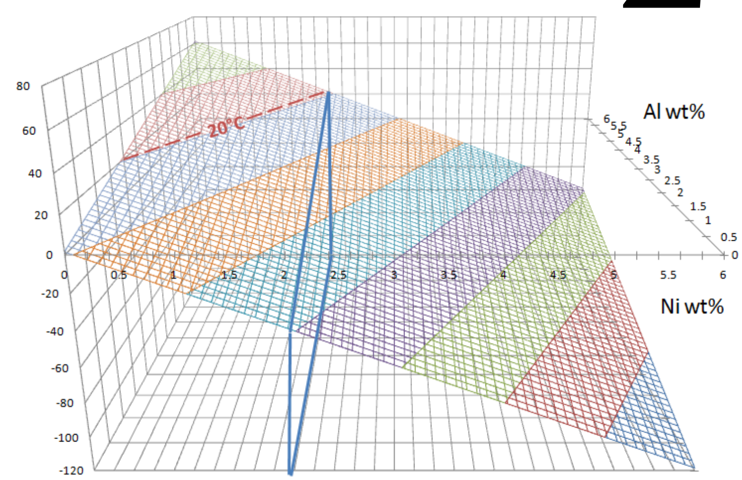
Low Temperature Toughness - DBTT

- DBTT a critical design factor for ferritic stainless steels
- Function of hardness, grain size, matrix composition
- DBTT model developed to optimize balance between alloy hardness and composition to minimize DBTT for a given level of strength

$$DBTT = DBTT_0 + f(Hardness) + f(Grain\ Size) + \sum k_i c_i$$

$(i = Ni, Al, Cr, etc)$

$$f(Hardness) = f\left(Vf, \langle R \rangle_{B2,L21}\right)$$

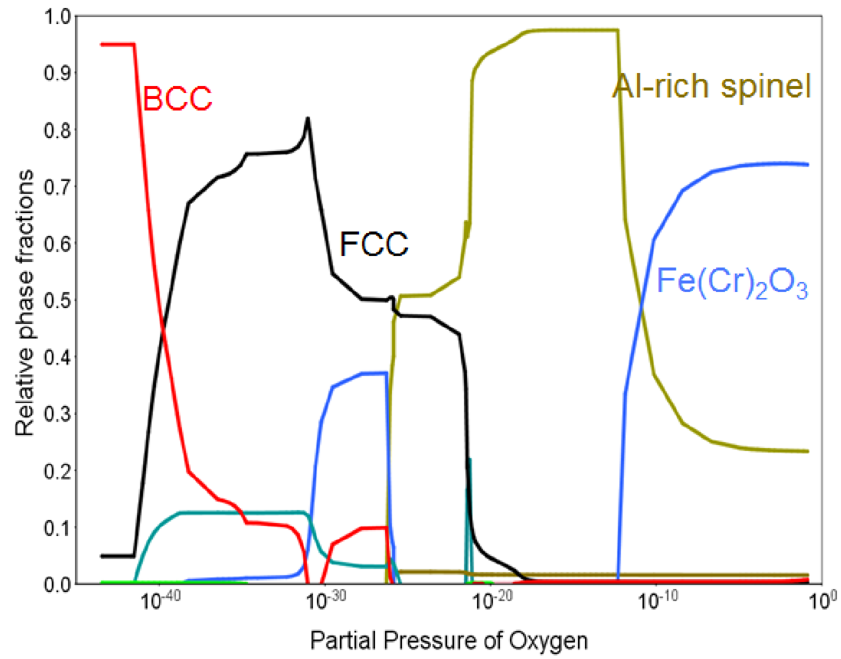


Oxidation Resistance

- Thermodynamic predictions of oxide stability vs chemistry
- **Goal: stable film formation at >700°C, minimize internal oxidation products**

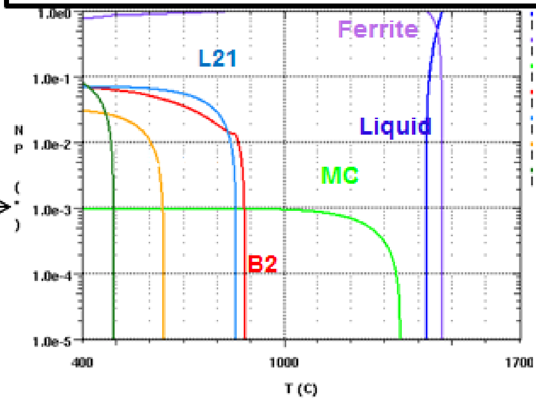
- Finding: (Fe,Cr)Al_2O_4 spinel oxide stable due to high Al contents
  - Cr_2O_3 present at highest O_2 (outer oxide layer)
  - Prohibitively high Cr needed to fully stabilize $(Cr,Al)_2O_3$ across all O_2
  - Similar behavior to P91/92 (Fe-Cr-Mn spinel - *protective*)

QT-BT: Oxide predictions at 700°C



Design Integration

Thermodynamic equilibrium calculations

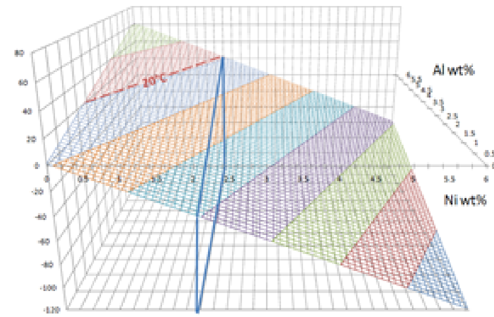


Improved matrix toughness by controlling composition and grain size

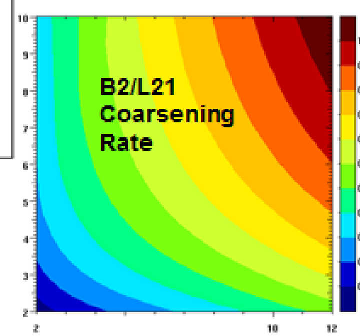
Destabilized Laves phase at operating temperature for optimal tertiary creep response

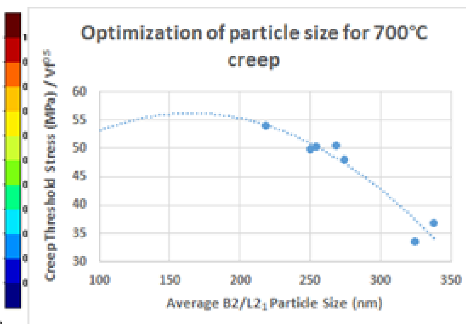
Fully ferritic to prevent recrystallization and allow robust PWHT

Reduced coarsening rate of strengthening phases and embrittling phases



DBTT calculations



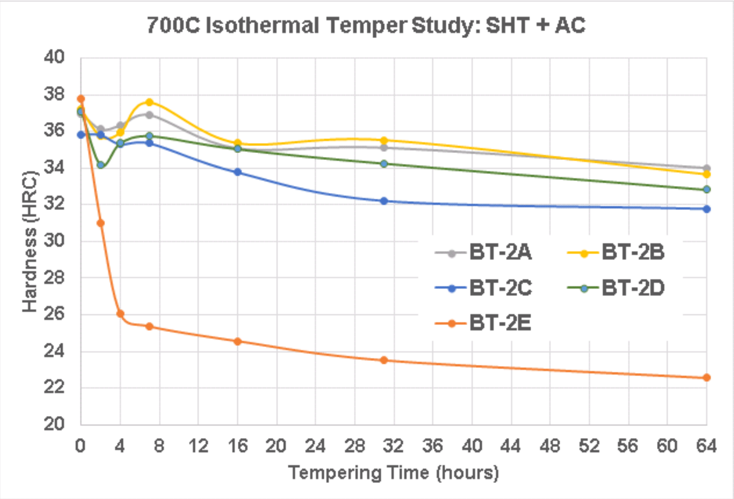


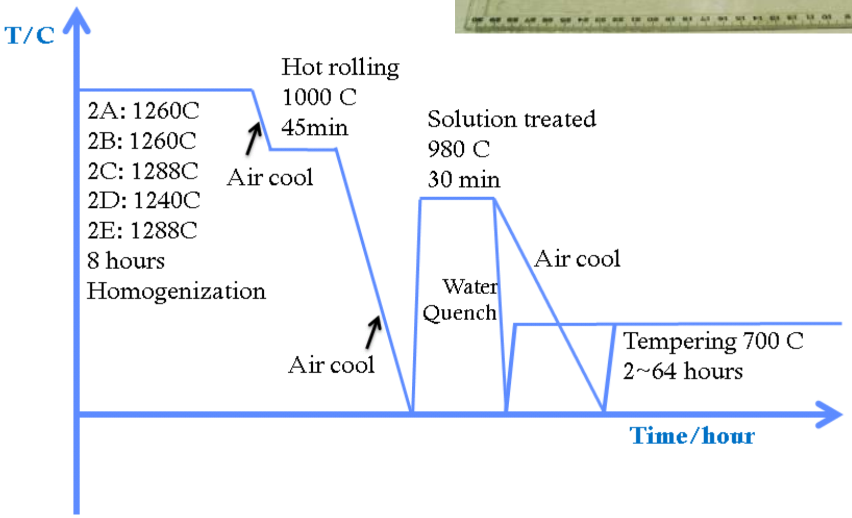
NiAl / Ni_2TiAl optimization
(lattice misfit, driving force, coarsening rate @ T, High-T low-σ Creep model)

Multiple prototype alloys were computationally designed and tested in two iterations

Prototype Evaluation

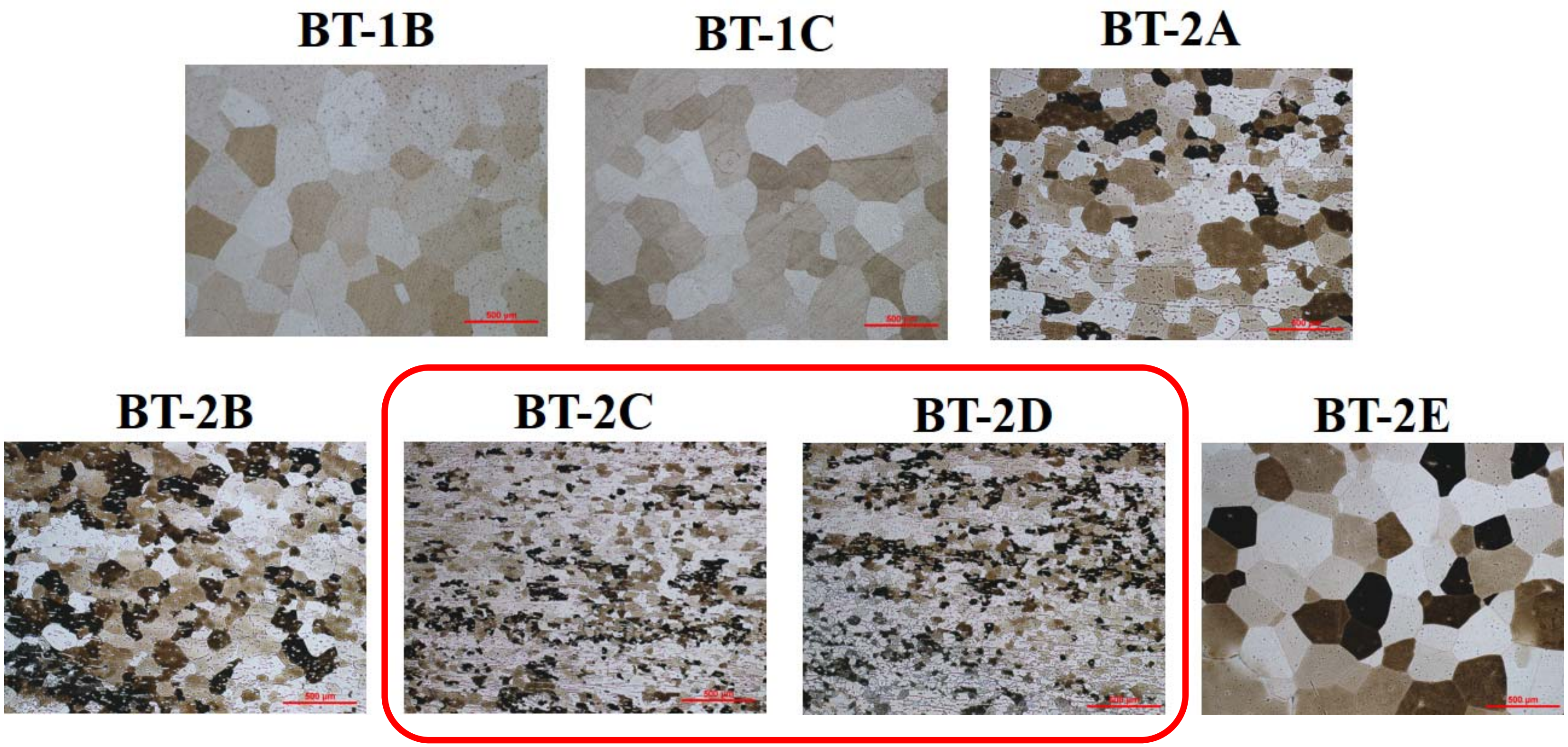
- Vacuum melted (VIM/VAR) at 30-lb scale (SAES)
- Homogenized and hot rolled into plate (Special Metals)
- Test coupons solution treated, air cooled and tempered at 700-750°C
  - Optimized to achieve "optimal particle size" for minimal creep threshold stress





Characterization of alloy microstructure

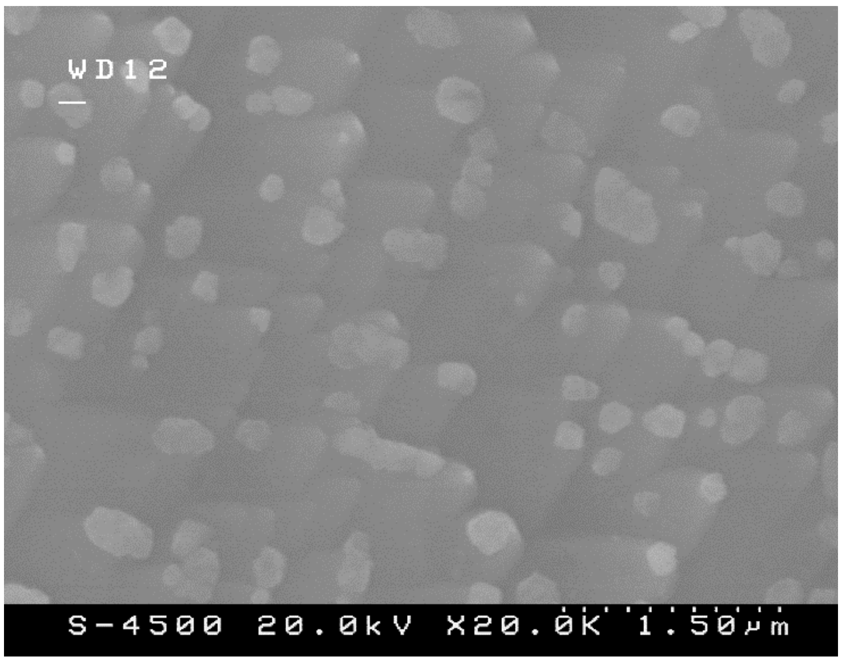
- Fully ferritic matrix validated
- Various designs achieved different levels of grain refinement

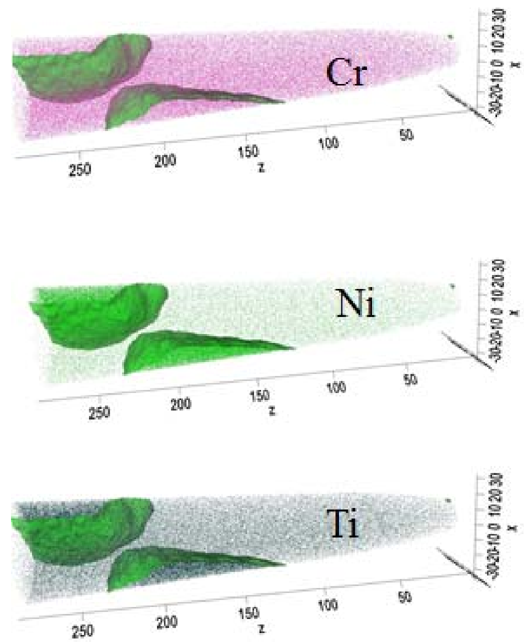


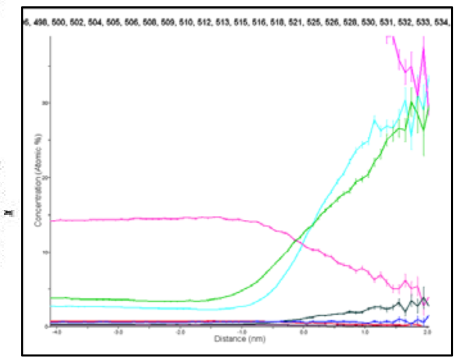
Grain refined (ASTM~5) alloys demonstrate significant RT ductility!

Characterization of alloy nanostructure

- Ferritic matrix validated
- B2 (NiAl) / $L2_1$ (Ni_2TiAl) precipitation validated
  - ~150-200 nm after tempering @ 700°C: design target particle size for optimal σ_{TH} achieved

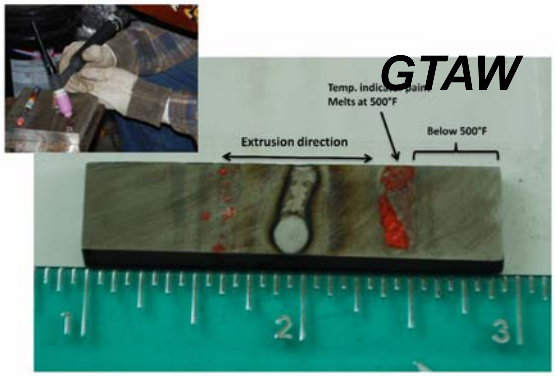


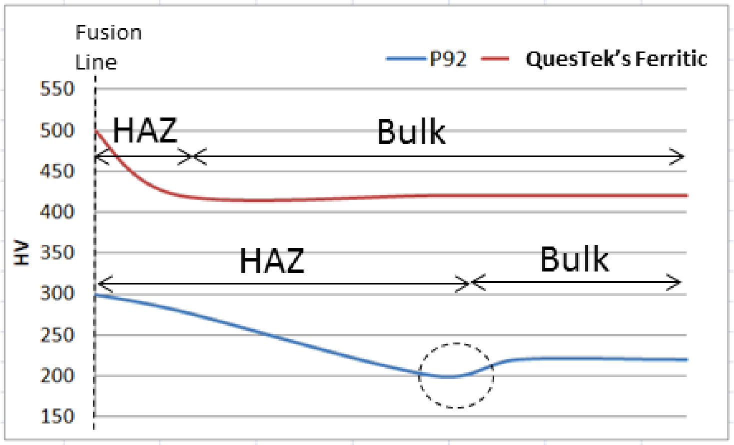


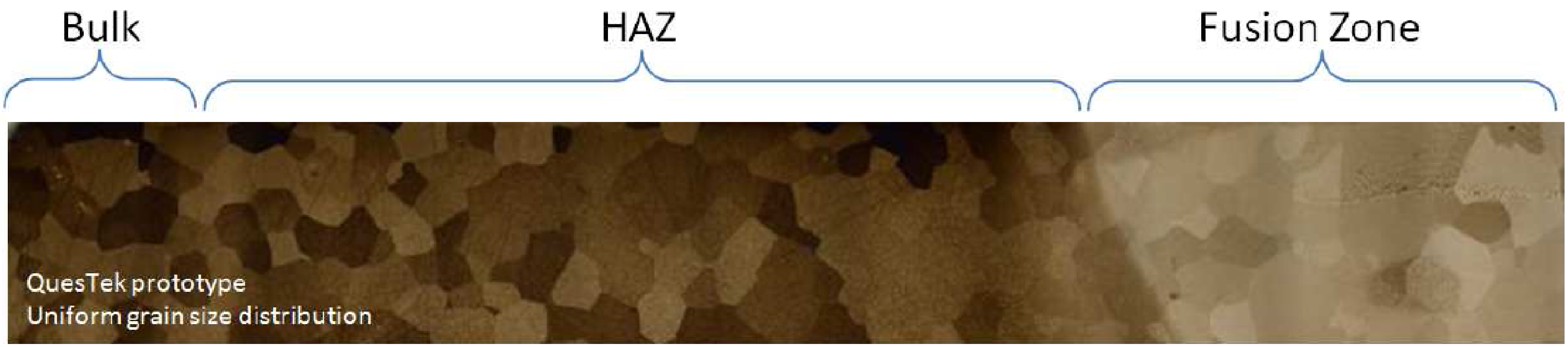


Initial Weld Demonstration

- Robust as-welded microstructure
  - No Fine-grain or Intercritical HAZ
  - No over-tempered HAZ
  - **Fusion and HAZ strengthened on cooling from weld: *post-weld stress relief only to restore toughness***



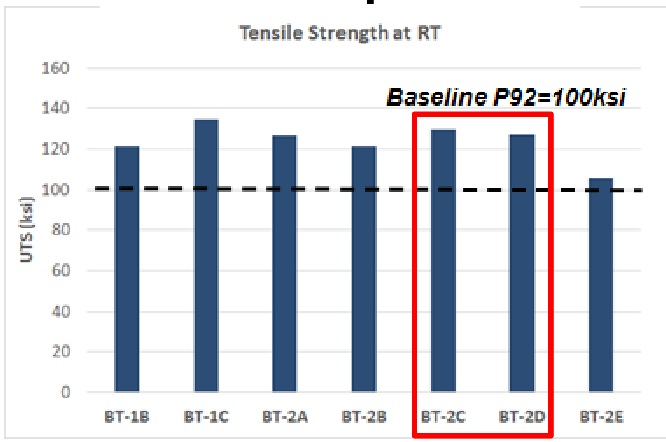


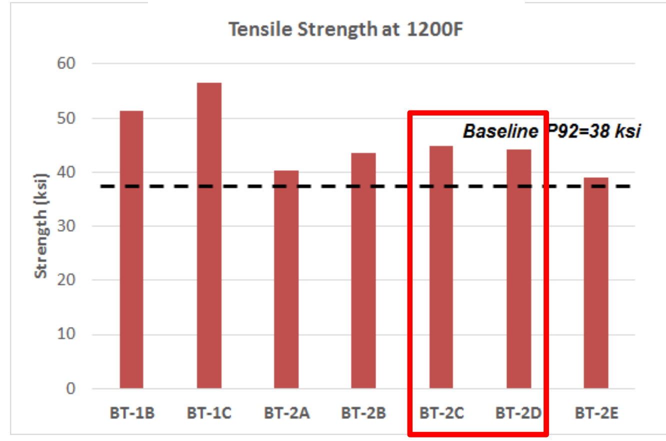


Initial Tensile Properties

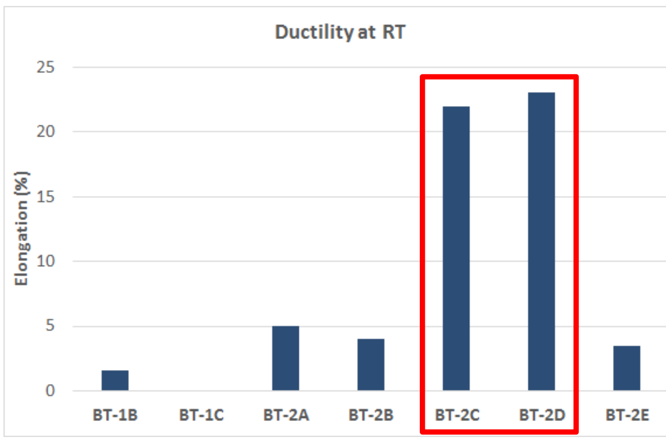
Room Temperature | 650°C (1200°F)

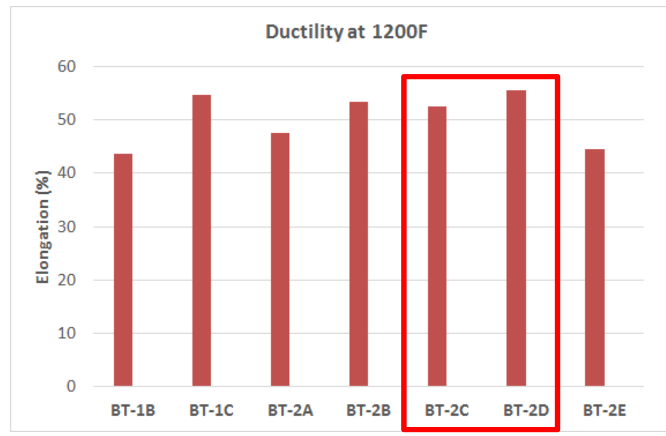
Tensile Strength





Tensile Ductility

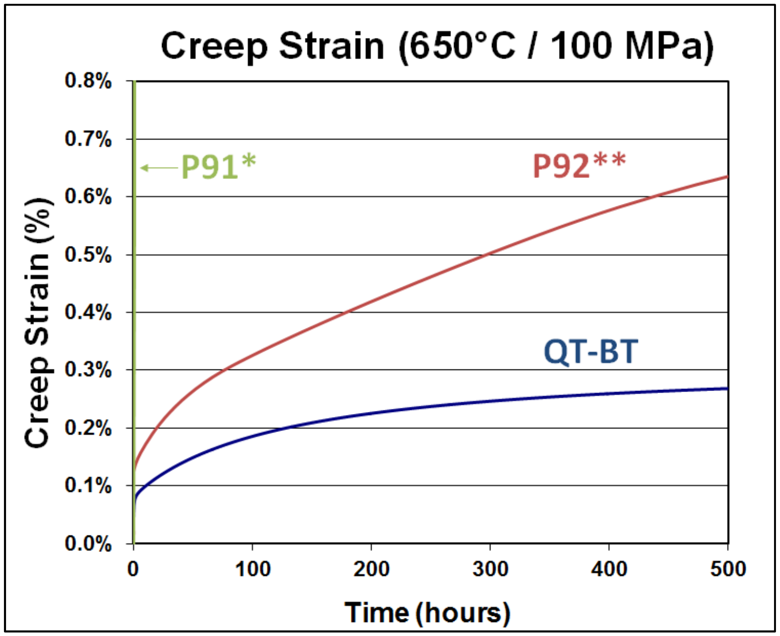


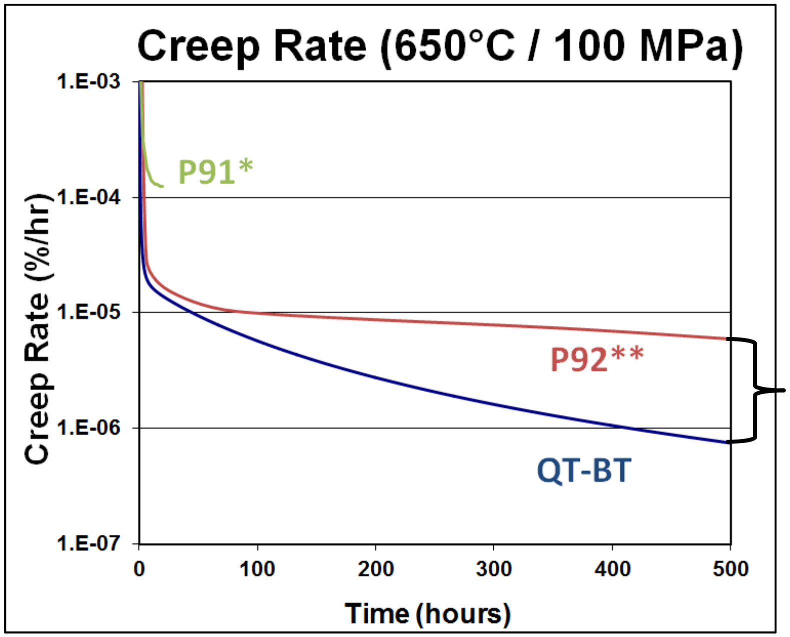


Variants BT-2C and BT-2D possess excellent RT and high-T strength and ductility, well in excess of baseline P92

Initial Creep Behavior

- Short-term creep testing to screen designs for down-selection
  - *Example 650°C/100 MPa, discontinued at 500 hours*
  - *Broader creep test matrix (incl. longer-term testing) in process on scaled-up lot*





≥Order of magnitude lower than P92

QuesTek's ferritic alloy shows promise of improved creep resistance over baseline P92

*Potirniche et.al, NUEP 2009 Project 09-835 (2013)
**Hald, 3rd EPRI conference on Advances in Materials Technology for Fossil Power Plants, Swansea UK (2001) p 115

Initial Oxidation – *Steamside Oxidation Testing*

- Steamside oxidation and Fireside corrosion testing conducted at Babcock & Wilcox
- Oxygenated H_2O + HN_3 to simulate OT fossil boiler water conditions
- Tested at 680-700°C for ~1000 hours

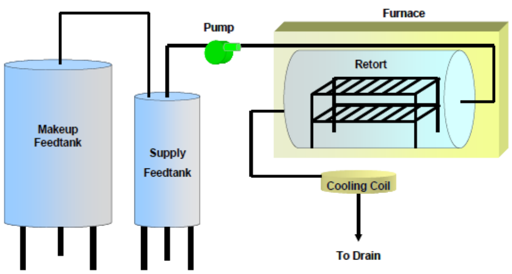
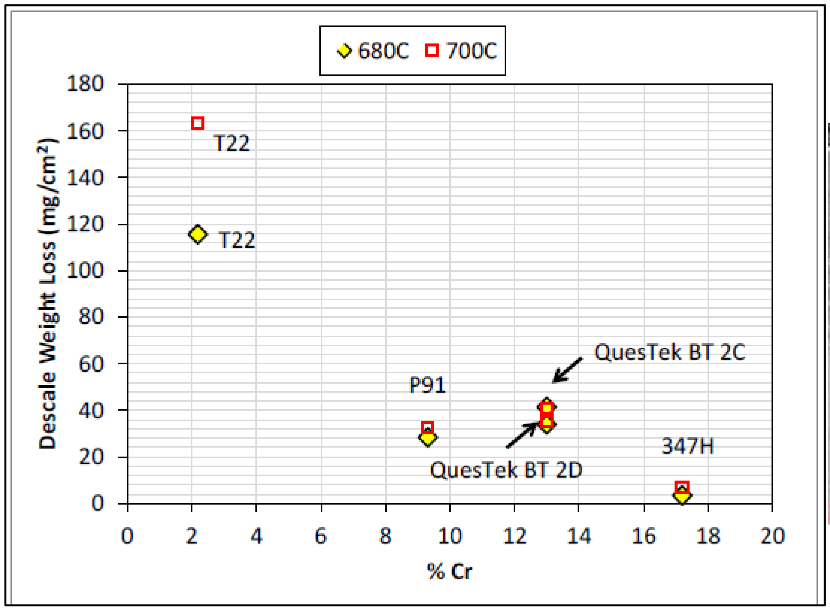
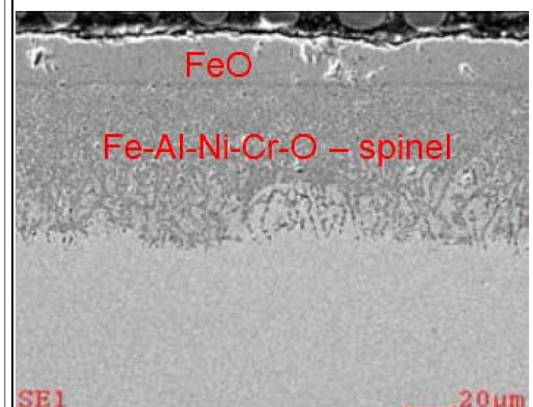


Figure 1. Steamside Oxidation Test Setup

Figure 2. Test Rack with Coupons



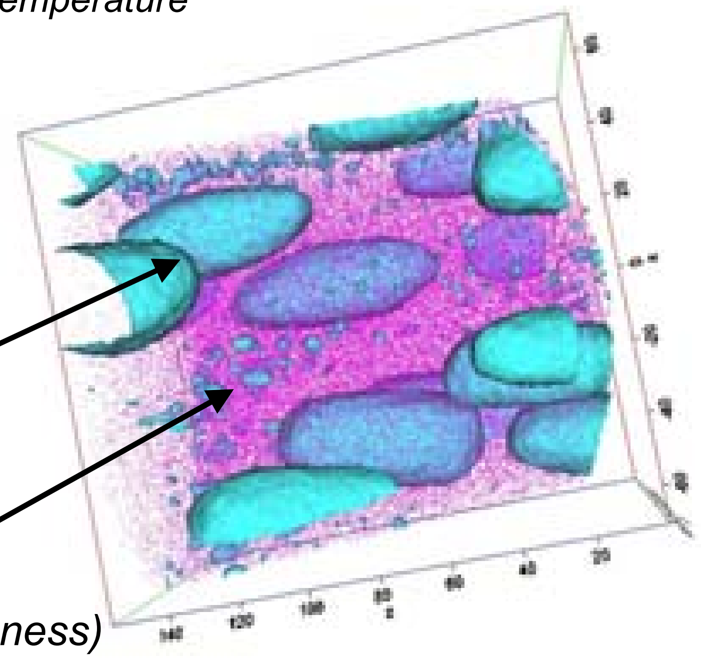


Oxidation predictions validated

- ***QuesTek's Ferritic alloy performed satisfactorily in oxidation (similar to legacy P91)***
- ***More careful consideration of pretreatment needed to avoid excess transient FeO***

Key learnings from initial prototype iterations

- Following extended service exposure (≥700°C), bimodal B2 distribution observed upon cooling to room temperature
  - “Secondary” B2 present at service temperature – *100-200 nm*
  - “Tertiary” B2 that forms on cooling to room temperature – *1-4 nm*
    - Fine B2 imparts significant RT strengthening– ***primary factor for RT toughness***
    - *Caused by excess supersaturation below service temperature*
  - *Solution:* ***redesign for lower supersaturation***



“Secondary” B2
(for creep)

“Tertiary” B2
(no benefit to creep, detrimental to toughness)

Next steps

- Final redesign completed
  - Focus on resolving tertiary B2 issues (toughness)

- In-process: Final design scale-up
  - ~500 lb VIM scale with prototype producer
  - Processing trials

- Detailed creep evaluations (~1000s hour)
  - Weld and parent

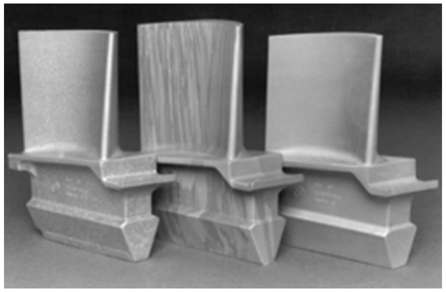
Case Study #2

Design of Castable SX Ni-based Superalloys for IGT Blade Components

Acknowledgment: "This material is based upon work supported by the Department of Energy under Award Number DE-SC0009592”

SBIR Program PHASE II, DOE PM: Steven Richardson

Siemens SGT5-8000H 375MW Gas Turbine



NETL SBIR: Single Crystal (SX) Ni Superalloy for IGT

- High-performance SX-Ni preferred choice for aeroturbine blades (*small*)
- **IGT blade castings are large > 8 inches**
  - Slower solidification / cooling rates exacerbate processing issues
- Adoption of high performance SX aeroturbine alloys for IGT currently limited by low casting yields
  - **High susceptibility to *Freckle formation***

PCC Airfoils, LLC
A Division of Precision Castparts Corp.

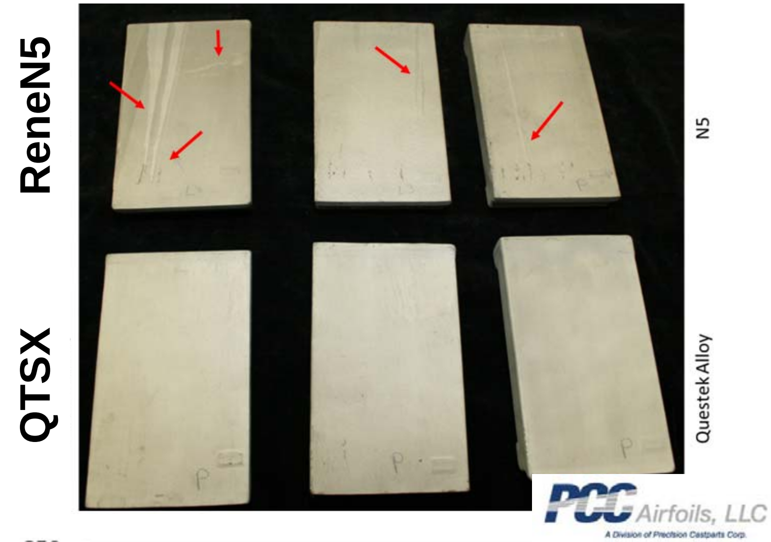
SIEMENS

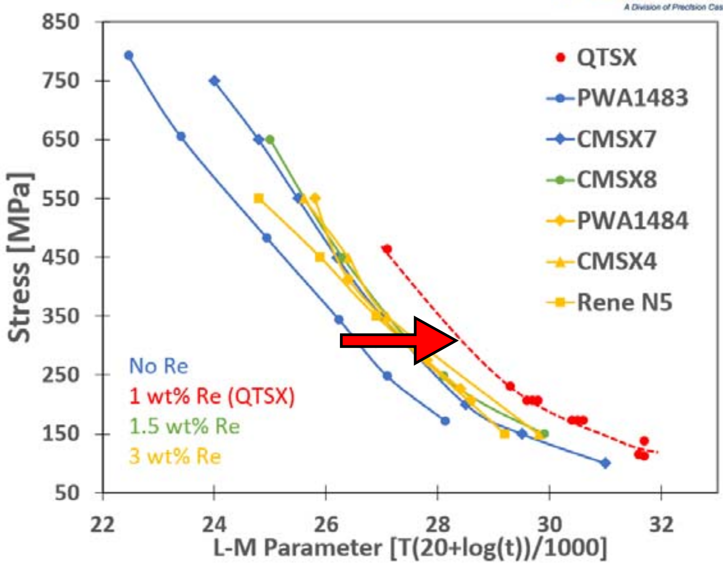
QuesTek's proposed approach: ICME-based design of a new processable, high-performance single crystal alloy tailored for IGT applications

Initial Progress to date

- QuesTek's designs based on a computational optimization between freckle resistance and creep strength
- ***Target: Castability of low-Re SX alloys, creep resistance of high-Re ("3rd Generation") aero SX alloys***
- ***Lab-scale demonstration of freckle-free castability under IGT-relevant conditions, with equivalent / improved creep resistance vs 3rd Generation aeroturbine alloys***
- *Full-scale IGT blade demonstrations in process*

Lab-scale blade castings of Rene N5 (freckled) and QTSX (freckle-free)



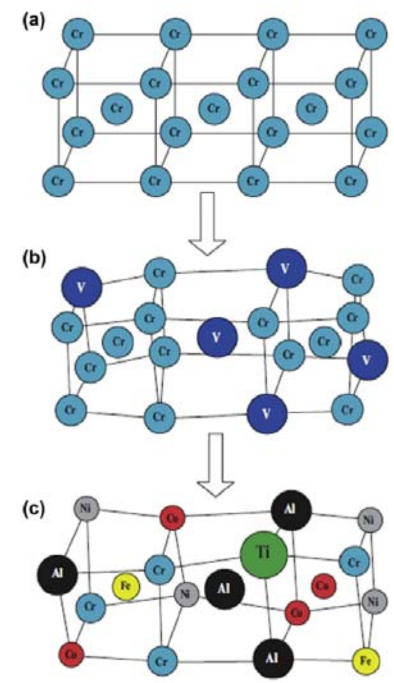


Case Study #3

Exploration of High-Entropy Alloys for Turbine Applications

Acknowledgment: "This material is based upon work supported by the Department of Energy under Award Number DE-SC0013220"

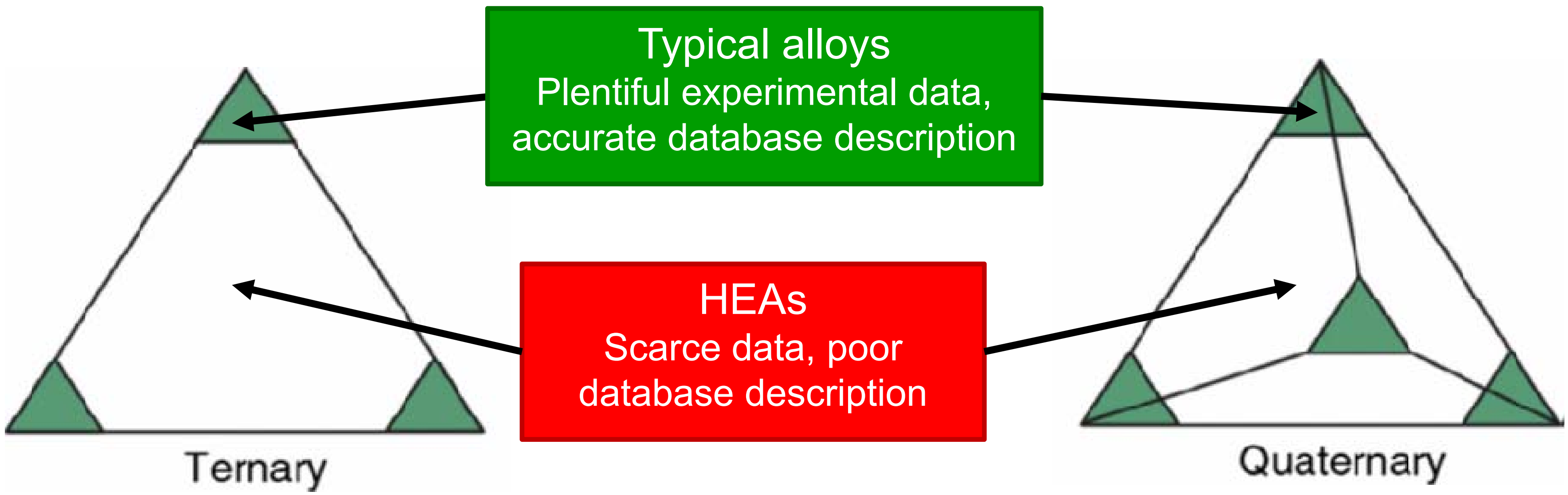
SBIR Program PHASE I, DOE PM: Mark Freeman



Zhang, Yong, et al. "*Prog Mater Sci* 61 (2014): 1-93

High Entropy Alloys (HEAs) for Industrial Gas Turbines

- HEAs are stable single phase FCC, BCC, or HCP solid solutions at or near equiatomic compositions in multicomponent (≥5) systems
- HEAs considered for high-temperature, oxidizing environments in IGTs
  - Better stability at higher temperatures
  - Better thermodynamic compatibility with bond coat
- **Primary Design Challenge: Limited CALPHAD Databases**

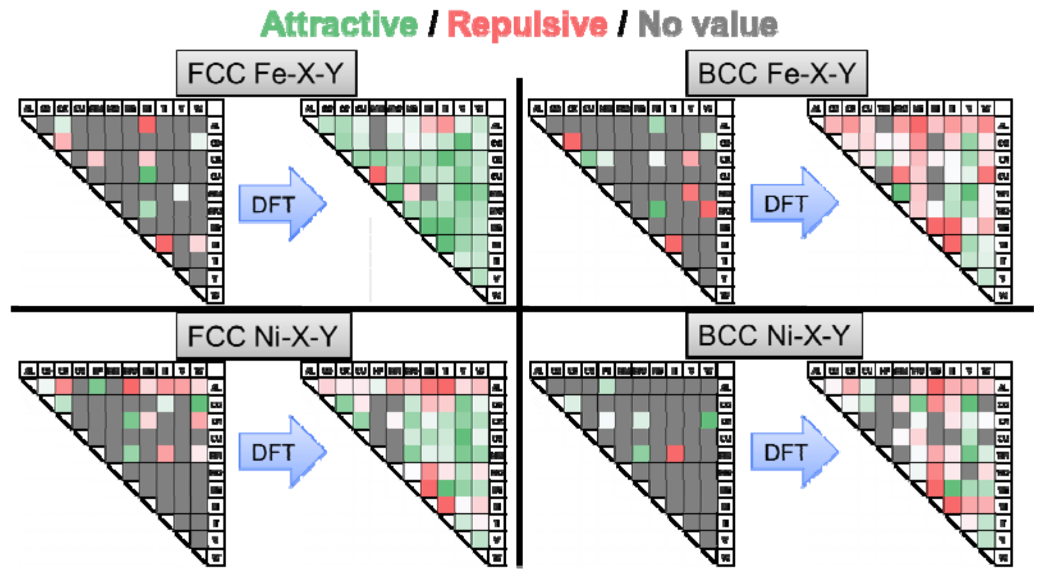


Phase I Overview: Couple high-throughput DFT thermodynamics with CALPHAD to accelerate HEA database development

High-performance Computing

CALPHAD Database Update

(ternary interaction parameters)



Improved accuracy of new database over current databases

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

Effect of CALPHAD + DFT

2x improvement in HEA predictability

Phase II Plan: Use Updated Database For Alloy Design

- Collaboration with Peter Liaw at University of Tennessee, recognized expert in HEAs
- Extend HEA CALPHAD database with additional elements using DFT
- Integration of Process-Structure and Structure-Property predictions into a preliminary HEA IGT design (in collaboration with OEM)
- Feasibility demonstration via scaled-up prototype production
- Preliminary application development

Closing Remarks

- ICME methodologies and tools have been developed and applied to the design of alloys with customized properties for critical applications in power generation
- Initial properties have been demonstrated at laboratory scales
  - Scaled-up production and longer-term testing in process
- Feasibility of meeting property goals demonstrated in <3 design iterations, demonstrating utility of ICME methodologies