Modeling Creep-Fatigue-Environment Interactions in Steam Turbine Rotor Materials for Advanced Ultrasupercritical Coal Power Plants

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Acknowledgment:
Vito Cedro and Patricia Rawls, NETL
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Outline

1. Technical background of the project
2. Potential significance of the results of the work
3. Statement of project objectives,
4. The project team
5. Technical approach to achieving the project goals
6. Project budget and schedule
7. Project management plan
8. Project risks and risk management plan
9. Project status

imagination at work

GE Global Research – GE's Innovation Engine

Global Research Center
Niskayuna, NY

John F. Welch Technology Center
Bangalore, India

China Technology Center
Shanghai, China

Global Research – Europe
Munich, Germany

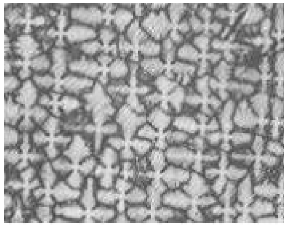
- 2,600 research employees (nearly 1,000 PhDs)
- 27,000 GE technologists worldwide
- $5.7 billion technology spend

Cornerstone of GE's commitment to technology

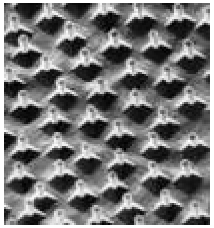
Ceramic & Metallurgy Technologies – Metallic Materials

Materials Development

- Steels
- Superalloys
- Metal Matrix Composites
- Light Metal Alloys
- Intermetallics



SX Superalloy

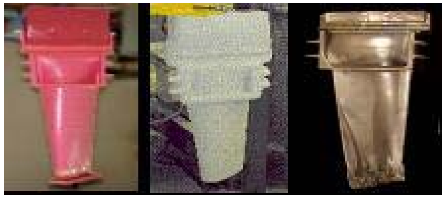


DS Eutectic Alloy

Disk Alloy

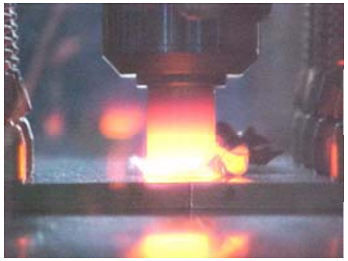
Materials Processing

- Investment Casting
- Rapid Solidification
- Forging
- Extrusion
- Joining



Wax, Mold, and Blade

Forging

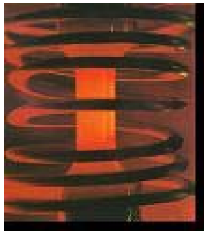


Friction Stir Welding

Materials Behavior

- Environmental, including Nuclear SCC
- Lifing Prediction & Extension
- Fracture/Deformation Mechanisms
- Micro-scale Testing

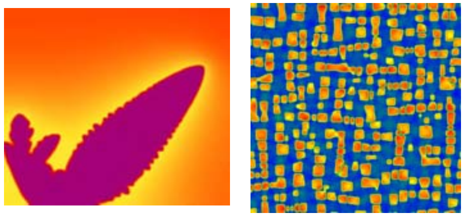
Thermal Mechanical Testing



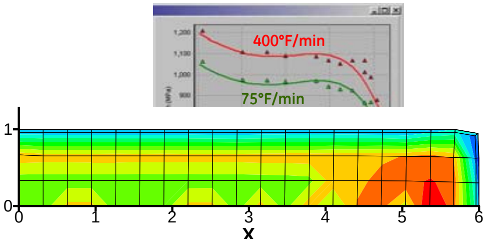
Environmental Mechanical Testing

Computational Materials Design

- Fundamental Property Prediction
- Microstructure Evolution Simulation
- Mechanical Property Modeling
- Process Simulation

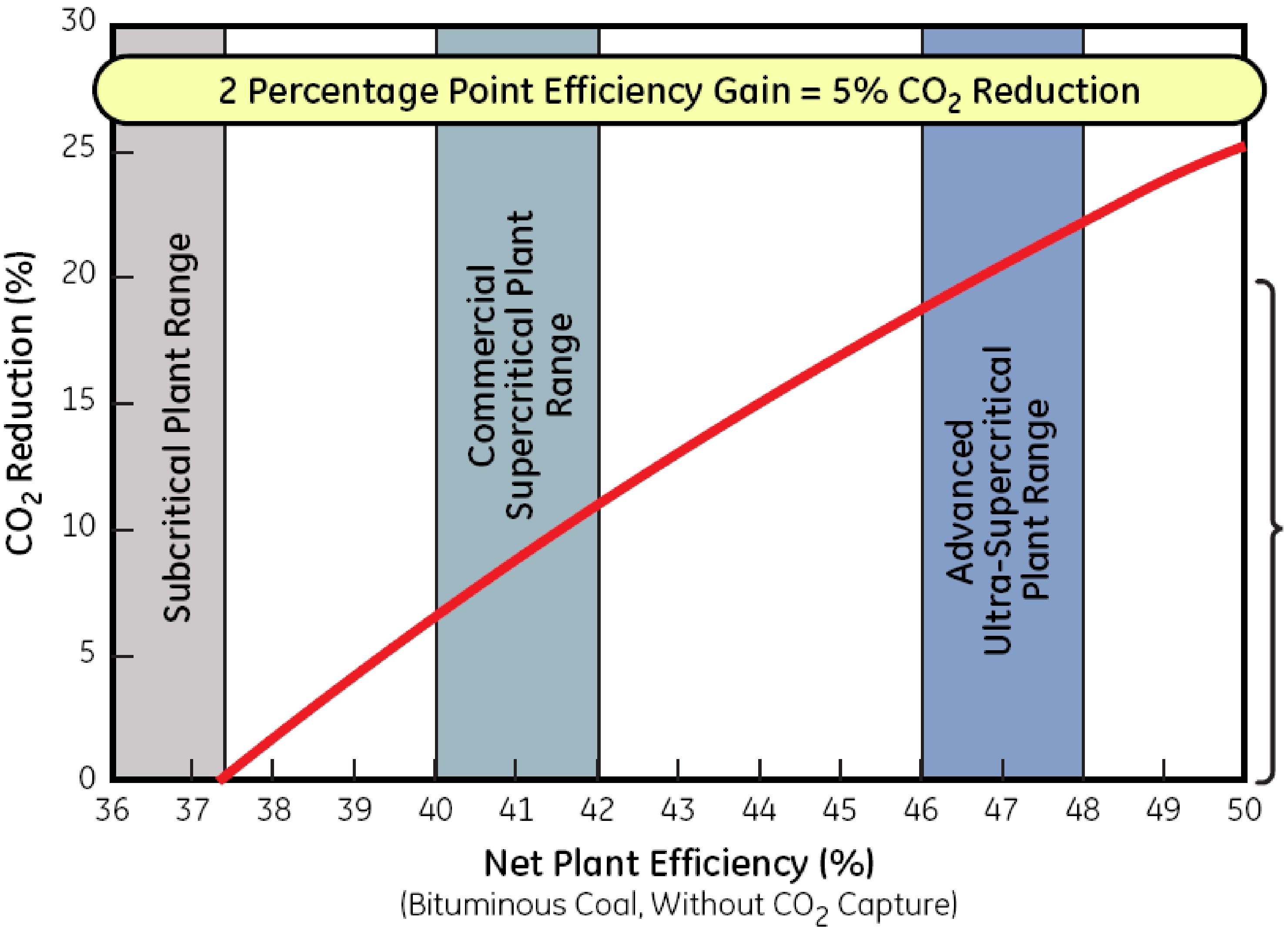


Microstructure Prediction



Mechanical Property

Advanced Ultra-Supercritical Steam Turbine

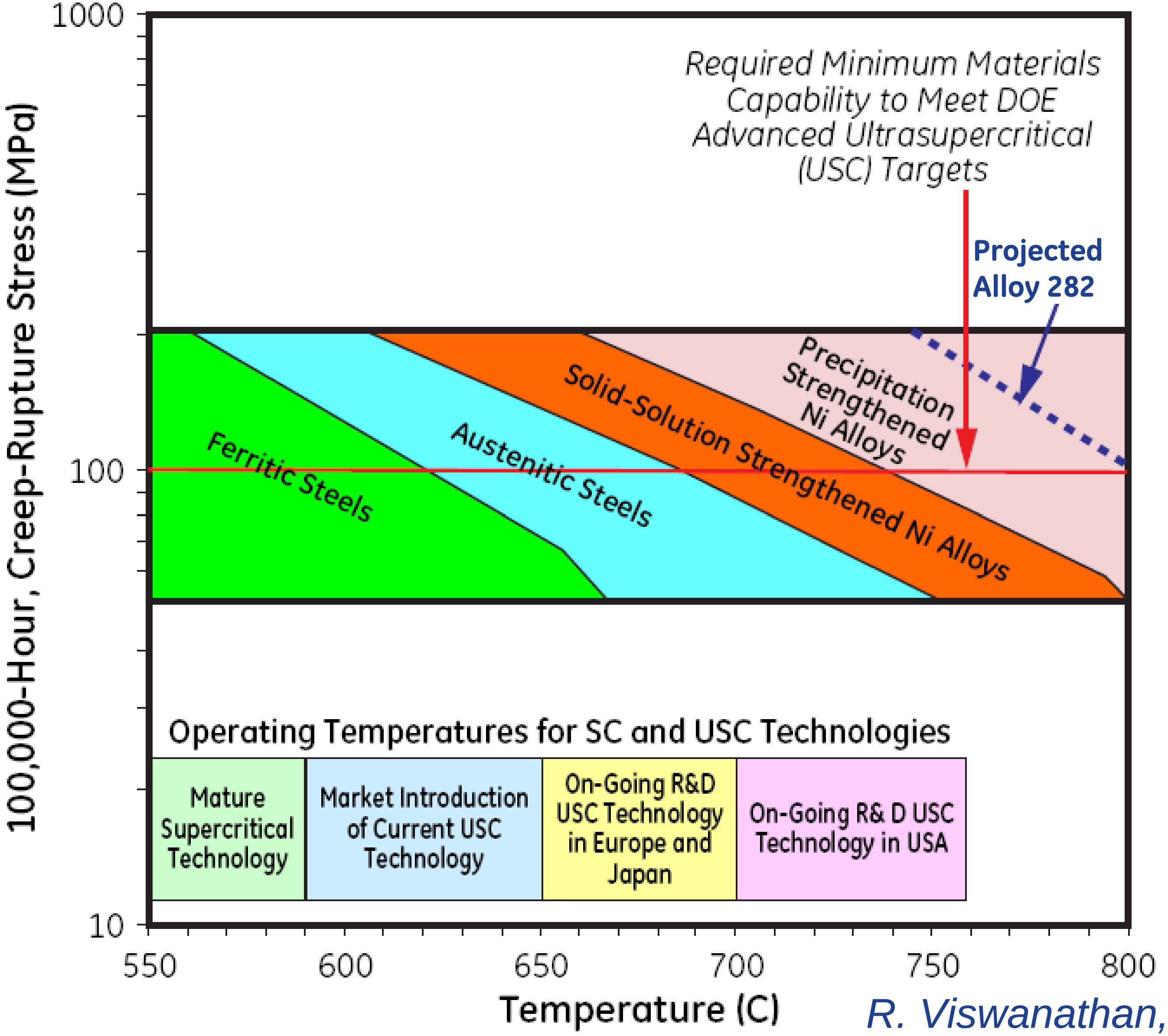


20% reduction in CO_2 corresponds with similar reductions (per MWh) in consumables including coal and limestone (reducing front-end equipment size), flue gas volume (reducing back-end and emission control equipment size), and overall emissions, water use, and waste generation

R. Romanosky, 2010

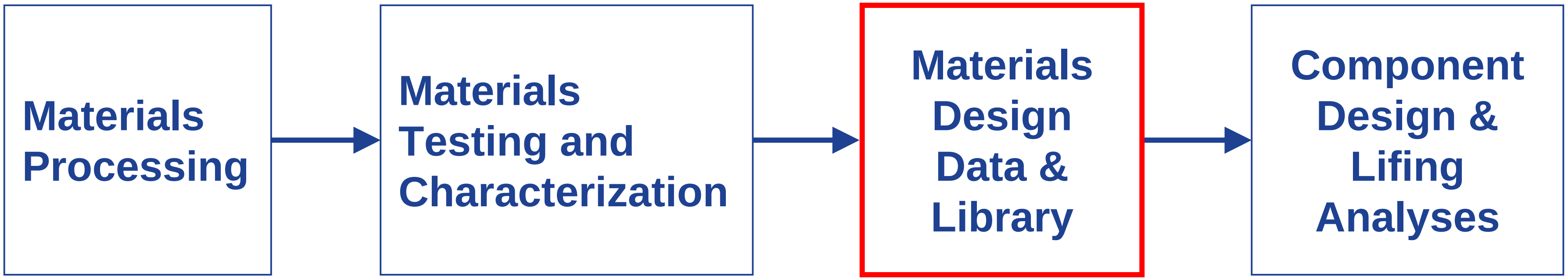
imagination at work

A-USC Rotor Materials



R. Viswanathan, 2007, 2009

Existing Materials and Design Practice



Materials Processing

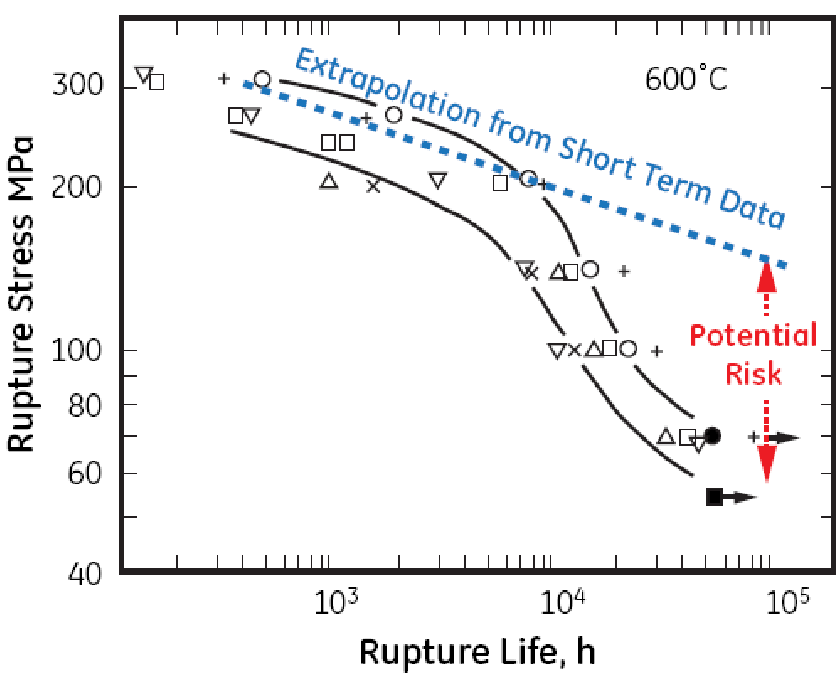
Materials Testing and Characterization

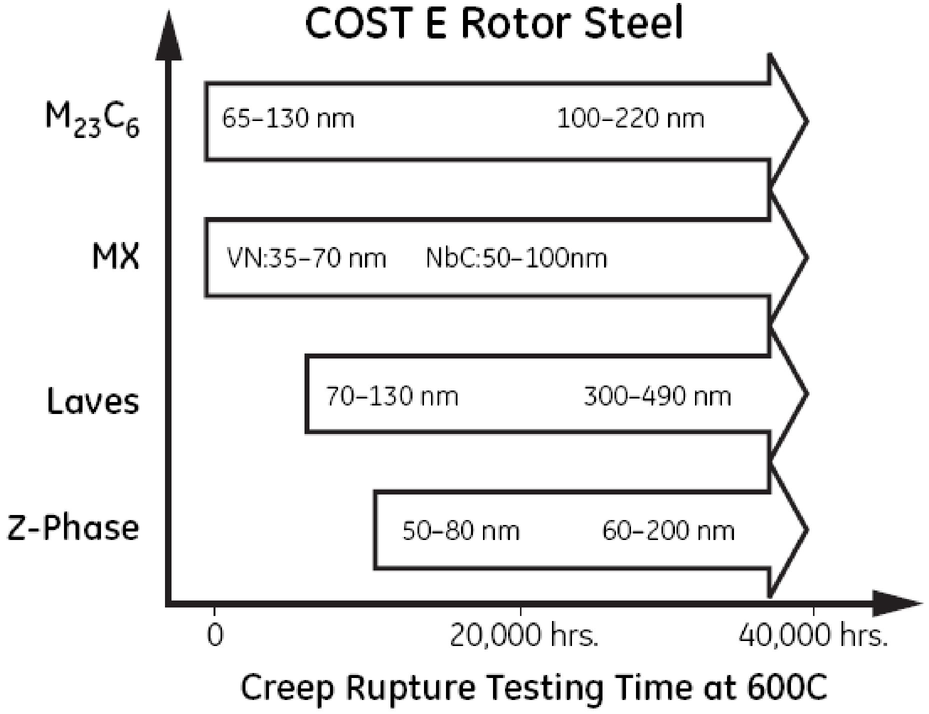
Materials Design Data & Library

Component Design & Lifing Analyses

imagination at work

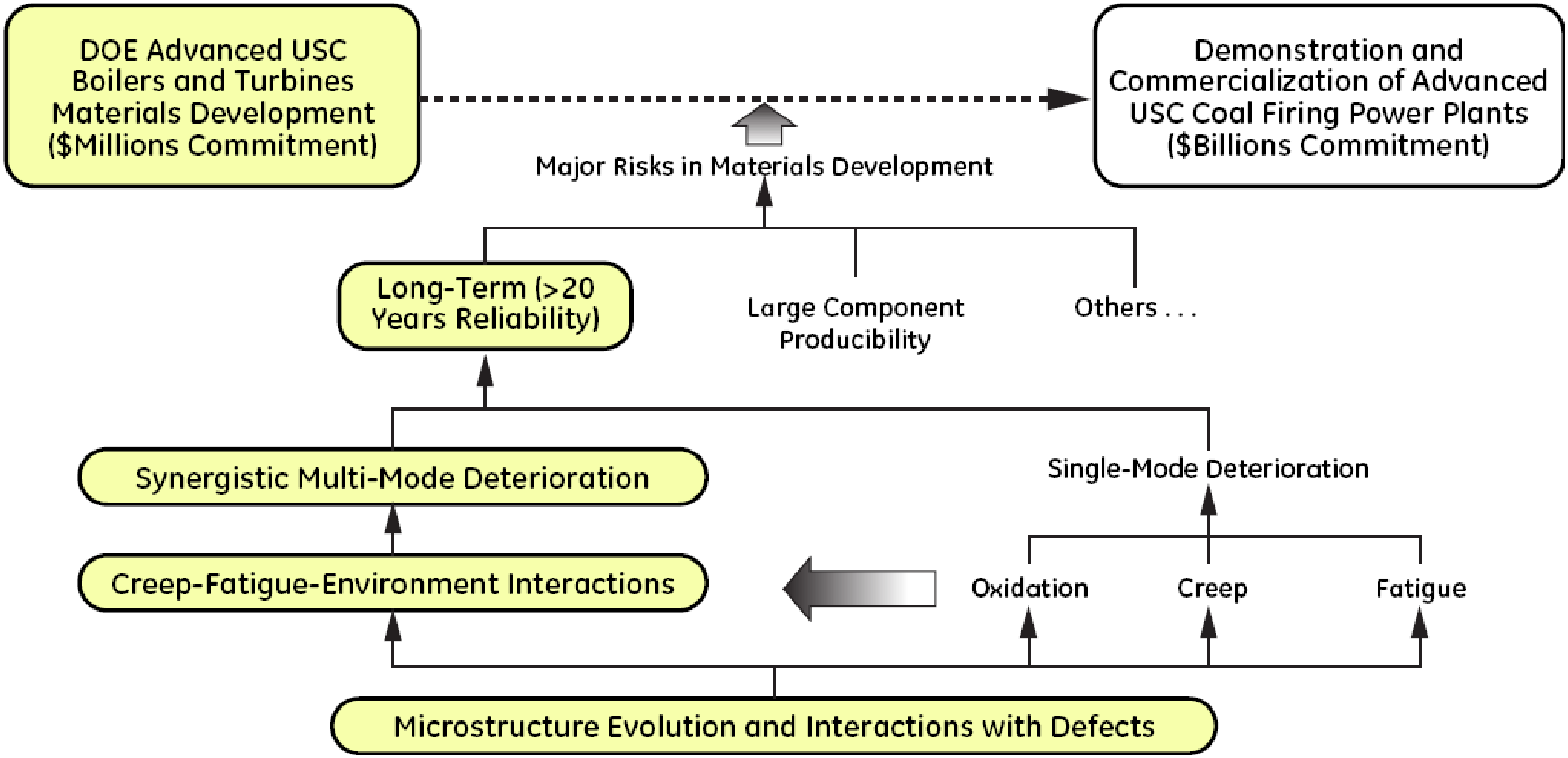
Prior USC Materials Development Experience





R. W. Vanstone, 1998

Challenge – Long-Term Reliability



DOE Advanced USC Boilers and Turbines Materials Development ($Millions Commitment)

Demonstration and Commercialization of Advanced USC Coal Firing Power Plants ($Billions Commitment)

Major Risks in Materials Development

Long-Term (>20 Years Reliability)

Large Component Producibility

Others . . .

Synergistic Multi-Mode Deterioration

Single-Mode Deterioration

Creep-Fatigue-Environment Interactions

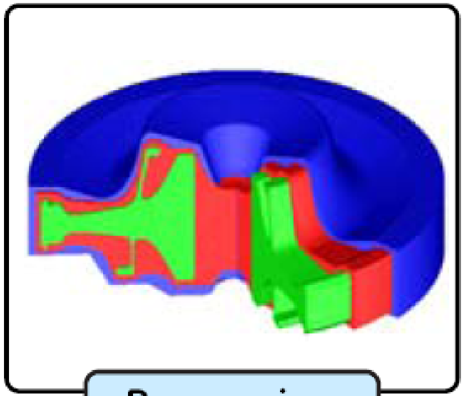
Oxidation

Creep

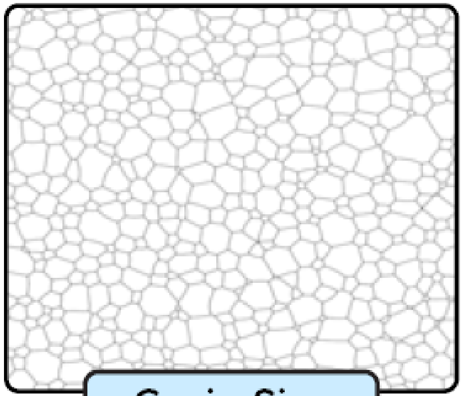
Fatigue

Microstructure Evolution and Interactions with Defects

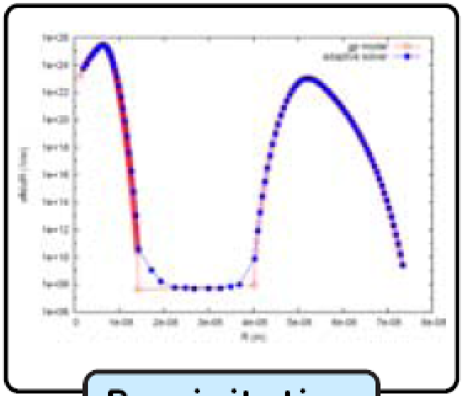
Build Upon Current Computational Framework



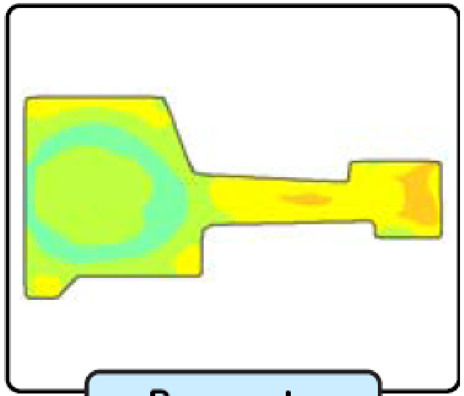
Processing Simulation →



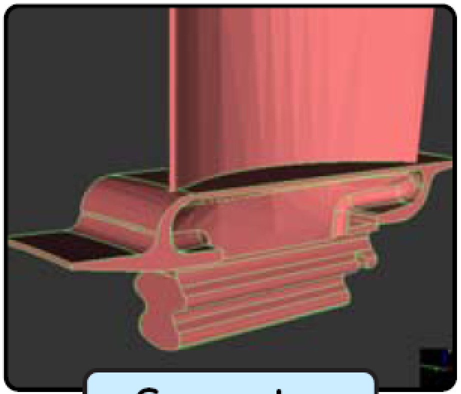
Grain Size Modeling →



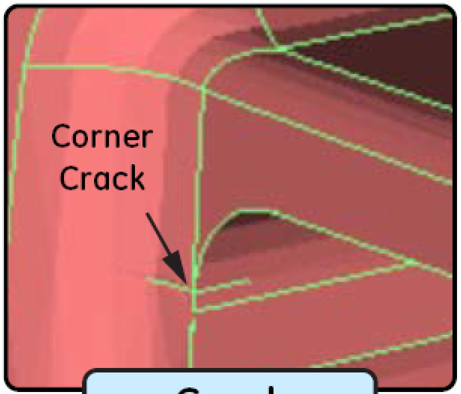
Precipitation Modeling →



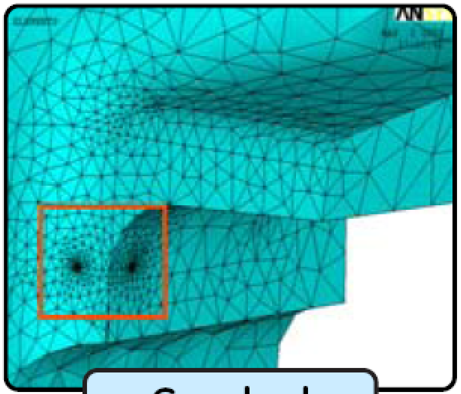
Property Prediction



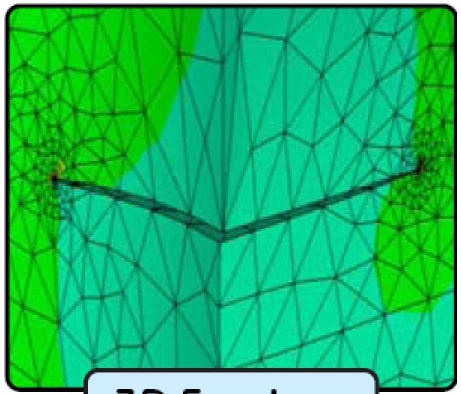
Geometry Model →



Crack Insertion →



Cracked FE Mesh →



3D Fracture Analysis

Project Objectives

Model creep-fatigue-environment interactions in steam turbine rotor materials for advanced ultra-supercritical (AUSC) coal power plants

- develop and demonstrate computational algorithms for alloy property predictions
- determine and model key mechanisms that contribute to the damages caused by creep-fatigue-environment interactions

Project Tasks

1. Project Management and Planning
2. Failure Mechanism and Microstructural Characterization
3. Atomistic and First Principles Modeling of Crack Tip Oxygen Embrittlement
4. Modeling of Gamma- Prime Microstructures and Mesoscale Microstructure-Defect Interactions
5. Microstructure and Damage-Based Creep Prediction
6. Multi Scale Crack Growth Modeling Considering Oxidation, Viscoplasticity and Fatigue

Time and Length Scales of Modeling Methods

Time Scale

years

days

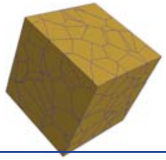
sec

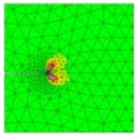
ms

ms

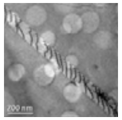
ps

Crack Growth Due to Creep-Fatigue-Environment Interactions
(Multi-Scale,
Finite Element Modeling)

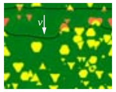




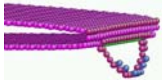
Creep Damage
(Microstructure-Based, Cumulative Damage Modeling)



Microstructure Evolution and Interactions with Defects
(Phase-Field Modeling)



Crack Tip Oxygen Embrittlement
(Atomistic and First-Principles Modeling)



nm

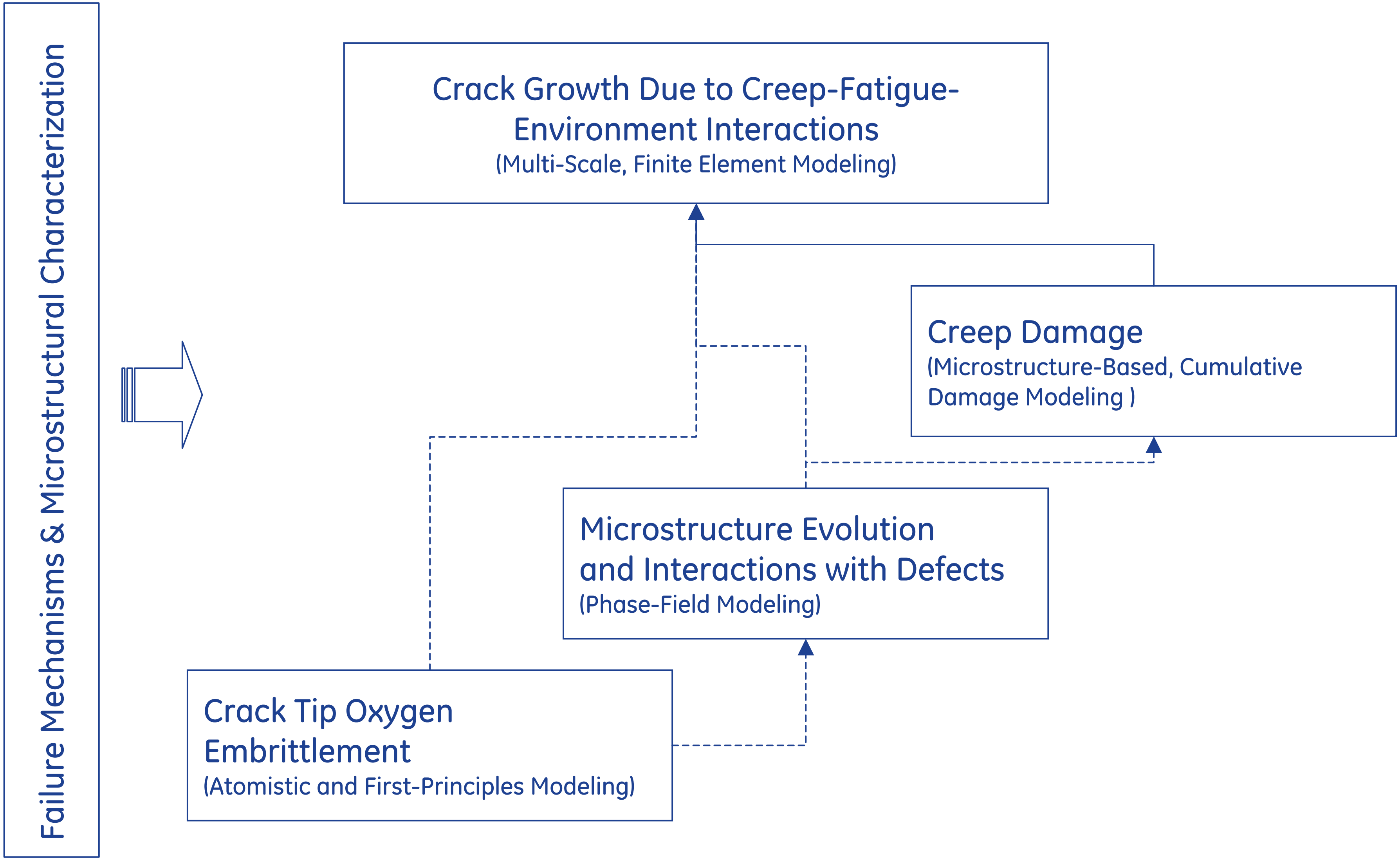
mm

mm

m

Length Scale

Project Approach and Interactions



Failure Mechanisms & Microstructural Characterization

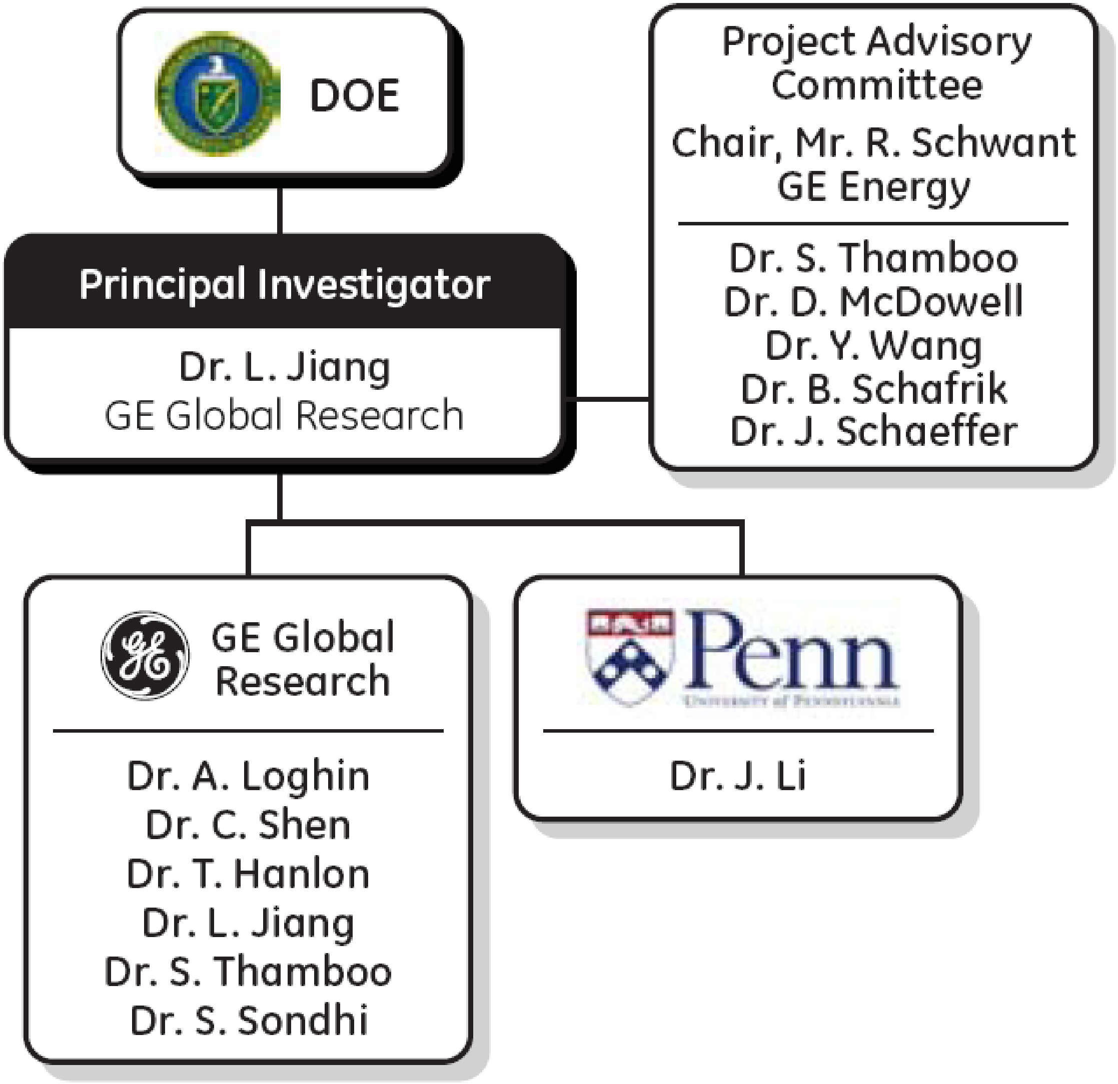
Crack Growth Due to Creep-Fatigue-Environment Interactions
(Multi-Scale, Finite Element Modeling)

Creep Damage
(Microstructure-Based, Cumulative Damage Modeling)

Microstructure Evolution and Interactions with Defects
(Phase-Field Modeling)

Crack Tip Oxygen Embrittlement
(Atomistic and First-Principles Modeling)

Project Team



DOE

Principal Investigator

Dr. L. Jiang
GE Global Research

Project Advisory Committee

Chair, Mr. R. Schwant
GE Energy

Dr. S. Thamboo
Dr. D. McDowell
Dr. Y. Wang
Dr. B. Schafrik
Dr. J. Schaeffer

GE Global Research

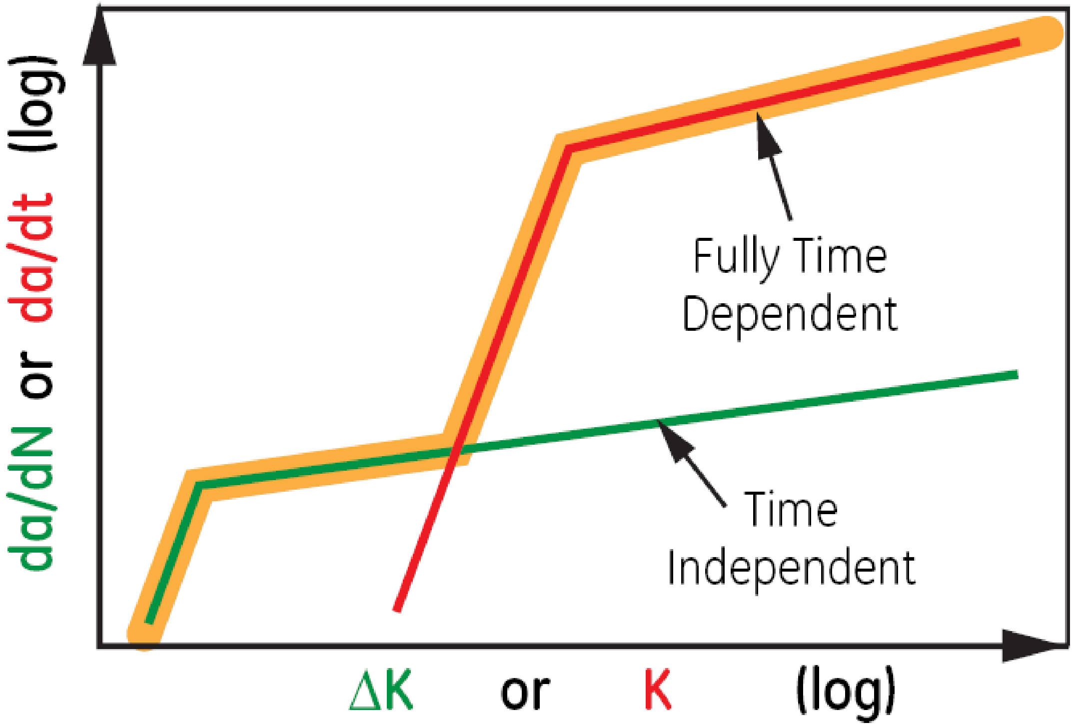
Dr. A. Loghin
Dr. C. Shen
Dr. T. Hanlon
Dr. L. Jiang
Dr. S. Thamboo
Dr. S. Sondhi

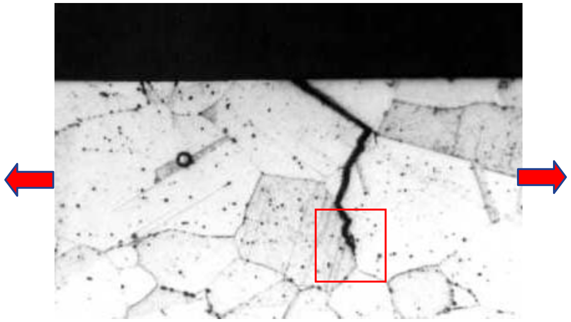
Penn

Dr. J. Li

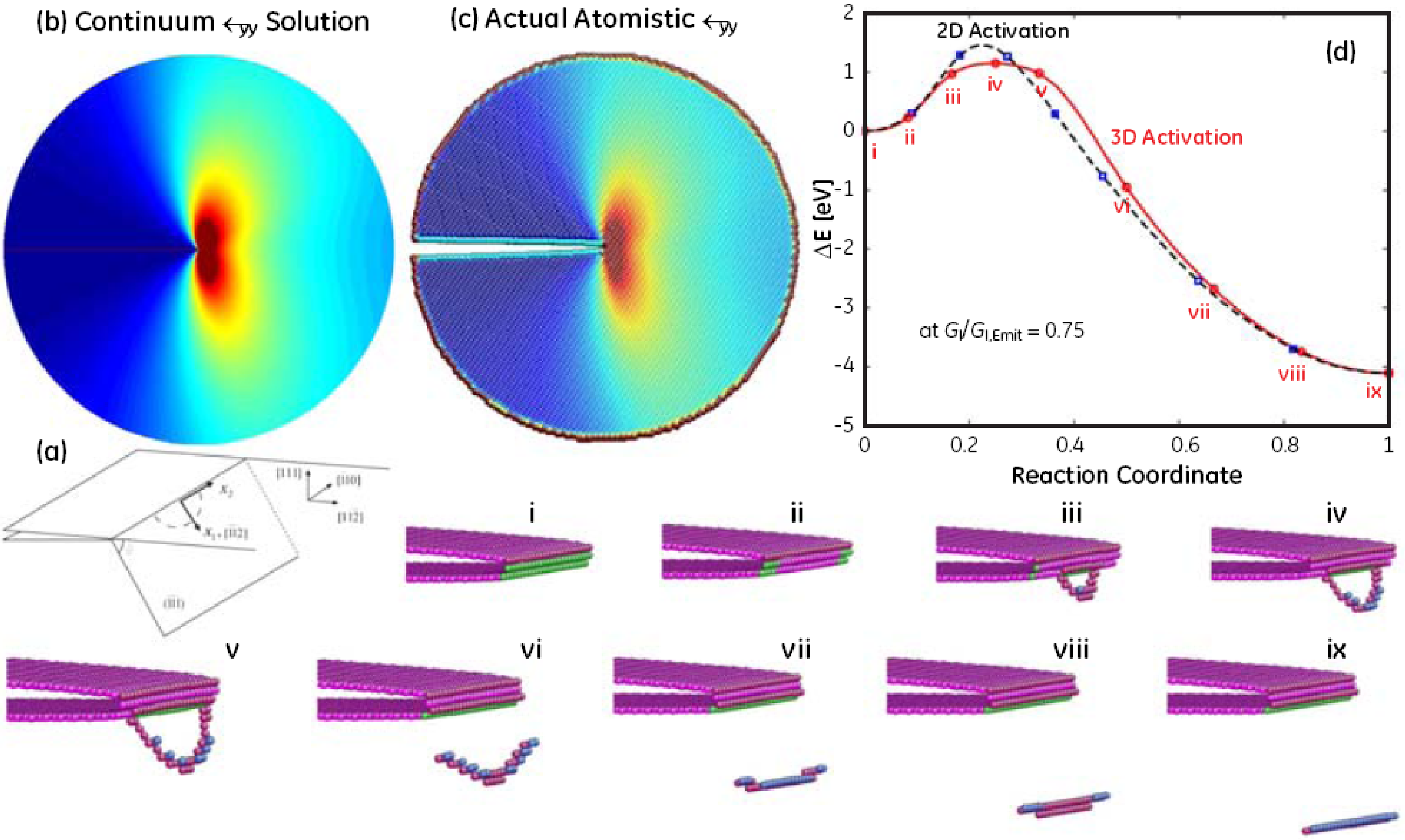
Failure Mechanism Characterization

Cracks growing in hold time fatigue follow the upper bound of the time independent and time dependent curves

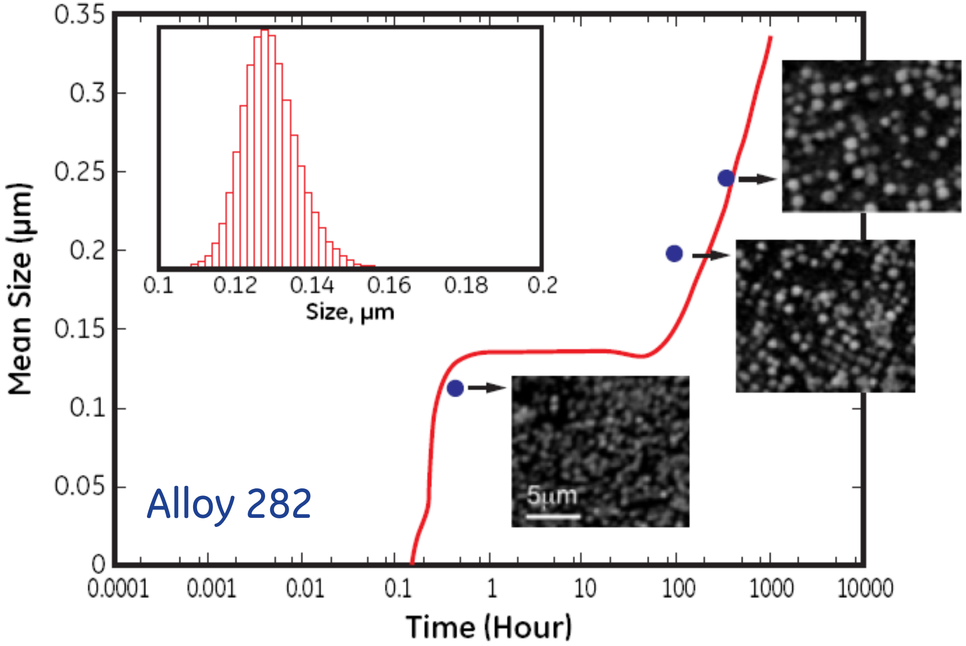


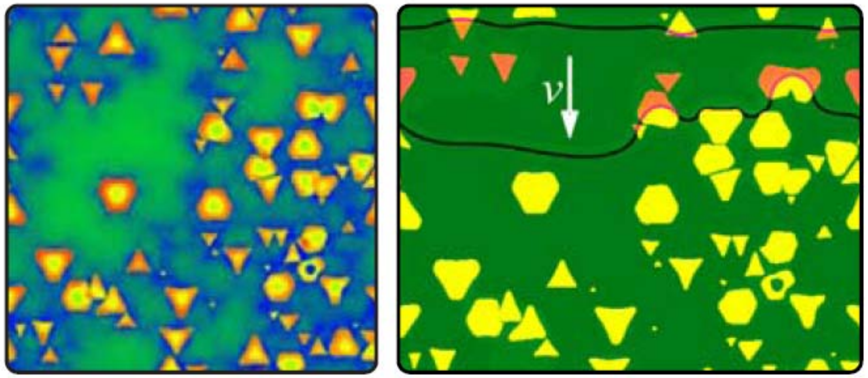


Atomistic Scale Simulation

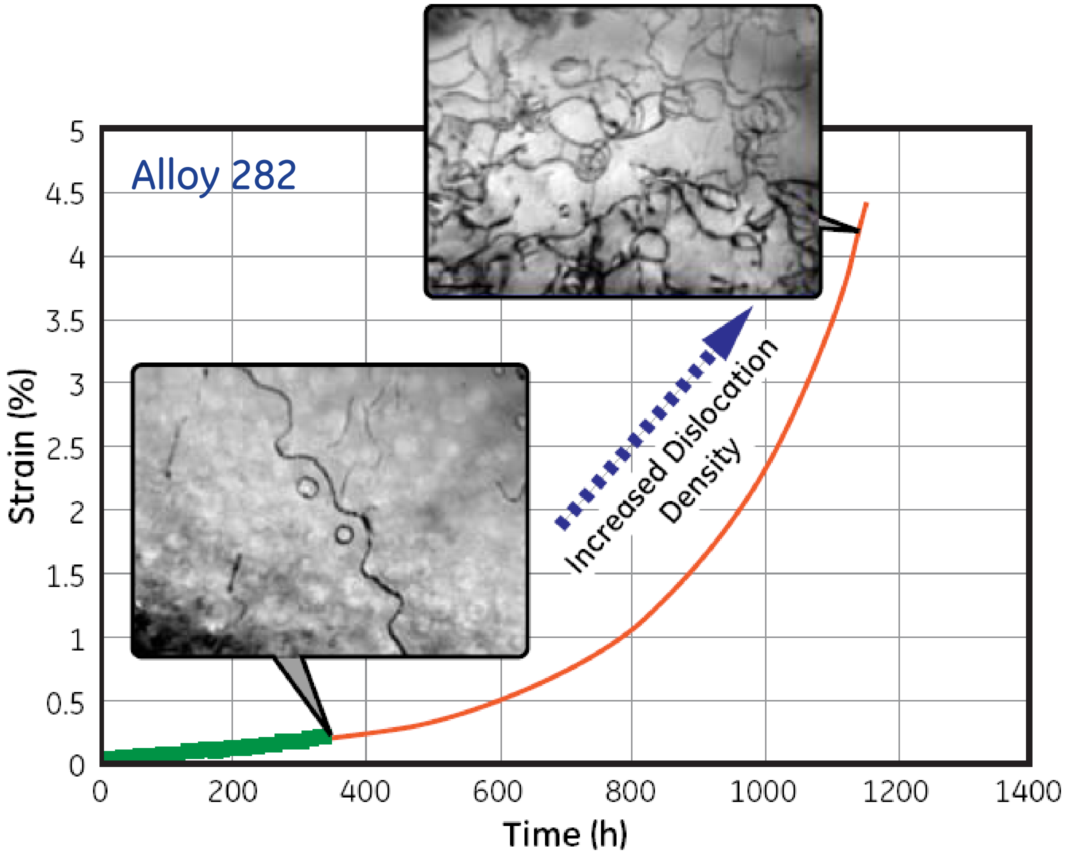


Microstructure Evolution and Interaction with Defects

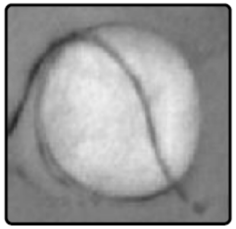




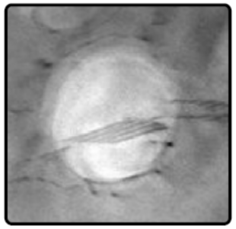
Microstructure and Damage-Based Creep Prediction



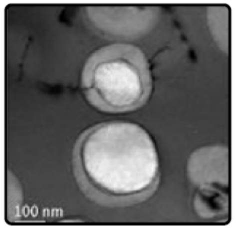
Dislocation Climb



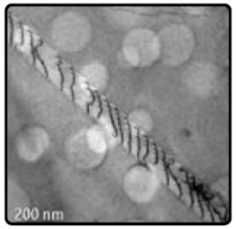
Shearing by Superdislocations



Shearing by Superpartials

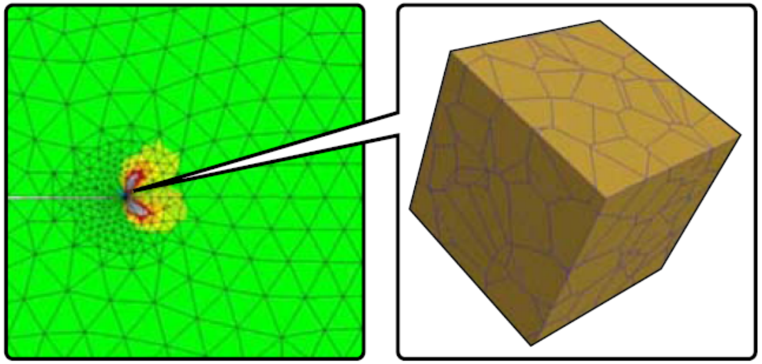


Micro-Twinning

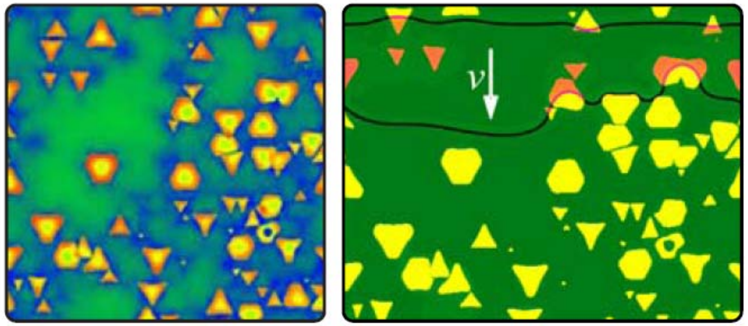


Multi-Scale Crack Growth Modeling

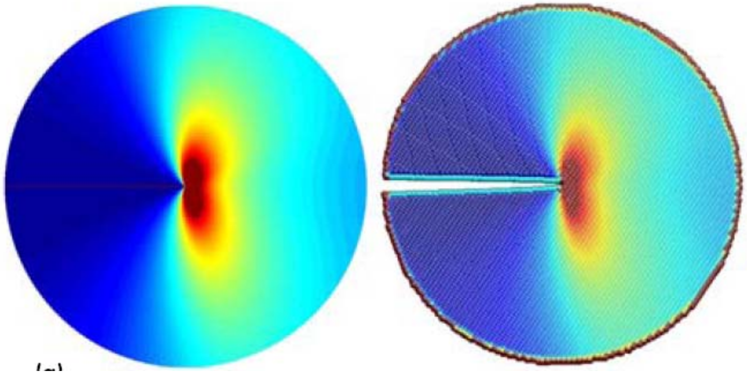
Macro-Scale



Meso-Scale



Atomistic-Scale



Modeling Creep-Fatigue-Environment Interactions

Program Team

GE Global Research
GE Energy

Penn
University of Pennsylvania

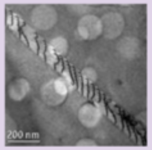
Relevant Prior Work

- DOE steam turbine materials for ultra supercritical cool power plants project
- GE materials design acceleration tools
- DARPA accelerated insertion of materials program

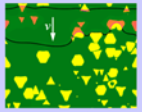
Modeling Creep-Fatigue-Environment Interactions in Steam Turbine Rotor Materials for Advanced Ultrasupercritical Coal Power Plants

Modeling Creep-Fatigue-Environment Interactions

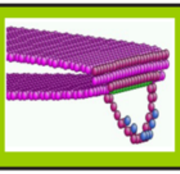
Creep Damage (Microstructure-Based, Cumulative Damage Modeling)

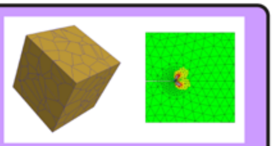


Microstructure Evolution and Interactions with Defects (Phase-Field Modeling)

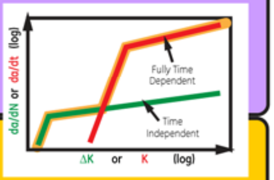


Crack Tip Oxygen Embrittlement (Atomistic and First-Principles Modeling)





Crack Growth due to Creep-Fatigue-Environment Interactions (Multi-Scale, Finite Element Modeling)



Failure Mechanism and Microstructural Characterization

Technical Approach

- Micro/macro-scale modeling for alloy property predictions
- Atomic/meso-scale modeling for mechanistic understanding
- Diagnostic experiments to validate, guide, and refine models

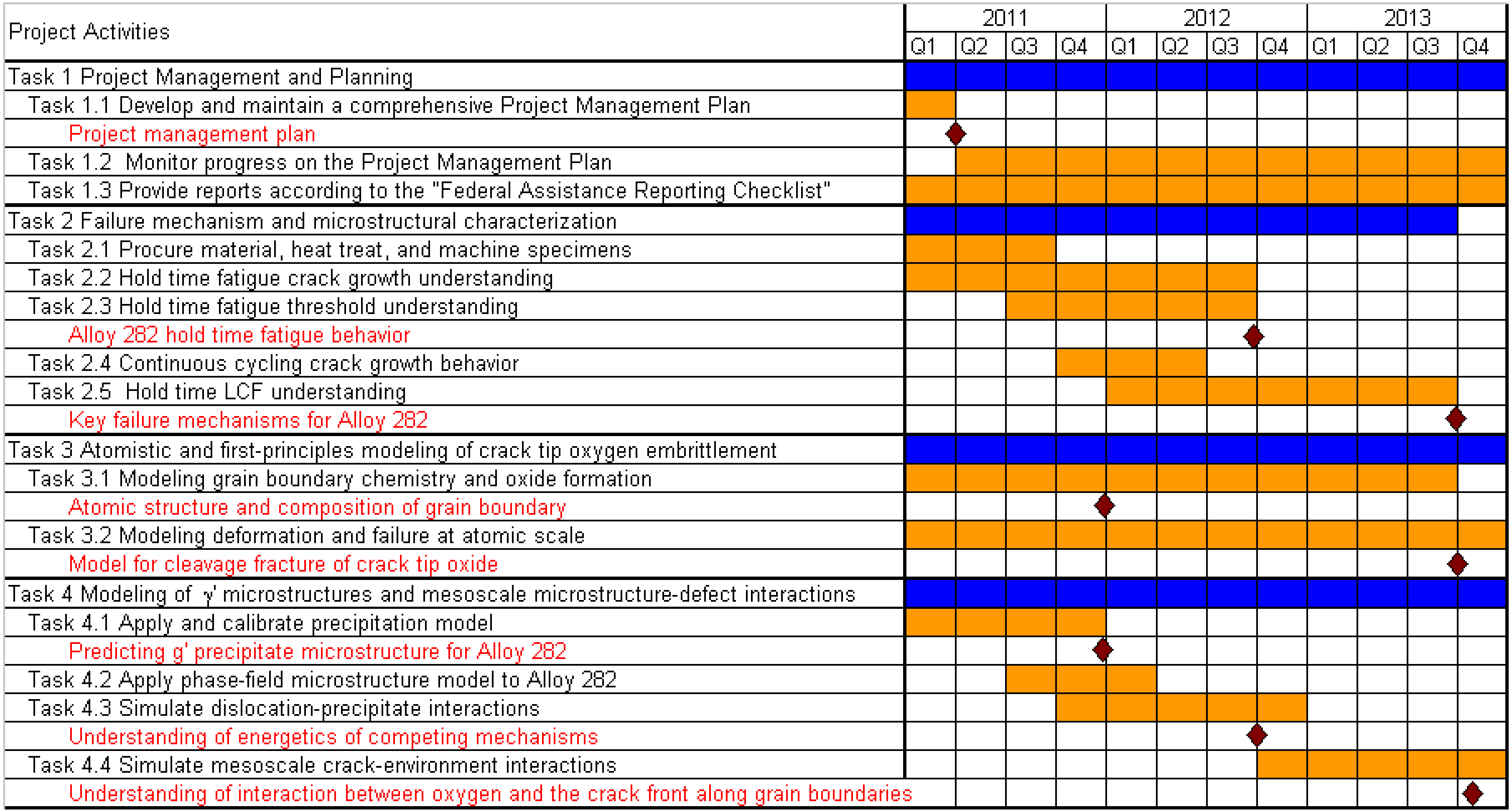
Program Deliverables

- Demonstration of computational modeling algorithms for alloy property predictions
- Determination of key mechanisms contributing to the damages of creep-fatigue-environment interactions

Anticipated Benefits of the Proposed Technology

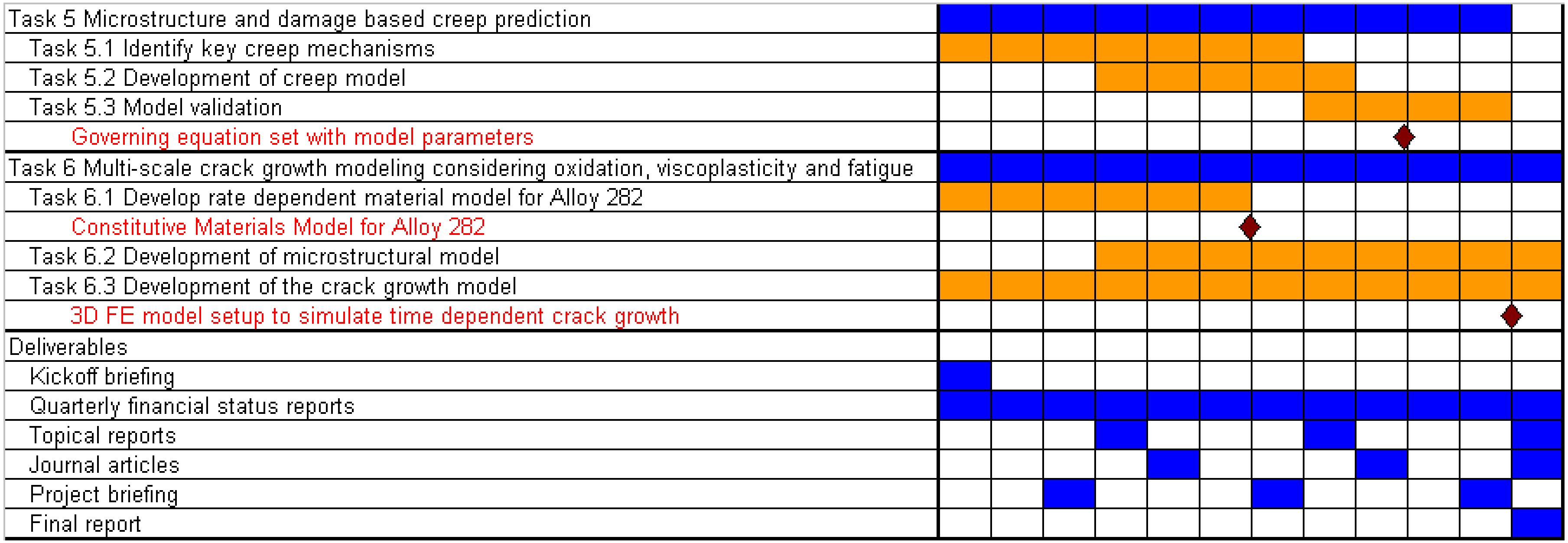
- Accelerate the materials development and enable lifetime/reliability prediction methods for the next generation fossil energy power systems
- Establish key computational technology for development in materials area of DOE NETL Advanced Research
- Enable advanced fossil energy systems to achieve the DOE efficiency and environmental goals

Project Schedule



Project Activities	2011				2012				2013			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 1 Project Management and Planning	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Task 1.1 Develop and maintain a comprehensive Project Management Plan	🟧											
Project management plan	◆											
Task 1.2 Monitor progress on the Project Management Plan		🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧
Task 1.3 Provide reports according to the "Federal Assistance Reporting Checklist"	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧
Task 2 Failure mechanism and microstructural characterization	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	
Task 2.1 Procure material, heat treat, and machine specimens	🟧	🟧	🟧									
Task 2.2 Hold time fatigue crack growth understanding	🟧	🟧	🟧	🟧	🟧	🟧	🟧					
Task 2.3 Hold time fatigue threshold understanding			🟧	🟧	🟧	🟧	🟧					
Alloy 282 hold time fatigue behavior							◆					
Task 2.4 Continuous cycling crack growth behavior				🟧	🟧	🟧						
Task 2.5 Hold time LCF understanding					🟧	🟧	🟧	🟧	🟧	🟧	🟧	
Key failure mechanisms for Alloy 282											◆	
Task 3 Atomistic and first-principles modeling of crack tip oxygen embrittlement	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Task 3.1 Modeling grain boundary chemistry and oxide formation	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	
Atomic structure and composition of grain boundary				◆								
Task 3.2 Modeling deformation and failure at atomic scale	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧
Model for cleavage fracture of crack tip oxide											◆	
Task 4 Modeling of γ' microstructures and mesoscale microstructure-defect interactions	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Task 4.1 Apply and calibrate precipitation model	🟧	🟧	🟧	🟧								
Predicting g' precipitate microstructure for Alloy 282				◆								
Task 4.2 Apply phase-field microstructure model to Alloy 282			🟧	🟧	🟧							
Task 4.3 Simulate dislocation-precipitate interactions				🟧	🟧	🟧	🟧	🟧				
Understanding of energetics of competing mechanisms							◆					
Task 4.4 Simulate mesoscale crack-environment interactions								🟧	🟧	🟧	🟧	🟧
Understanding of interaction between oxygen and the crack front along grain boundaries												◆

Project Schedule (continued)



Task 5 Microstructure and damage based creep prediction	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	
Task 5.1 Identify key creep mechanisms	🟧	🟧	🟧	🟧	🟧	🟧	🟧					
Task 5.2 Development of creep model				🟧	🟧	🟧	🟧	🟧				
Task 5.3 Model validation								🟧	🟧	🟧	🟧	
Governing equation set with model parameters									◆			
Task 6 Multi-scale crack growth modeling considering oxidation, viscoplasticity and fatigue	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Task 6.1 Develop rate dependent material model for Alloy 282	🟧	🟧	🟧	🟧	🟧	🟧						
Constitutive Materials Model for Alloy 282						◆						
Task 6.2 Development of microstructural model				🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧
Task 6.3 Development of the crack growth model	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧
3D FE model setup to simulate time dependent crack growth											◆	
Deliverables												
Kickoff briefing	🟦											
Quarterly financial status reports	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Topical reports				🟦				🟦				🟦
Journal articles					🟦				🟦			🟦
Project briefing			🟦				🟦				🟦	
Final report												🟦

imagination at work

Project Risk and Risk Management Plan

Task (Stakeholder)	Risks (Risk Level)	Impact if risk not addressed	Mitigation Plan
Task 1–Project Management and Planning (Liang Jiang)	• Program direction and technical coordination • (Risk level: medium)	Unclear responsibilities and less team interaction	• Work with project team in the preparation of the statement of work for each task to ensure clarity and task details • Lead and enforce technical collaboration
Task 2–Failure mechanism and Microstructural Characterization (Tim Hanlon)	• Resource availability in testing and materials • (Risk level: medium)	Delay in testing	• Work with suppliers early and up front
Task 3–Atomistic and First-Principles Modeling of Crack-Tip Oxygen Embrittlement (Ju Li)	• The alloy chemistry at grain boundary is too complex for accurate prediction by *ab initio* calculations • (Risk level: high) • The dislocation plasticity in front of crack tip consists of dislocation nucleation and dislocation propagation processes, and to model dislocation propagation may involve larger spatial scales and longer timescale than what molecular dynamics can handle • (Risk level: medium)	Understanding of crack-tip oxygen embrittlement mechanism	• While the multi-component, large unit cell DFT calculations are very expensive, it may not be required to get the chemistry completely correct in order to predict the mechanical impact of oxygen. We will use simple rules like grain boundary bond strength analysis to regress the results as a function of oxygen chemical potential. Accurate experimental characterizations may also help us in validating the grain boundary chemistry - mechanics model • Oxygen solubility in the bulk metal is very low. Thus the effect of oxygen should be concentrated on exposed crack-tip and in the grain boundaries. Dislocation propagation in the bulk should not be affected greatly, while dislocation nucleation may. Since dislocation nucleation is much more "local" atomic-scale process, we are reasonably confident that atomistic models can capture the main effect of oxygen

Project Risk and Risk Management Plan (continued)

Task (Stakeholder)	Risks (Risk Level)	Impact if risk not addressed	Mitigation Plan
Task 4– Modeling of γ' microstructures and mesoscale microstructure-defect interactions (Chen Shen)	• Simulation length scale of dislocation-precipitates interaction model is insufficient to represent the length scale of γ' microstructure in **Alloy** 282 • (Risk level: low-medium)	Understanding and modeling of microstructure and defect interaction	• Use scaling factor to increase the length scale of the dislocation model, perform a set of sub-scale simulations to derive the necessary correction factor for scaling up
Task 5– Microstructure and Damage Based Creep Prediction (Sanjay Sondhi)	• Multiple mechanisms operative for accumulating creep strain • (Risk level: medium)	Limit the predictive capability of the model, and less confidence in extrapolation	• Interrupted creep tests in the stress and temperature regime of interest over a range of starting microstructures. This will allow of the identify all key mechanisms and associated kinetics
Task 6–Multi-scale crack growth modeling considering oxidation, viscoplasticity and fatigue (Adrian Loghin)	• Some of the microstucture simulations are computationally expensive. • (Risk level: high)	Reliability of model prediction for creep-fatigue-environment interactions	• We will rely more on 2D simulations to simplify the analysis • Run critical 3D analysis to verify 2D results and to identify critical mechanisms

Project Status

1. Opened project, Feb 19th, 2011
2. FOA000260 Awardees Project Kickoff Meeting, Feb 23rd, 2011
3. Project kickoff at GE Global Research, March 18th, 2011
4. Discussion with DOE A-USC Materials Team, 1Q, 2011
5. Project Management Plan, March 31st, 2011
6. Procure Alloy 282, machine, and test
7. Literature review of Alloy 282
8. Move forward with modeling efforts