



## ***eXtremeMAT Computational Materials Discovery for Existing & Advanced Power Cycles***

***Computational Materials Discovery & Design  
2019 TMS Annual Meeting & Exhibition  
March 12, 2019***

## Acknowledgement:

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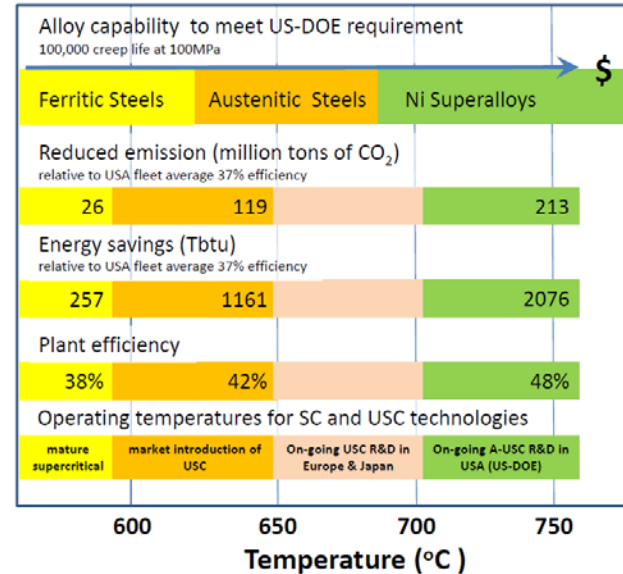
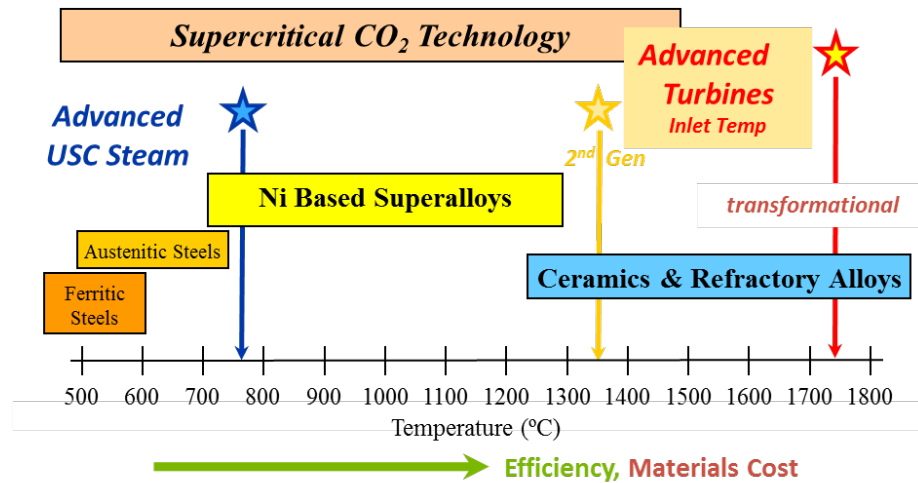
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## Consortium Task Leads/Executive Committee

- Jeffrey Hawk, NETL, Project Technical Lead & Manufacturing Task Lead
- Laurent Capolungo, LANL, Physics Based Modelling & Simulation Task Lead
- Ram Devanathan, PNNL, Steering Committee & Data Science & Machine Learning Task Lead
- Edgar Lara-Curzio, ORNL, Steering Committee & Validation Task Lead
- David Teter, LANL, Steering Committee Chair
- Tom Lograsso, Ames Laboratory, Steering Committee
- Gabriel Ilevbare, INL, Steering Committee
- Sergei Kucheyev, LLNL, Steering Committee
- David Alman, NETL, Steering Committee

## Materials Under Extreme Environments



### Materials Challenges

- High Temperatures, High Pressures, Corrosion, Oxidation
- Large Components
- Manufacturability
- Long Service Life  $\geq 100,000$  hrs
- Cycling of plants designed for base load

**Technology Enabler**  
**Affordable, Durable and Qualified**  
**Structural Materials for Harsh**  
**Service Life**

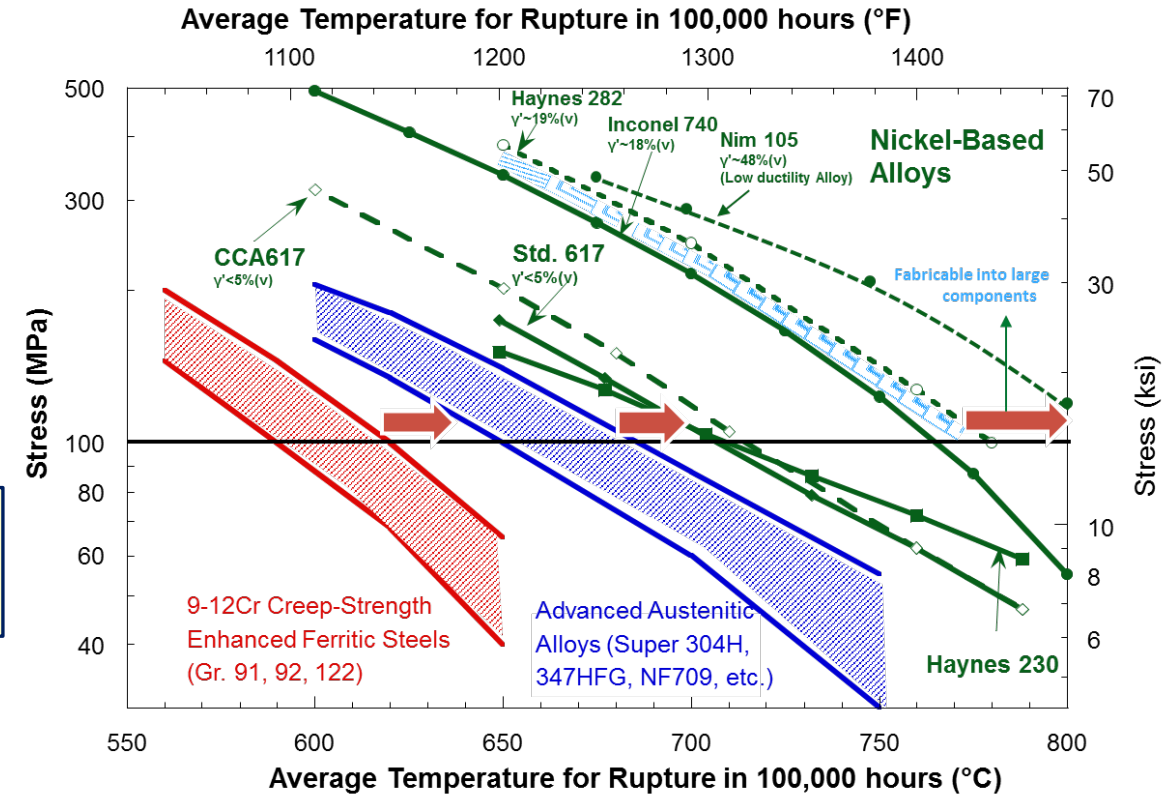
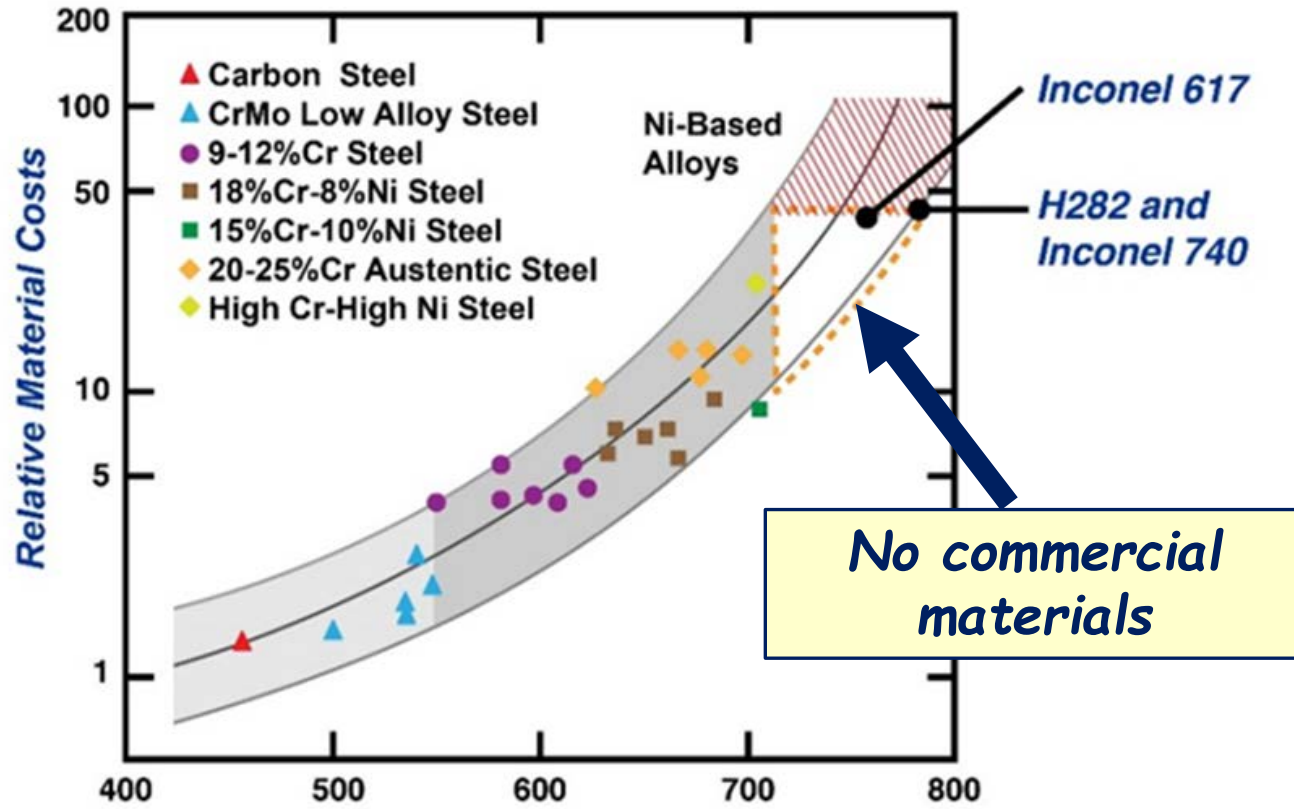


# eXtremeMAT

Accelerating the Development of Extreme Environment Materials



U.S. DEPARTMENT OF ENERGY



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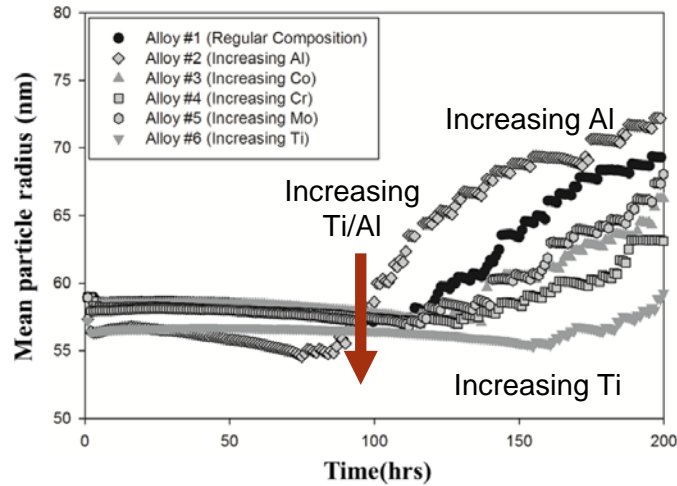
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Application	Benefit/Opportunity	Alloy Needs
Advanced Steam Plants	A-USC steam at 760°C and 35 MPa; 47% plant efficiency.	Low-cost, durable, high-strength, & qualified steels, and Ni-base superalloys (at 760°C) for 100,000 h creep life at 100 MPa stress at use temperature.
<b>Industrial &amp; Waste Heat Recovery</b>	<b>Recover 0.3 Quads energy T &gt; 650°C</b>	<b>Low-cost, corrosion, erosion, fouling resistant alloys for heat exchangers.</b>
sCO <sub>2</sub> Power Cycles	9 percentage points increase in plant efficiency compared to PC oxyfuel combustion with 20% lower LCOE for near 100% carbon capture at 800°C in high pressure CO <sub>2</sub> atmospheres	Qualified, high-temperature, oxidation, corrosion, & carburization resistant alloys, T > 700°C. Production level/ready materials in the US.
<b>Concentrating Solar Power (CSP)</b>	<b>Receivers: ≤ \$150/kW<sub>th</sub>; Thermal Efficiency ≥ 90%; HTF exit T &gt; 720°C; ≥ 10,000 cycles (30 years)</b>	<b>High-temperature, stable alloys for receivers.</b>
<b>Transportation: Turbocharger &amp; Housing</b>	<b>Affordable, high-efficiency engines</b>	<b>High-performance Fe-base alloys to replace Ni-base alloys.</b>

Alloy	Al	Co	Cr	Fe	Mo	Ti	Ni
#1*	1.5	10.0	20.0	1.5	8.5	2.1	Bal
#2	<u>1.8</u>	10.0	20.0	1.5	8.5	2.1	Bal
#3	1.5	<u>11.0</u>	20.0	1.5	8.5	2.1	Bal
#4	1.5	10.0	<u>21.0</u>	1.5	8.5	2.1	Bal
#5	1.5	10.0	20.0	1.5	<u>9.5</u>	2.1	Bal
#6	1.5	10.0	20.0	1.5	8.5	<u>2.5</u>	Bal

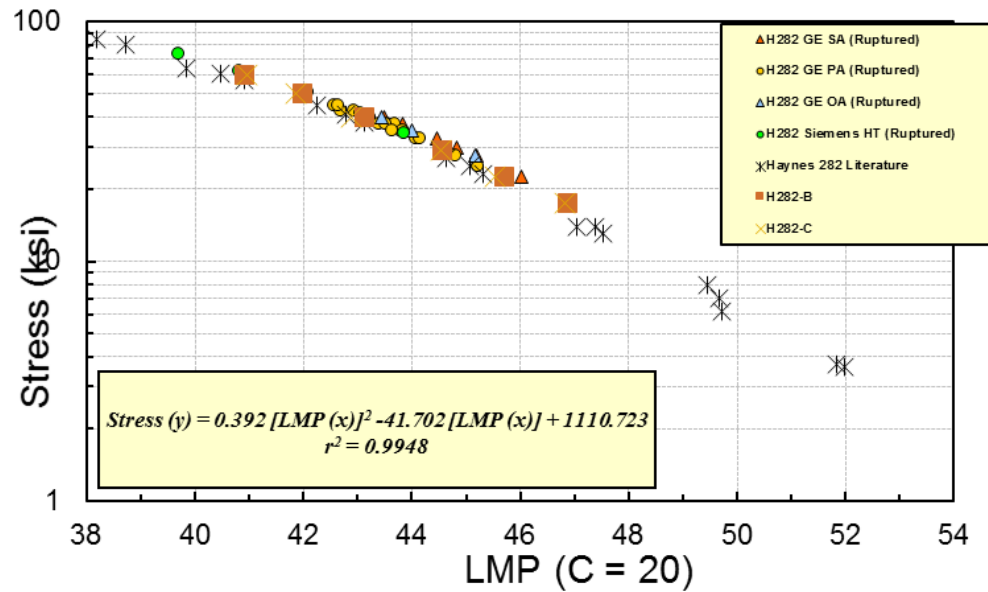
\*typical nominal composition of Haynes 282

Model predicts lower  $\gamma'$  coarsening rate with increasing Ti/Al ratio

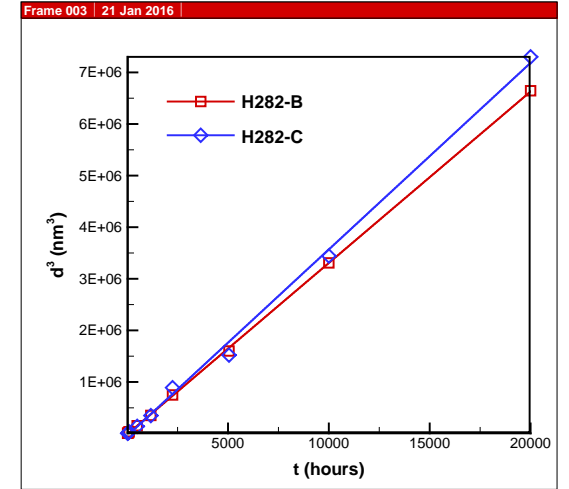


Youhai Wen, NETL

Alloy	Ni	Cr	Co	Mo	Ti	Al	Ti/Al
Nominal	Bal	18.5-20.5	9-11	8-9	1.9-2.3	1.38-1.65	
H282-B	Bal	19.22	9.86	8.49	2.22	1.27	1.75
H282-C	Bal	19.19	9.85	8.50	1.94	1.54	1.26



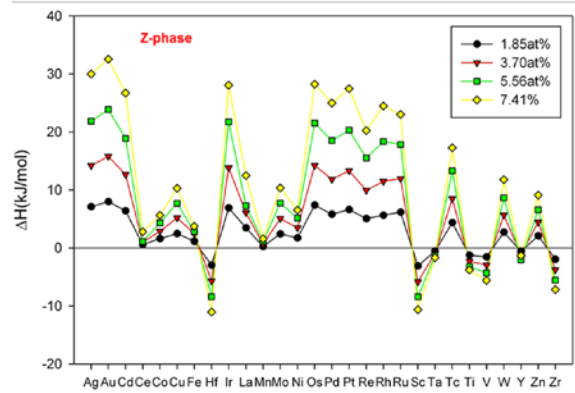
Slower  $\gamma'$  coarsening rate does translate into longer creep life! One more method for optimizing  $\gamma'$  nickel alloy creep life



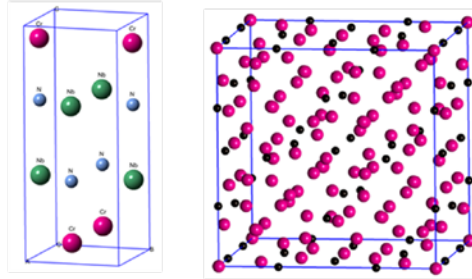
Creep Stress	H282-B $t_f$	H282-c $t_f$	$\Delta\%$
17.5	<u>18,578</u>	17,310	7.3
22.5	4,517	3,753	20.3
29	1,171	1,113	5.2
40	212	156	35.9
50	54	46	17.4
60	15	16	-6.3

Multi-scale computational modeling tools with best melt practice, heat treatment design & thermo-mechanical processing to produce optimal microstructures and highest possible alloy performance.

### Optimize composition

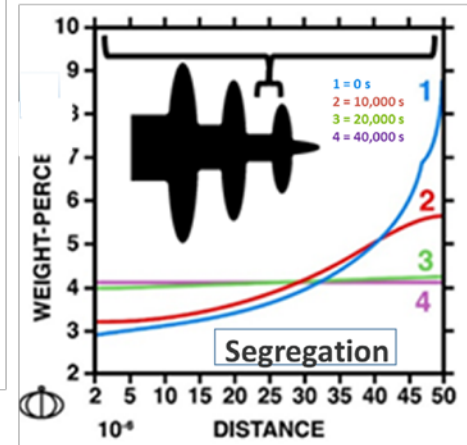


Z-phase (CrNNb)       $C_6Cr_{23}$  Carbide



DFT and CALPHAD used to optimize alloy composition. Simulations used to determine the effect of alloying elements on the formation and stability of unwanted (Z-phase) and desired strengthening phases (Carbides)

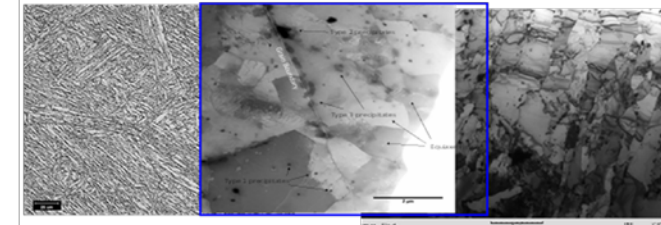
### Optimize processing



NETL's R&D 100 award winning computational tool used to guide heat-treating cycles to optimize the alloy's microstructure and properties.

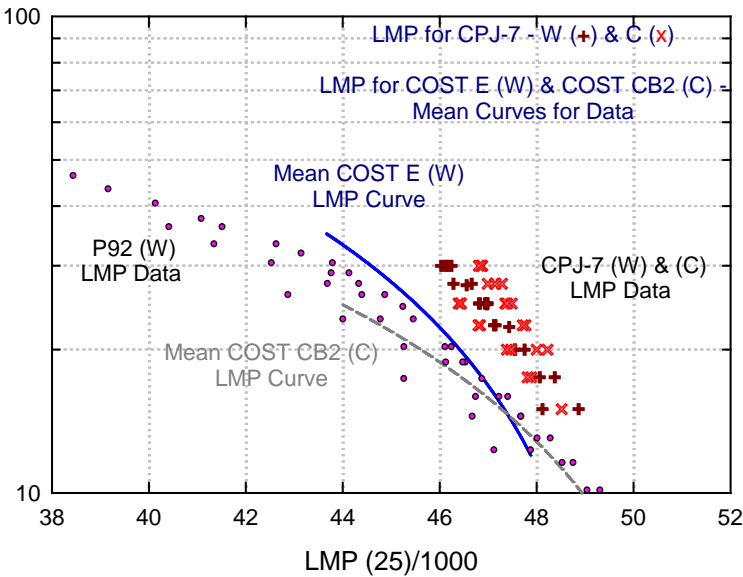
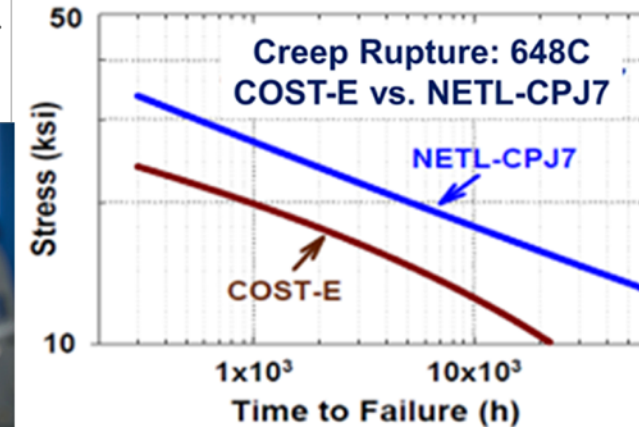


### Optimize microstructure



Outcome: NETL CPJ-7, New Fe-9Cr Alloy with an Increase Temperature Capability of ~ 50° F for this important class of power plant steel.

### Improve creep performance



**US Patent 9,181,597: Creep Resistant High Temperature Martensitic Steel Hawk, Jablonski, Cowen, NETL**



## Large Ni-Base Castings for A-USC Turbine Applications



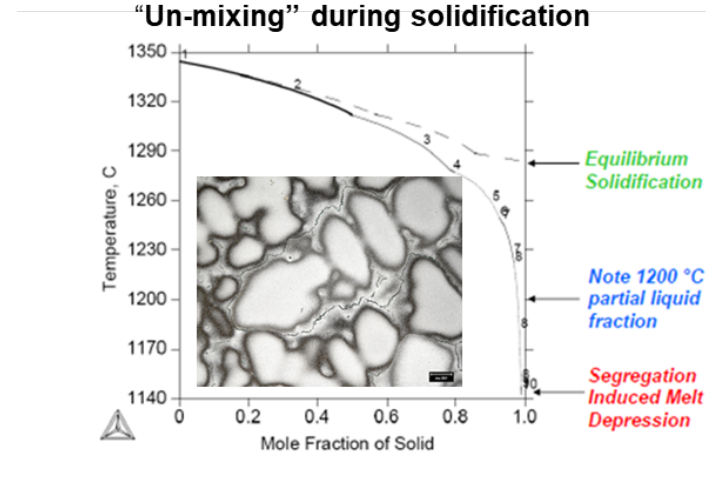
### Casting Challenges

1-15 tons; Up to 100 mm in thickness; slow cooling rates and segregation prone alloys

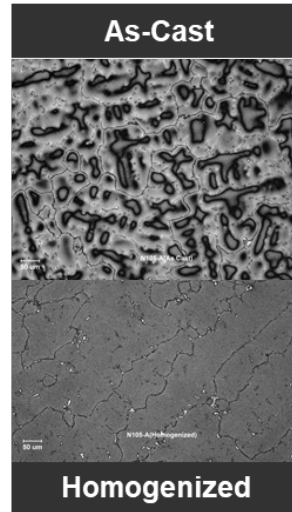
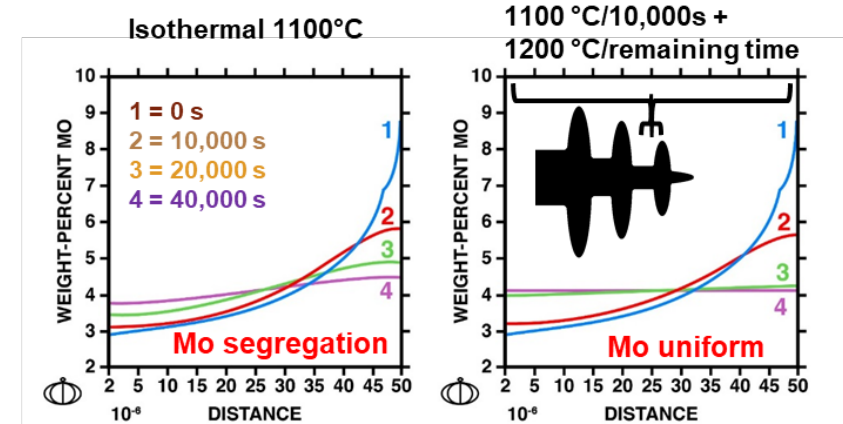
### Cast Version of Wrought Alloys

Wrought alloys considered due to proven weldability in thick sections

**Paul Jablonski, Jeff Hawk, NETL**

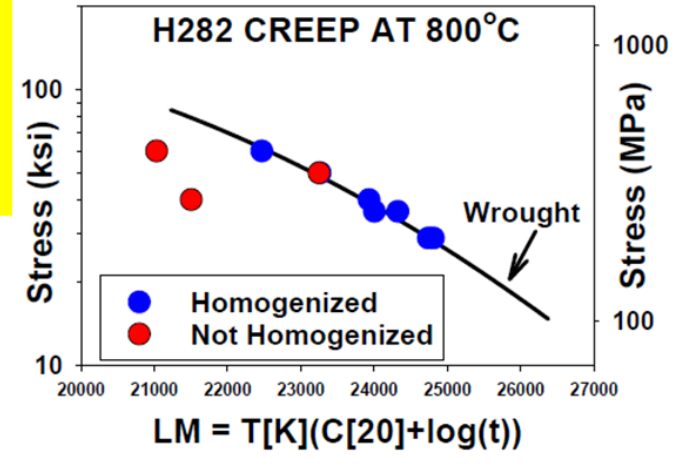


## CALPHAD Simulations of Mo segregation in Ni-alloy after heat-treatment



**Properly homogenized casting has comparable properties to wrought material**

Cast & heat-treated at NETL  
Creep testing at ORNL, GE, & NETL  
Homogenized: NETL multi-step solution treatment+ double aged  
Not Homogenized: traditional solution treatment + double aged



- **NETL Small Ingots (15 lb): 1100°C/3 h + 1200°C/9 h**

## Applied to industry casting for A-USC turbine components

- **Metaltex Step Block (300 lb): 1130°C/3 h + 1200°C/3 h + 1210°C/14 h**
- **Flowserve Step Block (1000 lb): 1100°C/6 h + 1200°C/48 h**
- **Special Metals ESR/VAR (10,000 lb): 1133°C/4 h + 1190°C/8 h + 1223°C/30 h**
- **GE: ½ actual size valve body for an A-USC turbine (18,500 lb casting)**



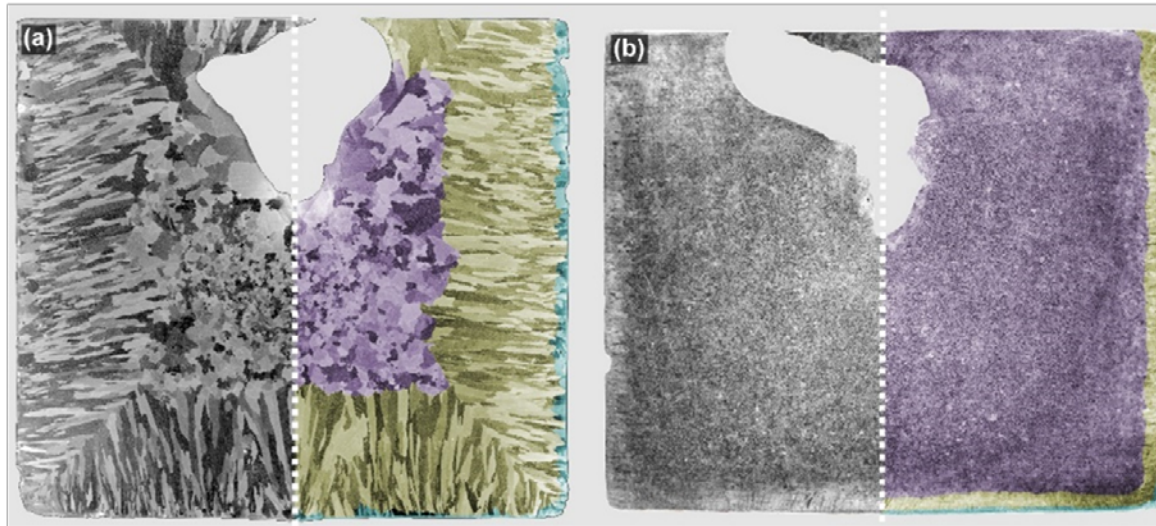
Temp (C)	Time (h)	IMP-T (C)
1115	3	54.4
1165	3	50.6
1175	3	51.2
1190	8	47.9
1205	12	50.6
1220	24	47.0
1225	24	50.1
Overall	77	---

*Computation simulations specified heat-treating schedules.*

*Designed to match existing furnace capability at commercial heat-treating facilities!*

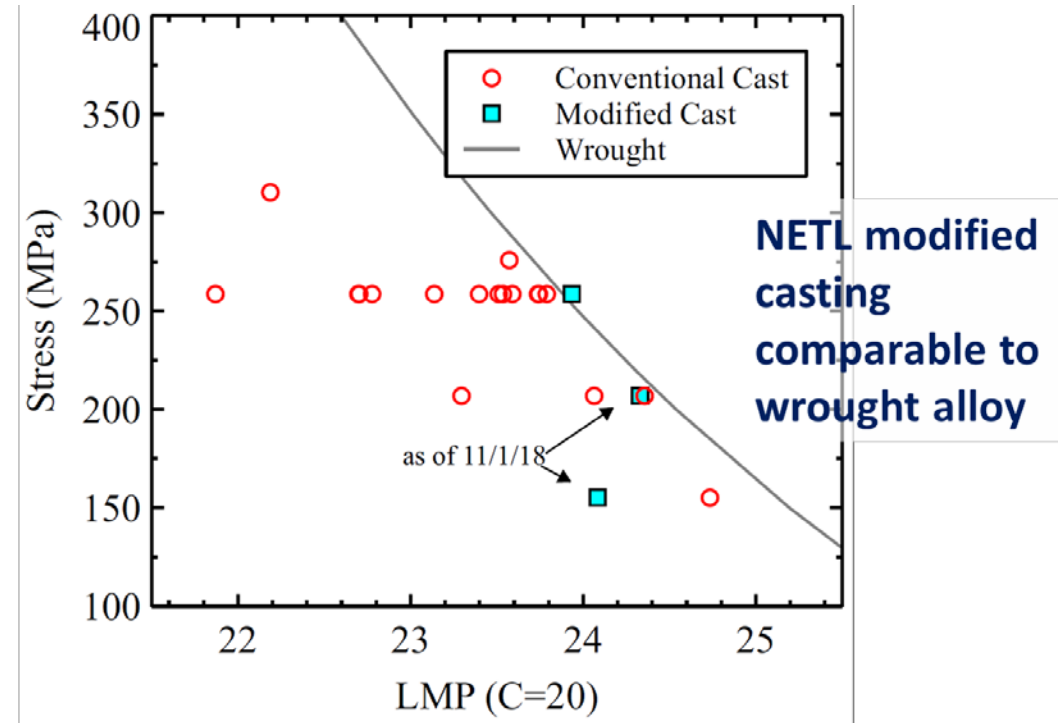


## Cast Version of 740H: Computational homogenization heat-treatment not effective H282 (GS & GB modification needed).



Conventional Casting:

Modified Casting:



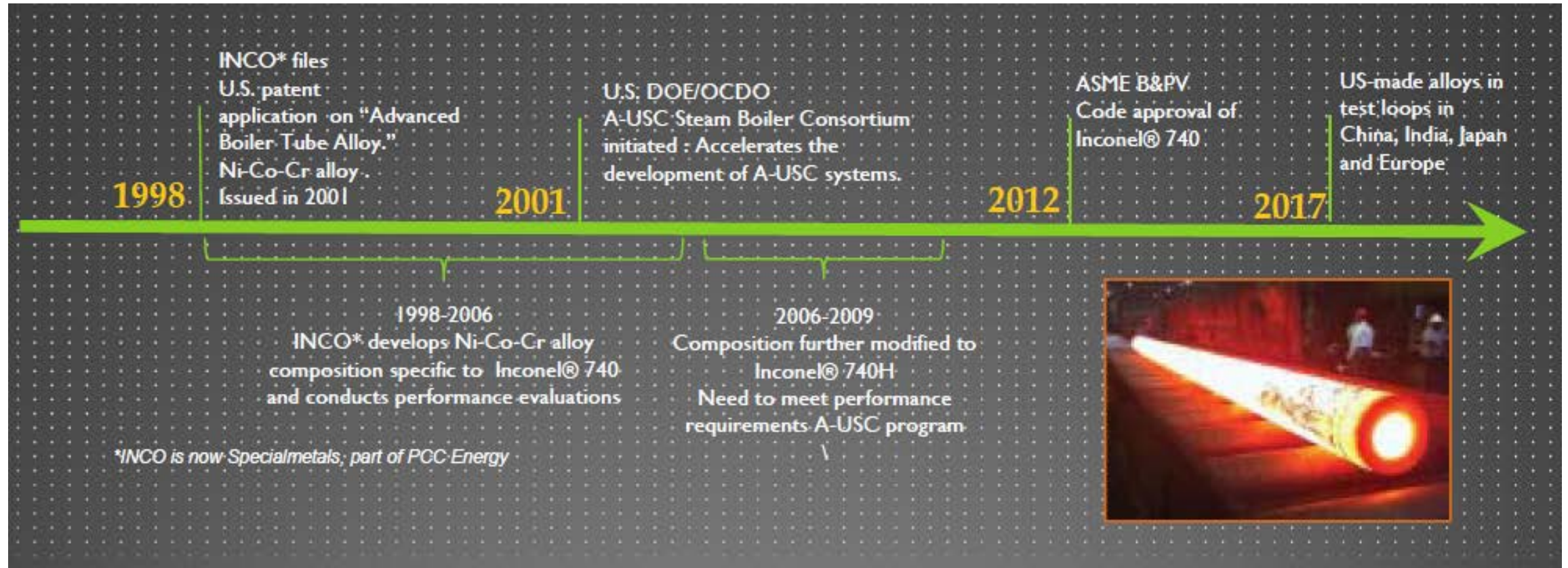
Ongoing research: Detrois, Jablonski, Hawk, NETL (2019)

# eXtremeMAT

Accelerating the Development of Extreme Environment Materials



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**Opportunity: Computational approaches to accelerate materials design, materials manufacturing, and performance prediction & qualification**

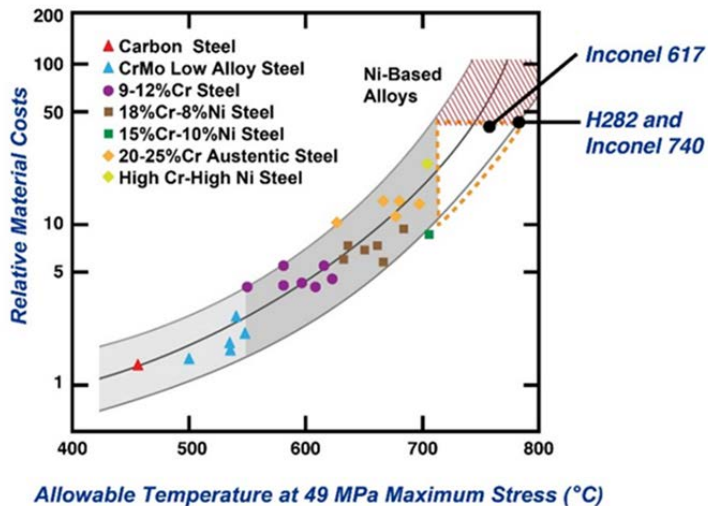
## For example, importance -

- Lower cost alloys for  $>650^{\circ}\text{C}$  service
- Thin section long-term integrity

✓ critical for advanced cycles (e.g.,  $\text{sCO}_2$  power cycles), but also valuable for existing FE power plants

## eXtremeMAT Objectives -

- Cost effective, heat-resistant materials
- Reliable life prediction models based on actual PP operation parameters



**POWER Engineering**

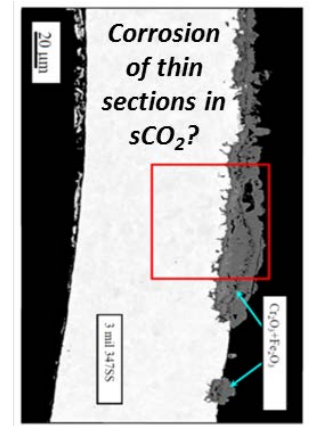
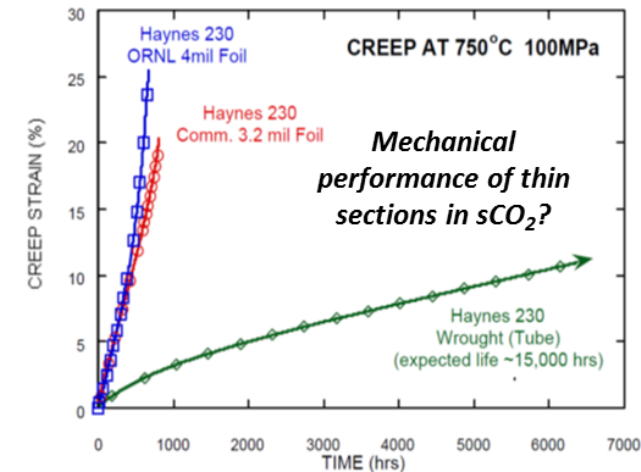
### Changing Mission Profiles

05/22/2017

By Mike Caravaggio and Norris Hirota, Electric Power Research Institute

Over the past decade, fossil and hydro generation plants have increasingly experienced significant changes in their operating strategies, or "mission profiles," compared to their original designs. These changes include new operating regimes with increased cycling, extended unit layups, and prolonged periods of low turndown.

The changes, in turn, are creating a multitude of challenges for the plants and their operating staff in areas ranging from component degradation to staffing levels, O&M budgets, and meeting environmental compliance under non-baseload conditions.



P.J. Masiasz, et al ORNL 2006

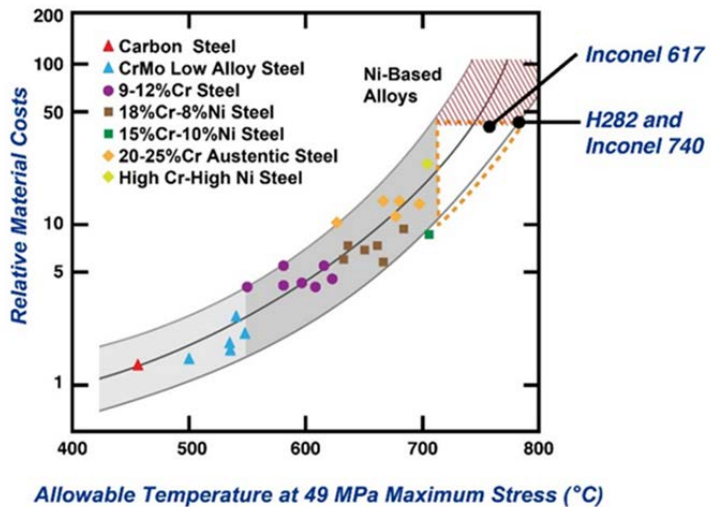
P.J. Masiasz, et al ORNL 2006

## Opportunities -

Lower cost, higher temperature austenitic alloys – reduce the cost of A-USC power cycles

Life prediction for critical components in plants undergoing cycling conditions (e.g., hold-time fatigue)

Performance of thin sheet used in recuperators in sCO<sub>2</sub> power cycles



**POWER Engineering**

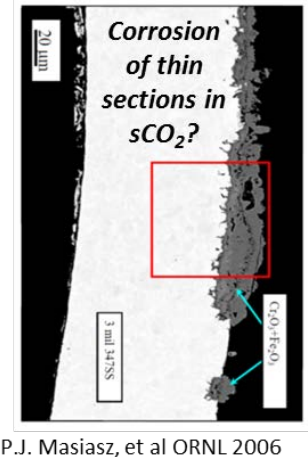
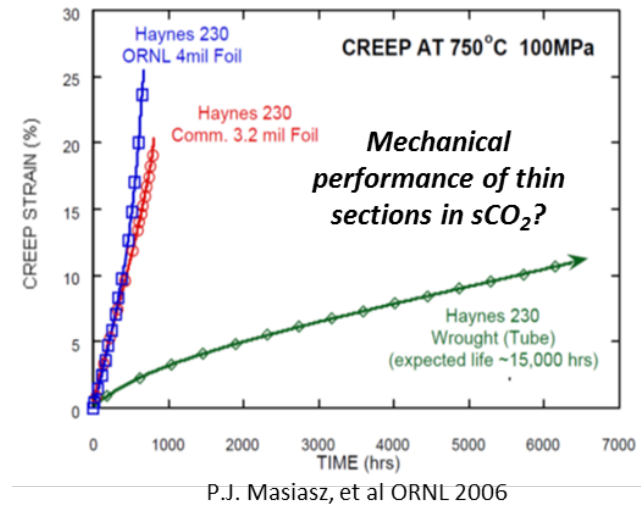
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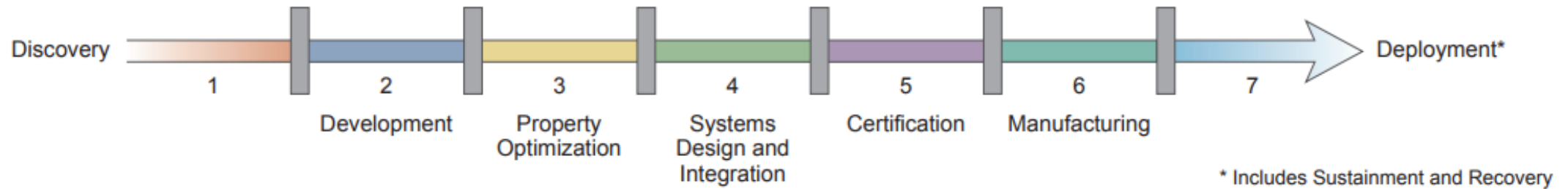
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## Going beyond empirical materials development



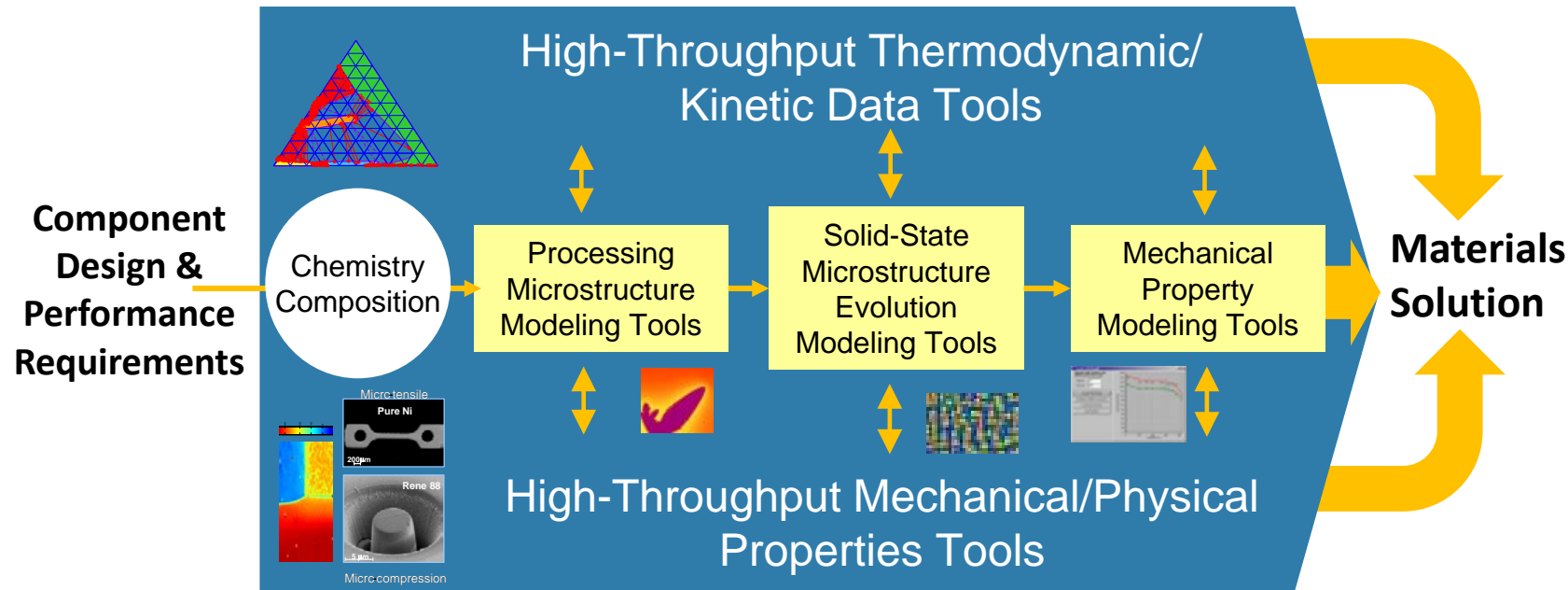
Traditional materials development takes 10-20 years (source: OSTP MGI White Paper, 2011)

Empirical lifetime prediction is unreliable and not transferable to new alloys.

**Solution: Use data management and analytics to integrate materials development.**

## Integrated Materials Engineering Approach

Physics-based modeling tools  
High-throughput screening tools + Data Analytics → Materials Solution



- New Alloys → Achieve Cost/Time Reduction
- Predict Materials Service Performance & Manage Part Life

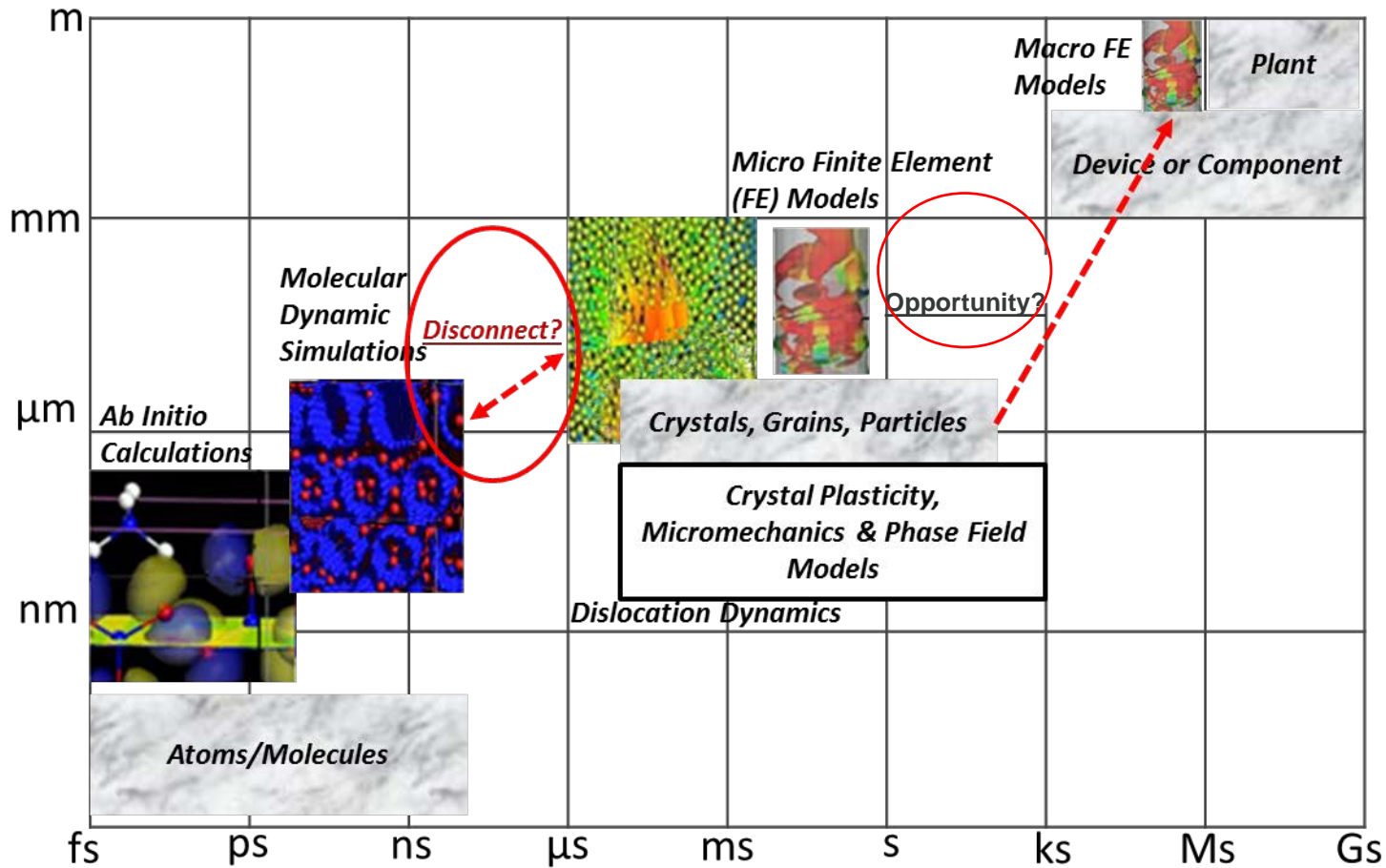
Utilize unique, world-leading US DOE - NL resources associated with:

- *materials design,*
- *HPC power,*
- *advanced processing & manufacturing,*
- *in-situ characterization*
- *performance assessment at condition*

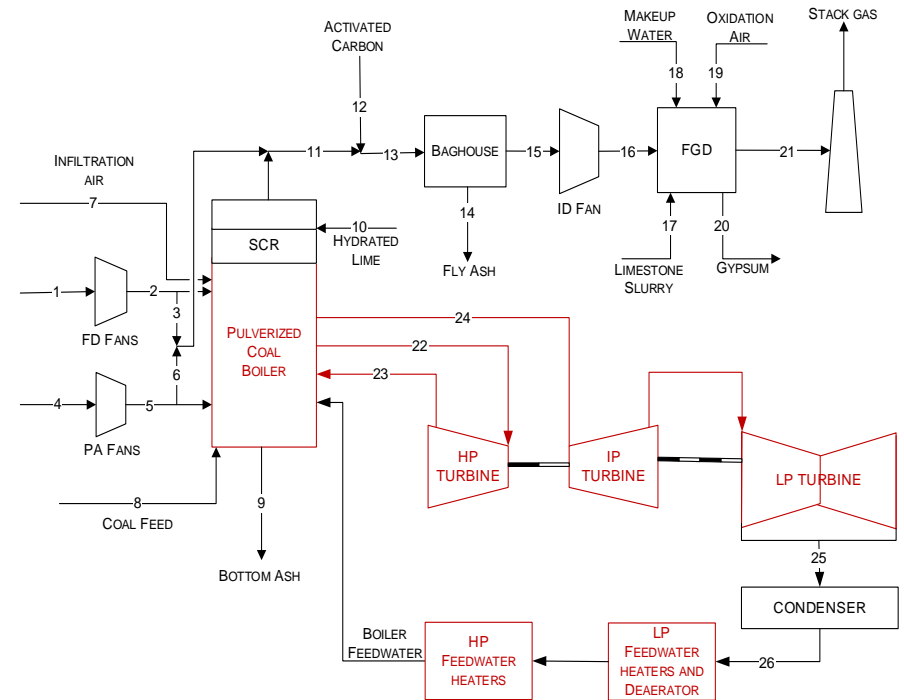
in a focused, coordinated, & collaborative way to demonstrate a methodology & framework for developing materials for any challenging FE power cycle.



## eXtremeMAT Challenge -



## General Requirements for Computational Tools & Analysis in Multi-time & Multi-dimensional Scales



Note: Block Flow Diagram is not intended to represent a complete material balance. Only major process streams and equipment are shown.

## Why physics based models?

- **Certain observations are counter-intuitive**
  - For example, increase in yield stress with increasing temperature
  - Tension-compression asymmetry (both in yield and creep)
  - Violation of Schmid's law
- **Increasing complexity**
  - (ordered) Precipitate strengthening
  - Lattice-mismatch effects
  - Cross-slip induced strengthening
  - Multi-modal dispersion of precipitate
- **Accelerated alloy design**
  - Identify vital microstructure X's (i.e., variables)
  - Their relative impact and their stability in the model

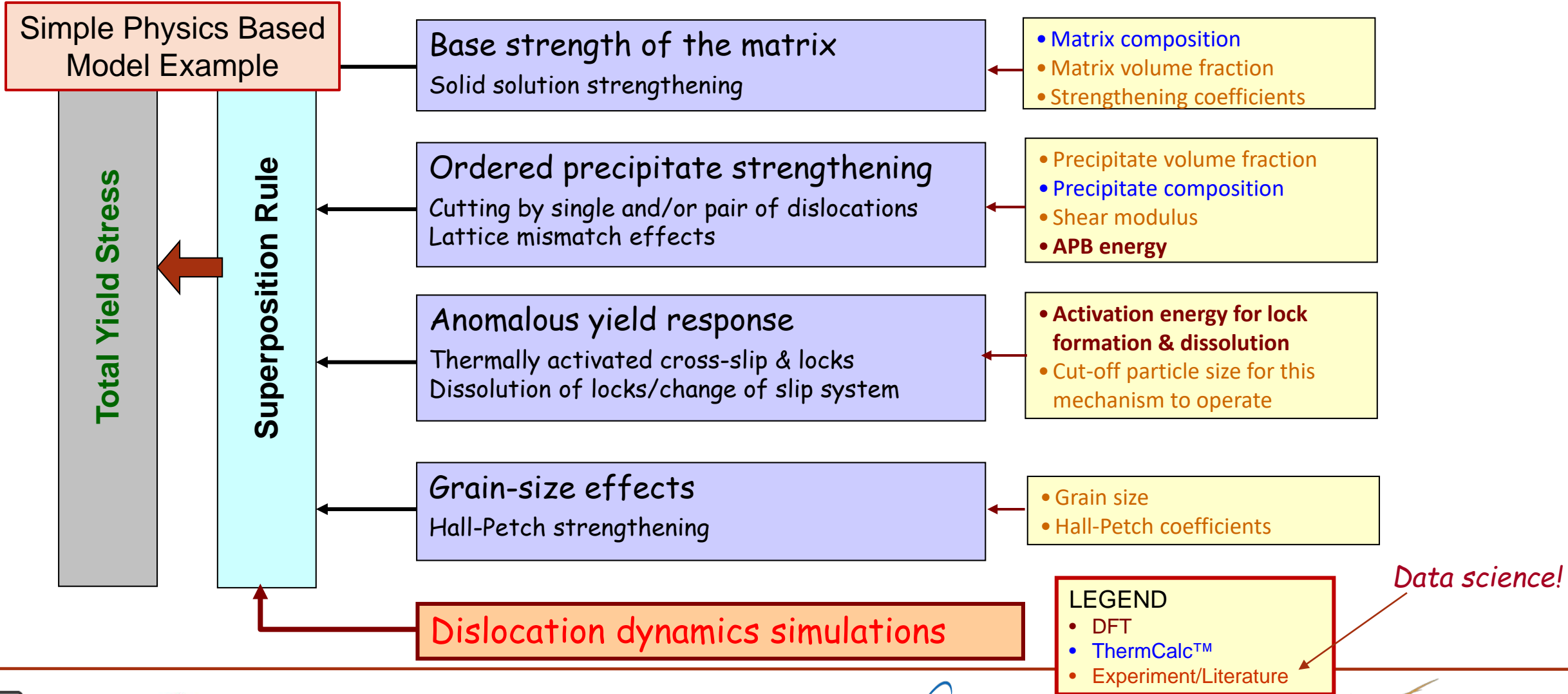
*All these processes can be described by physics-based models using constitutive equations. Early attempts used simple physical models. XMAT will use more state-of-the art, physically descriptive ones.*

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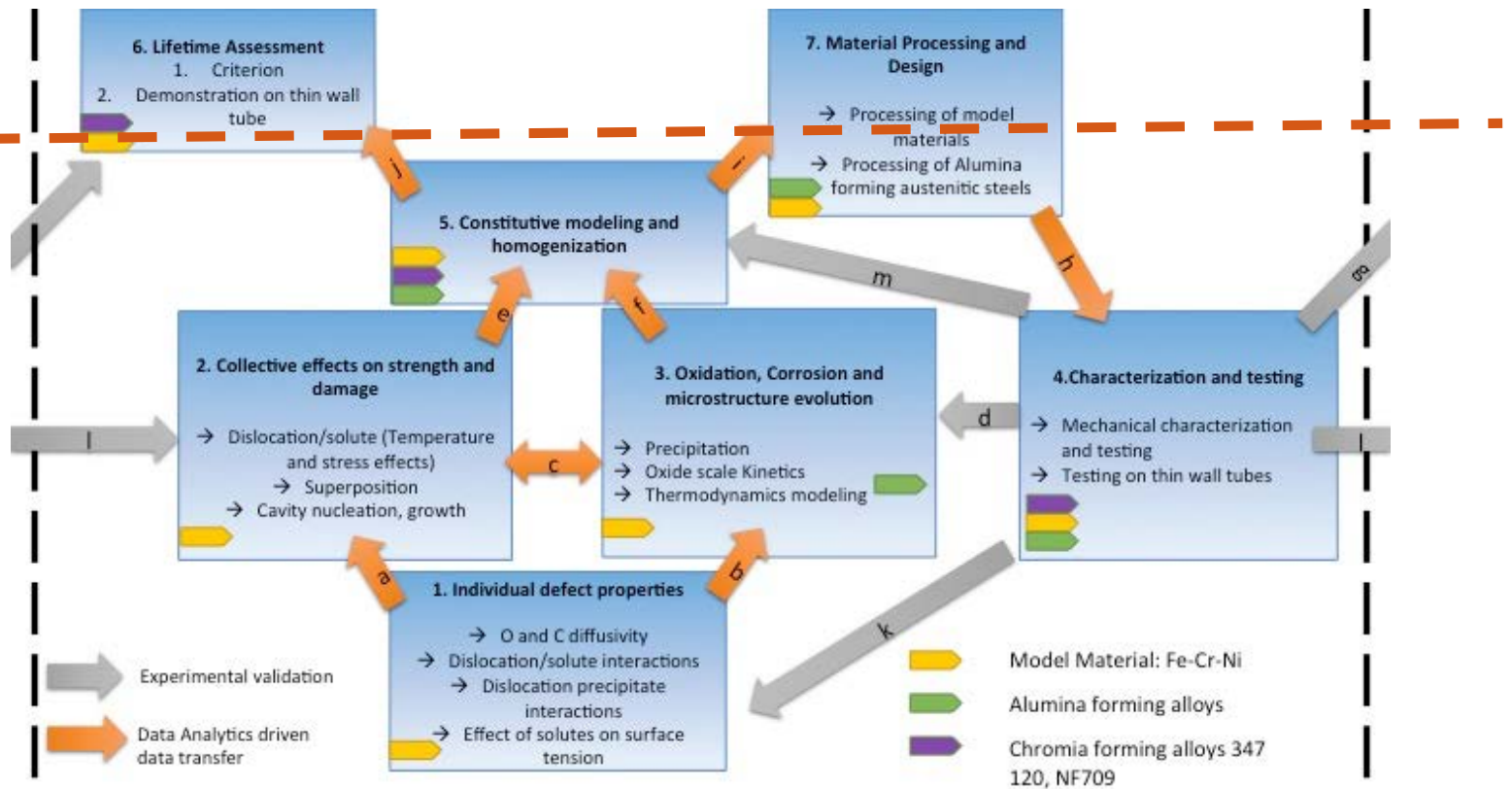
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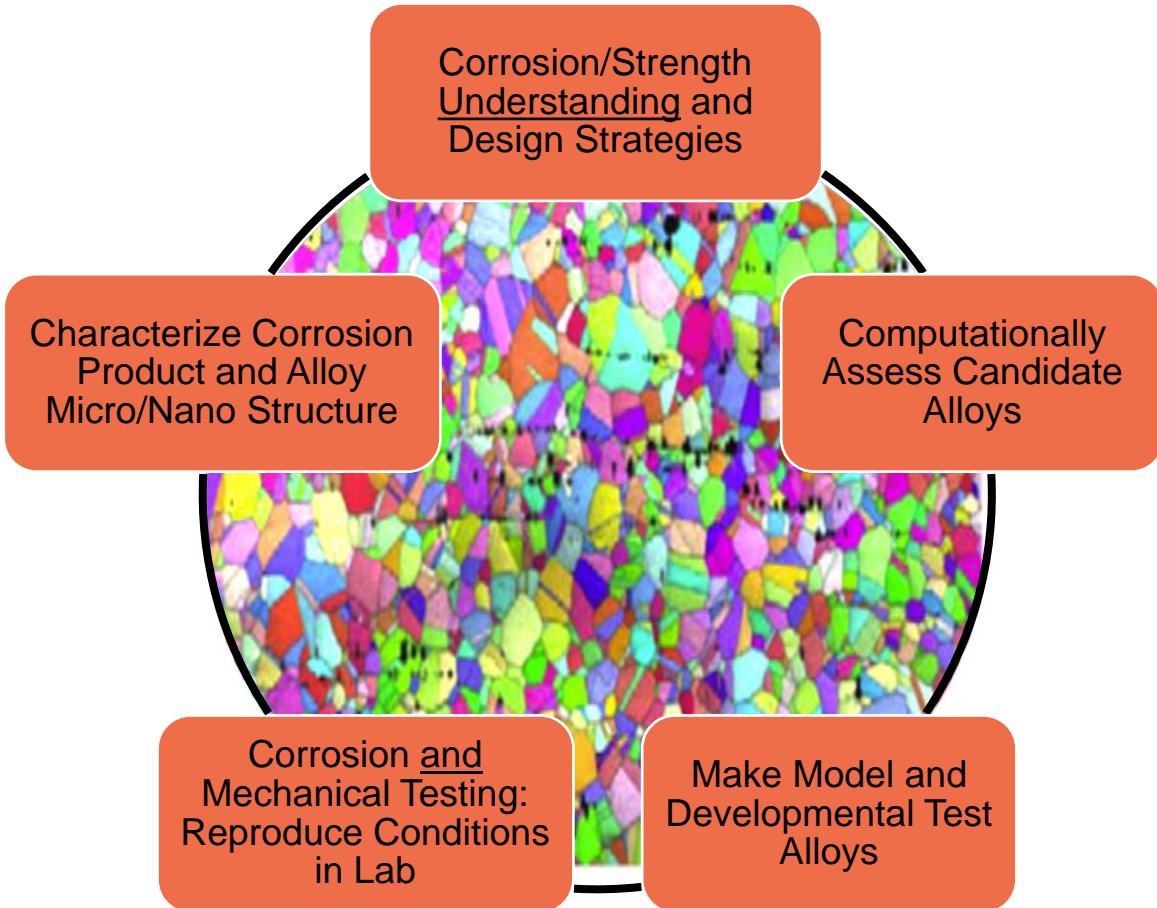


## Life Time Modeling & Performance ↔ Alloy Design

*Modeling Building Blocks*

Develop Basic Tool Sets:  
Computational Modeling  
& Data Science/Analytics





## *XMAT Physics-based Modeling*

*Develop a physics-based modeling framework using most appropriate & realistic constitutive equations describing quasi-static & dynamic deformation processes across all stress states & length/time scales. Use these models to predict component/material lifetime (e.g., ferritic, austenitic, etc., ppte strengthened or not, & the components made from those materials) as function of material chemistry, temperature, environment, operation history, etc.*

*→ Lifetime assessment*

*→ Material design*

## 2.5. Lifetime Assessment (H. Huang)

- Integration across length scales
- Multiphysics framework

## 2.4. Constitutive modeling and homogenization (R. Lebensohn)

- Polycrystal plasticity code
- Constitutive law
- Database
- Tertiary creep

*XMAT will look at a wide range of physics-based models over many length & time scales using appropriate constitutive equations that completely describe the physical loading situation & the evolution of microstructure over the operational lifetime. This schematic describes some of the physical models.*

## 2.2. Collective effects on strength and damage (R. LeSar)

- Coupled Cluster dynamics/ DDD tool
- Void formation model kinetics

## 2.3. Microstructure evolution (M. Brady)

- Thermodynamics based design
- Kinetic based design
- Strength based design
- Passivation layer formation

## 4. Characterization & Testing (E. Lara-Curzio)

- Mechanical characterization & testing
- Testing on thin wall tubes

## 2.1. Individual defect properties (B. Wood)

- Interatomic potential Fe-Cr-Ni
- C and O diffusivities in Fe-Cr-N
- Oxidation rate at free surfaces

*Data science as input & model validation*

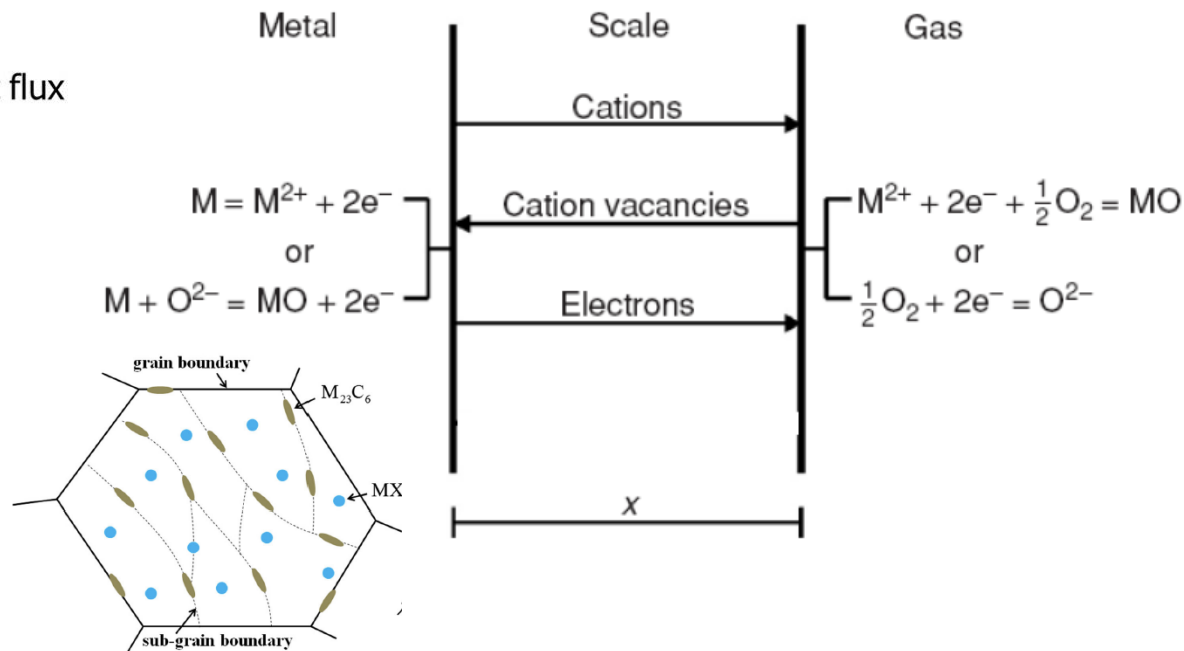
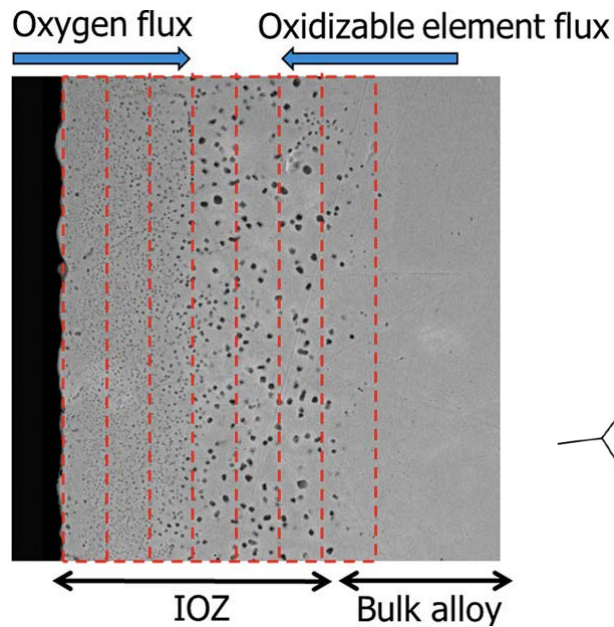
- Model Material: Fe-Cr-Ni
- Alumina forming alloys
- Chromia forming alloys

Mechanical Response as a function of microstructure and chemistry

Failure due to damage evolution as a function of composition

**Formation of oxide scale**

Failure prediction due to failure of the passivation layer



Our understanding of the phenomena leading to oxidation is mature (e.g. Wagner's theory.)

### Challenge:

Effects of trace elements.

Does stable scale form?

Connection with failure and chemistry is unclear.

# eXtremeMAT State of the art

Accelerating the Development of Extreme Environment Materials

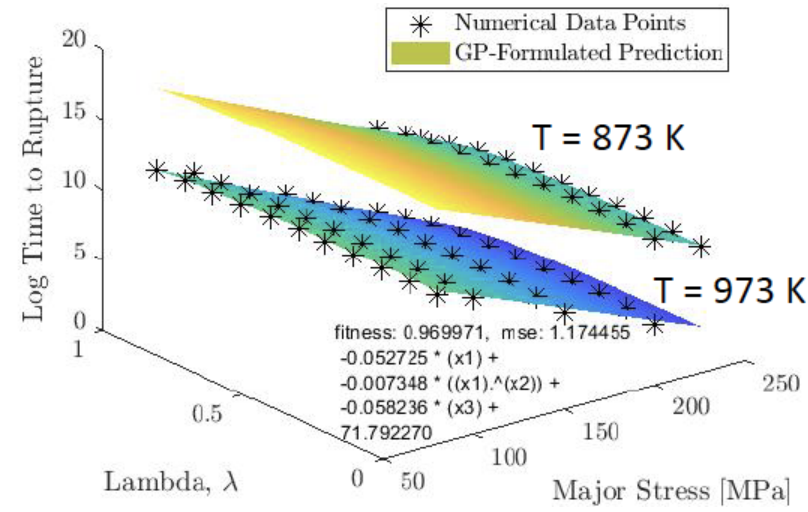
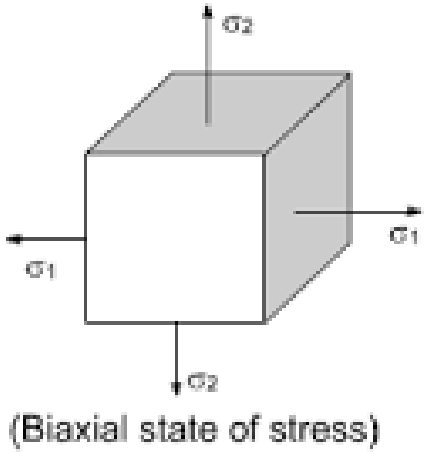


Mechanical Response as a function of microstructure and chemistry

Failure due to damage evolution as a function of composition

Formation oxide scale

Failure prediction due to failure of the passivation layer



Data analytics can yield new failure criteria



**New Lifetime Prediction Tool:**

$$\log(t_r) = A\sigma_1 + B\sigma_1^\lambda + C \cdot T + D$$

$A = -5.3 \times 10^{-2}$ ,  $B = -7.3 \times 10^{-3}$ ,  
 $C = -5.8 \times 10^{-2}$ ,  $D = 71.8$

Capolungo, LANL



# eXtremeMAT

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*Given the incredible complexity envisioned in the modeling activity, Reduced order Models (RoM) may be developed to facilitate acceptance by industry & standards committees to apply modeling approach to practical power cycle materials situations.*

P91 → ferritic  
347H  
316H

Constitutive law  
*with damage*

FFT

Joint effort with  
Task 3

ROM for  
mechanical  
response

VPSC (used for fitting)

*Reduced order Models (RoM) are not curve fitted data. These models provide a simplified pathway into the the modeling framework and eliminate the need for industry to know/provide all model variable information.*

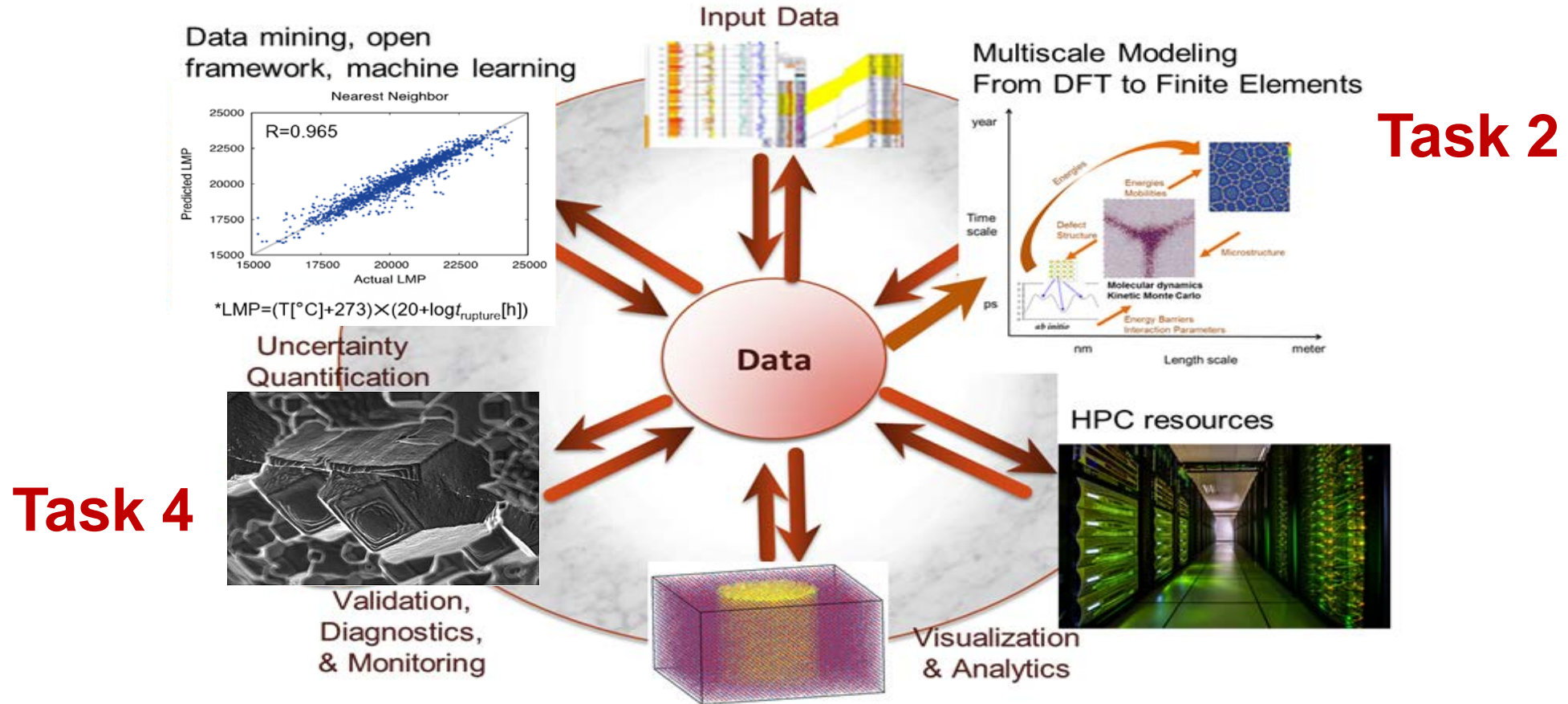
FEM

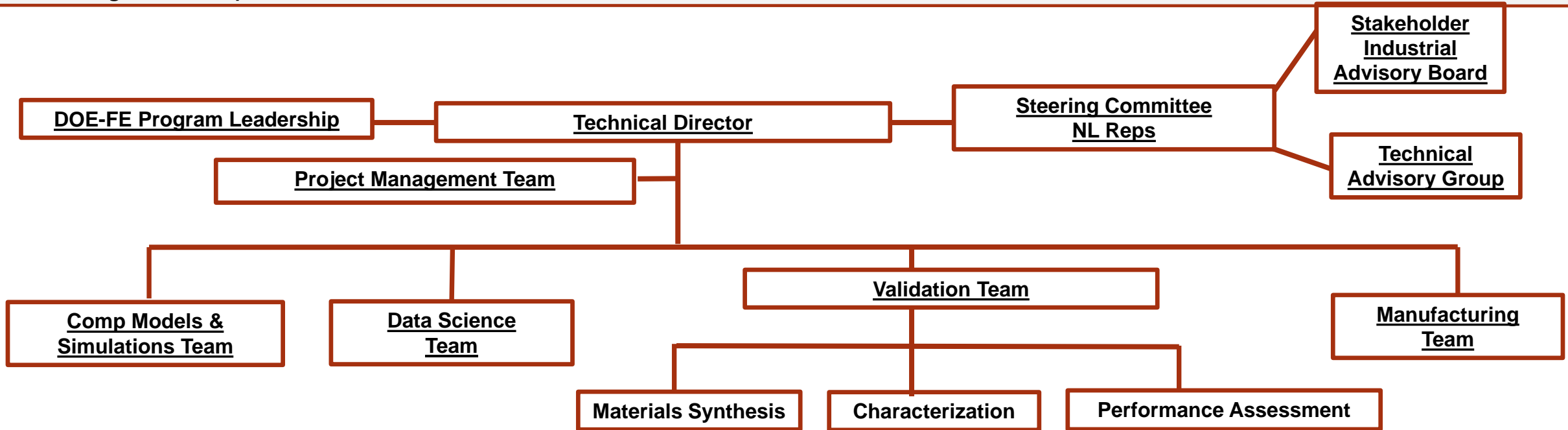
Limited to 2D microstructure  
Numerical efficiency

ROM rupture  
life

Joint effort with  
Task 3

*Data science will be used to reduce the time, and cost, for alloy design & development activities as well as provide lifetime prediction modeling simulation tools.*





*Challenge: Managing the seven DOE National Laboratories to facilitate and ensure communication, coordination, collaboration, research progress and project success.*

# eXtremeMAT

Accelerating the Development of Extreme Environment Materials



High Level Milestone/Accomplishment	2019				2020				2021				2022				2023			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Develop multiscale modeling integration strategy	→																			
Establish database of information on chromia- & alumina-forming alloys to be used for alloy design	→																			
Implement modeling strategy & first demonstration for mechanical response and failure of model alloys & chromia-forming alloys			→																	
Validate modeling strategy through experiment					→															
Complete identification of candidate alloys & share chemistry, microstructure and processing data for early baseline performance prediction					→															
Apply modeling strategy & formulate improved austenitic alloys					→															
Develop data-driven models to integrate with physics based models for reliable predictions. Document model assumptions & limitations in EDX									→											
Validate candidate austenitic alloy(s) formulated from modeling strategy									→											
Predict performance and failure of a component (thin wall tube) for several different environments									→											
Predict microstructural stability under performance conditions by combining microstructure data, simulation data & process models													→							
Demonstrate a full integrated & validated data analytics capability for alloy design & lifetime prediction													→							
Demonstrate manufacture of optimized austenitic alloy(s) formulated from computational and data analytics													→							

**Outcome**

*Improved Physics-based Materials Models* for predicting performance & service life.

*Computational Framework* for optimizing specific alloy performance.

Improved alloys with superior performance.



## Atoms to Metals

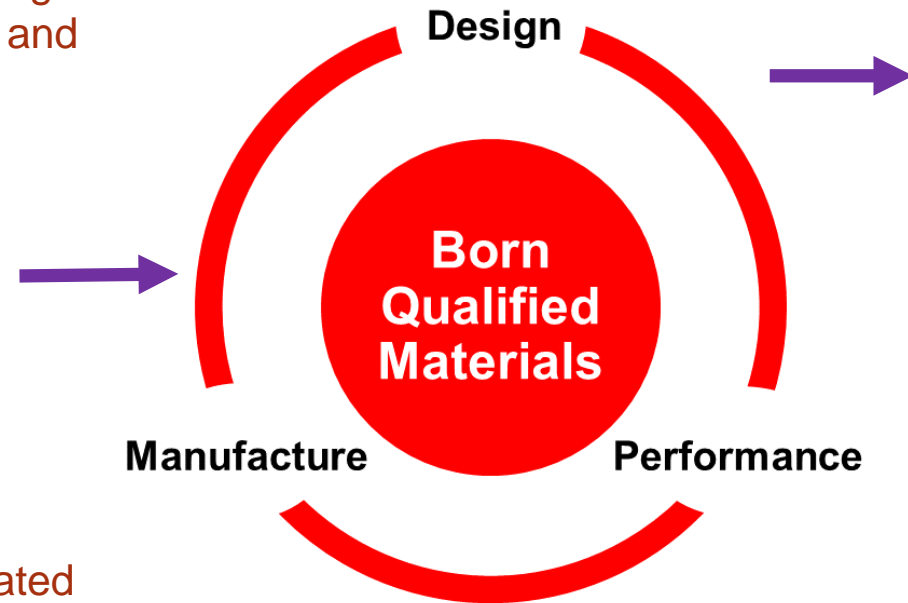
ICME multi-scale computational approaches incorporating best practice manufacturing and focused on performance evaluation and characterization.

## Targeted Validation Experiments

Conducted in industrial relevant environments and scales.

## Data Informatics and Analytics

Analyze the large volume of data generated from materials testing incorporate learning to improve predictive capability of simulations and reduce uncertainty.



Validated simulations linking structure, processing and performance.

Accelerate the identification and deployment of cost effective materials by 2X for extreme environment applications.

## Thank you

- Questions
- Comments
- Other thoughts & considerations

- **BACKUP SLIDES**

## Task 2: Multi-scale modeling

- **Objective:** (i) Deliver predictive criterion for the lifetime of materials as functions of chemistry & environment; (ii) Develop figures of merit for alloy design; (iii) Design an engineering-based approach for assessing performance of components in extreme environments.
- **Approach:** Development & use of hierarchical multi-scale / multi-physics framework for the prediction of mechanical response & microstructure evolution in alloys subjected to extreme environments. Integration strategy relies on multi-scale characterization (Task 4) & leverages data analytics methods for information transfer across length scales (Task 3).
- **Subtasks:**
  - 2.1 Individual defect properties
  - 2.2 Collective effects on strength & damage
  - 2.3 Oxidation, corrosion & microstructure evolution
  - 2.4 Constitutive modeling & homogenization
  - 2.5 Lifetime assessment



## Task 3. Data Analytics and Management

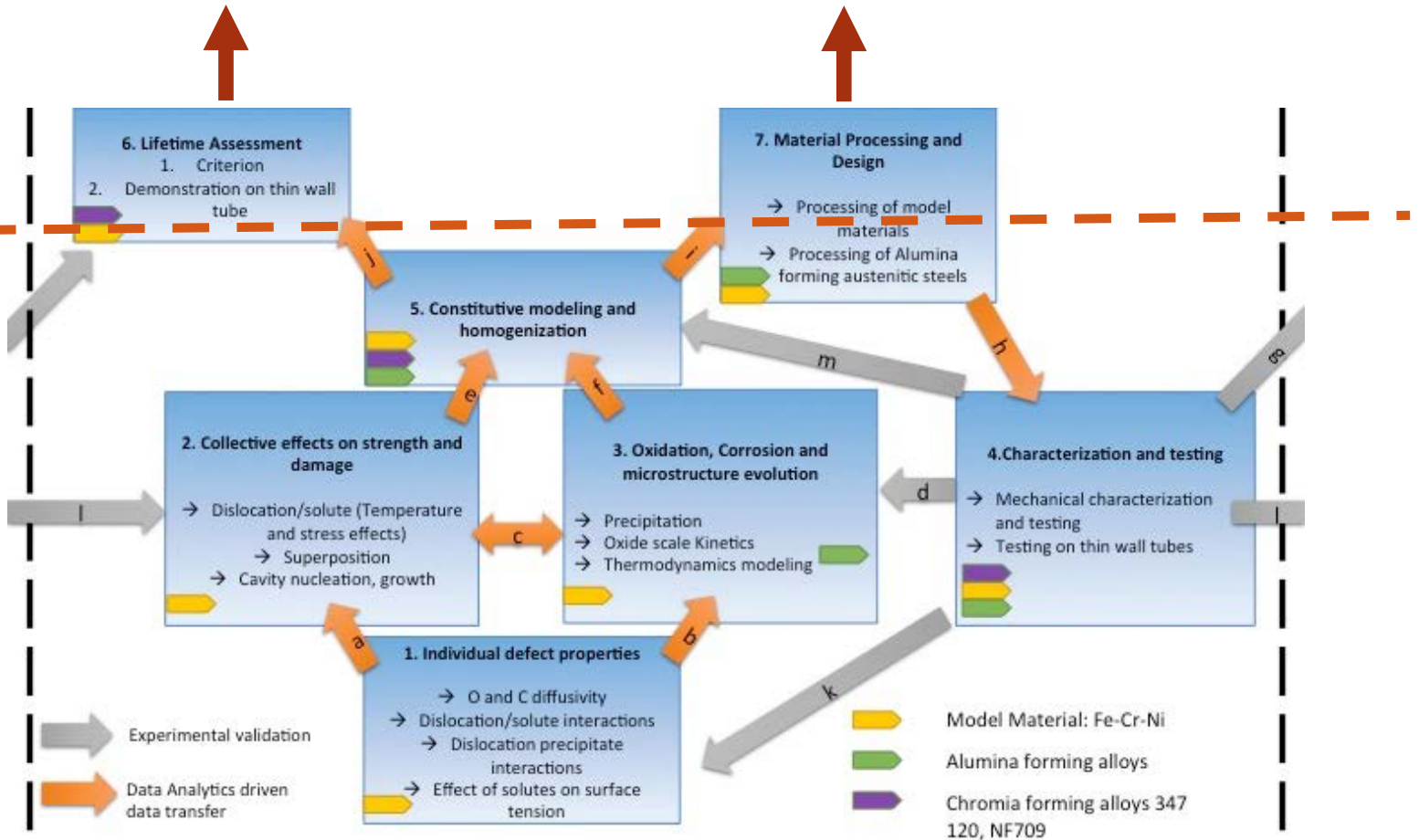
- **Objective:** Develop a data analytics framework to predict performance at extremes and design alloys with improved creep and oxidation resistance.
- **Approach:** Collect, curate and validate data; quantify uncertainty; analyze data; develop a user interface; and manage data lifecycle.
- **Subtasks**
  - 3.1 Data Assessment: Identify data gaps, collect and curate data (Tasks 2 and 4)
  - 3.2 Data Management: Develop data management framework with support for customizable workflows, visualization, user interfaces, and model setup. (Task 2)
  - 3.3 Data Analytics: Identify the main drivers of mechanical degradation in extreme environments.

## Modeling Building Blocks

Develop Basic Tool Sets:  
Computational Modeling  
& Data Science/Analytics

Life time predictions,  
including thin sections

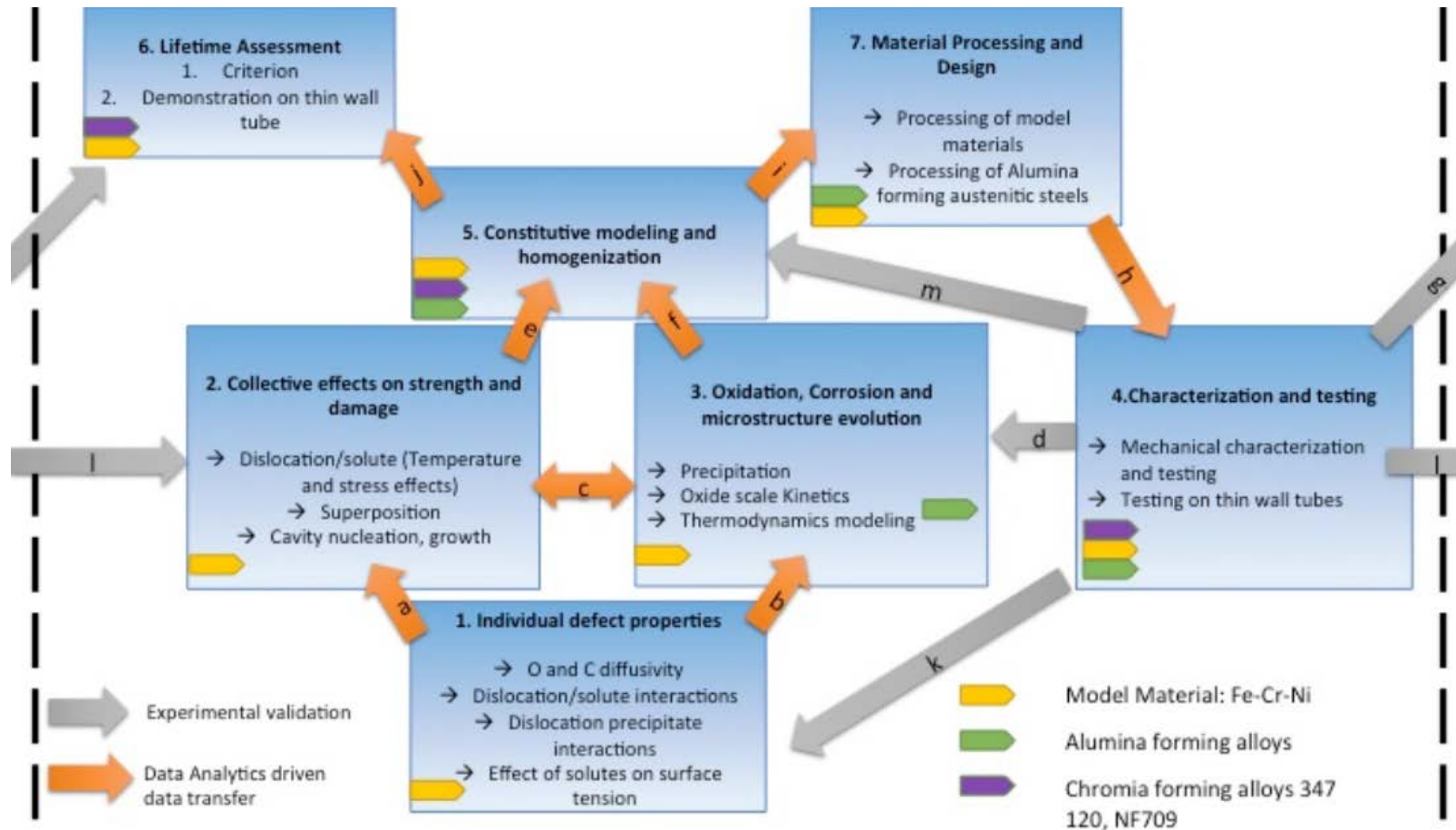
Apply to optimize (improve)  
347/316 (austenitic) type alloys



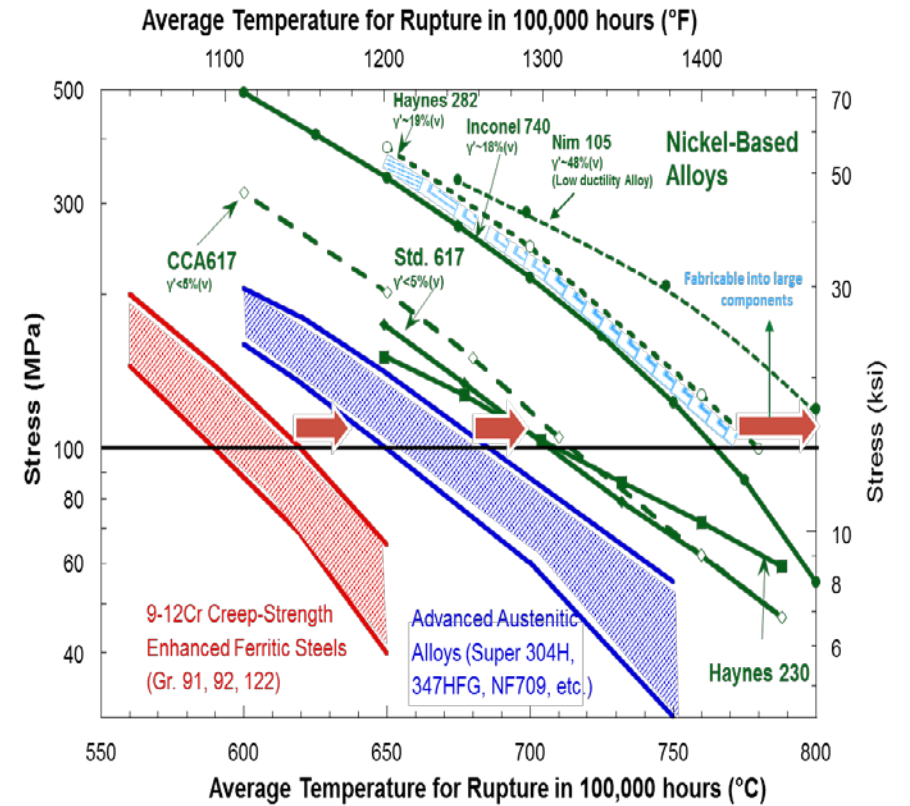
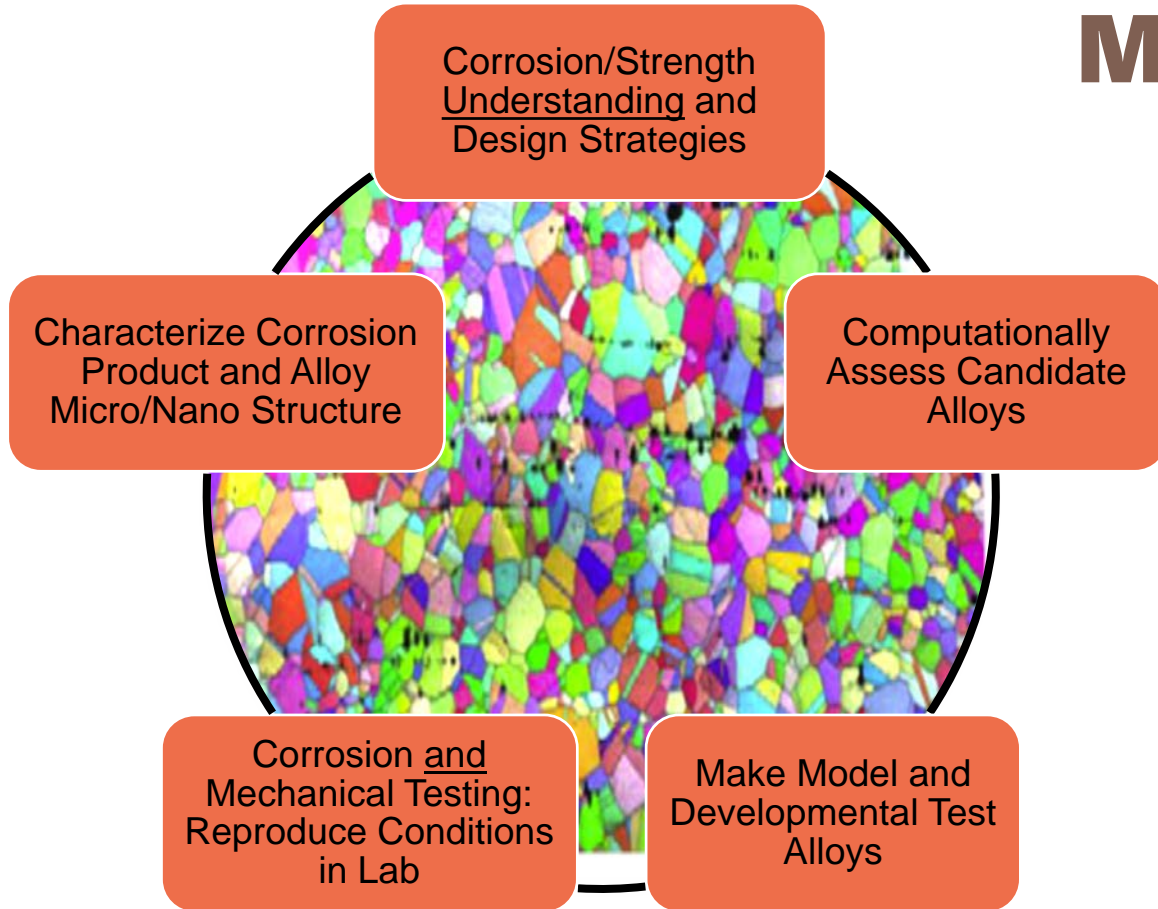
## Integrated Modeling Framework

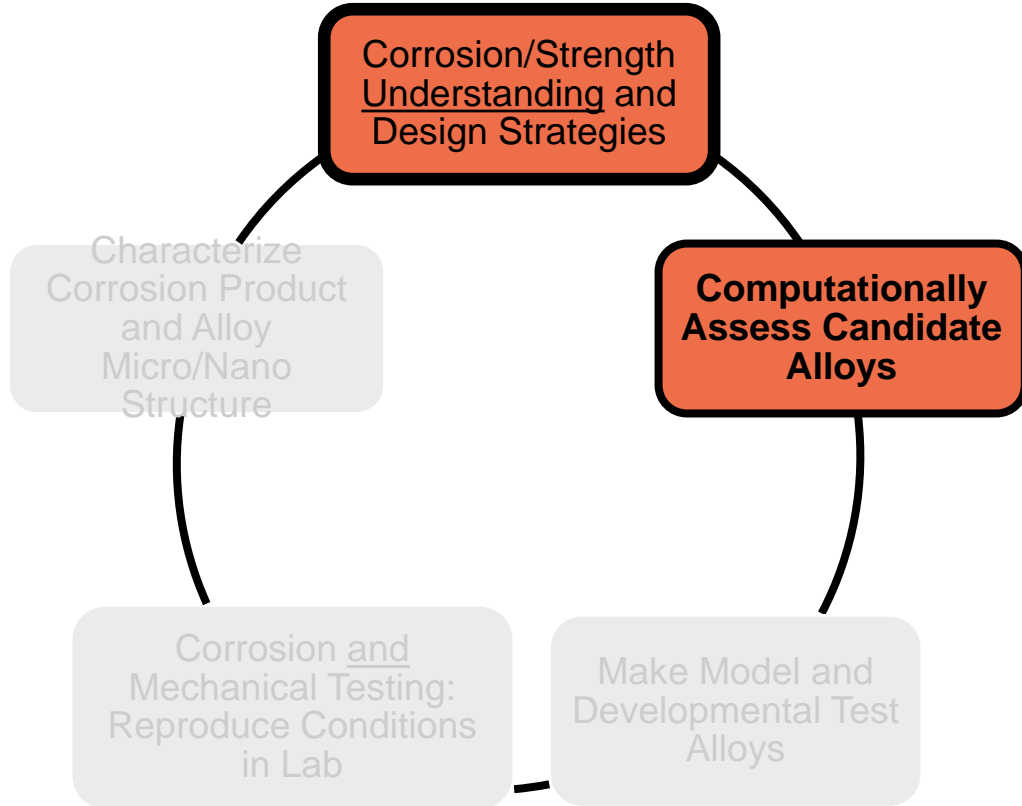
### Computational Modeling & Data Informatics/Analytics (entirety of project duration)

- Develop & Optimize Computational Frameworks
- Establish Targeted Validation Experiments
- Construct & Implement Data Science Resource for FE Materials



## Modeling and simulations

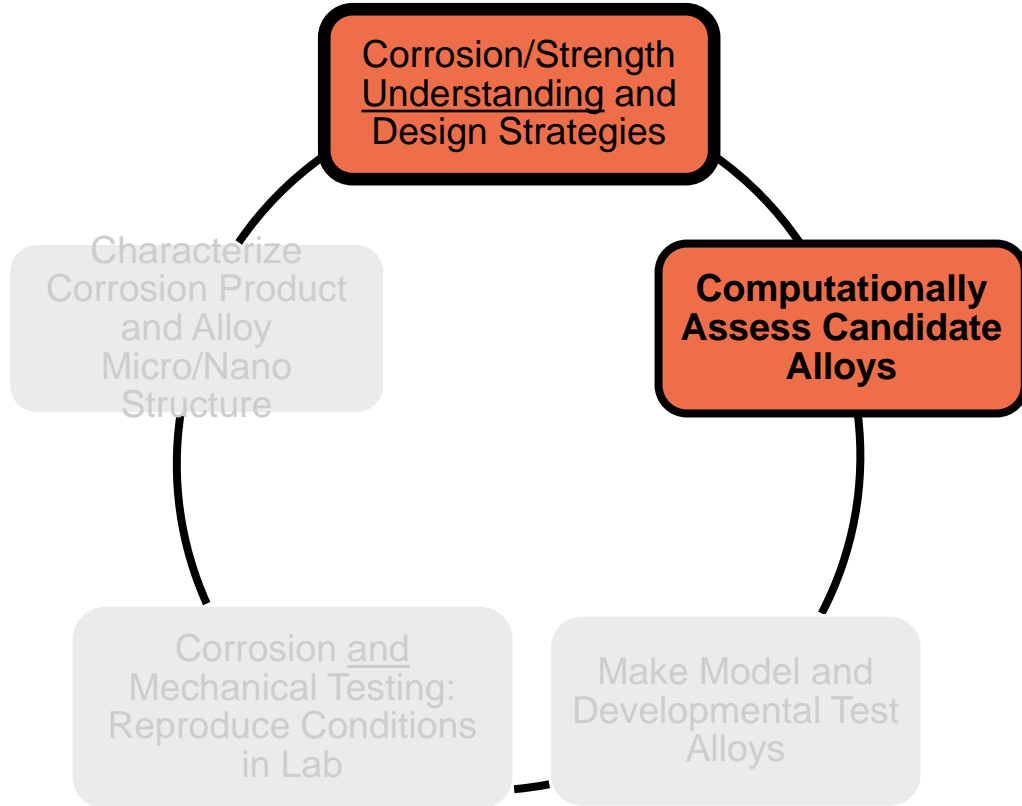




## Modeling and Simulations

Edisonian approaches to material design are reaching their limits.

Trace elements and many-body interactions between defects and chemical species can rarely be postulated *a priori*.



## *Modeling and Simulations*

Mod/Sim will deliver a framework for designing heat resistant alloys that fully accounts for metal chemistry, exposure, and cycling:

Generalized rupture life criterion sensitive to chemistry, stress, temperature and for environment.

Enhanced thermodynamic and kinetic database.

New alloy design guidelines.

Mod/Sim software/codes/tools to predict system performance.

