CITRINE INFORMATICS

THE OHIO STATE UNIVERSITY

ICME for Creep of Ni-Base Superalloys in Advanced Ultra-Supercritical Steam Turbines

Kickoff Meeting – Oct 5-6th 2016

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An OH·TECH Consortium Member

U.S. DEPARTMENT OF ENERGY

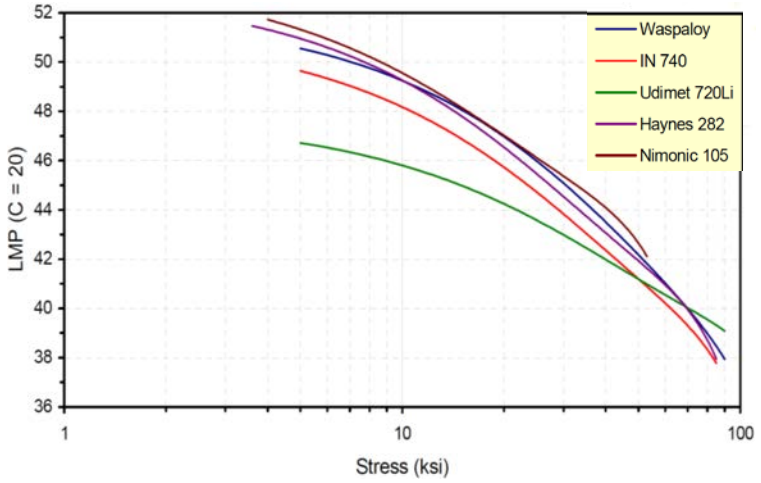
NETL

Outline

- Vision and Objectives
- Materials Informatics Strategy
- Advanced Modeling Strategy
- Project Details
  - Who's doing what
  - Project Tasks
  - Timeline and Milestones

Current Creep Modeling of Ni-base Superalloys

Larson-Miller parameter (LMP) vs stress for various Ni-base superalloys ($C_{LM} = 20$)



$$T[C_{LM} + \log t_r] = P_{LM} = f(\sigma)$$

- Parametric in nature: simple analytic models based on Larson-Miller parameter and experimental creep life data
- No microstructure information is considered
- No physics based creep mechanisms are involved
- Cannot provide feedback on optimization of improving Ni-base superalloys
- Rely on many experimental test data (not efficient)

R. Viswanathan, et al., Steam Turbine Materials for Ultrasupercritical Coal Power Plants, Energy Industries Of Ohio, Incorporated, 2009.

Program Vision and Objectives

- VISION: Combine materials informatics and physics based modeling for an ICME approach to predict long-term creep behavior in Ni based superalloys for Advanced Ultra-Supercritical Steam Turbine Applications
- Application of advanced materials informatics for critical assessment of existing experimental data
- ….. critical assessment of existing modeling capabilities
- Development of new modeling capabilities that are crucial but currently missing for predicting long-term creep behavior
- Long term application - Accelerate the development and qualification of new materials in next generation of A-USC steam turbine systems

Informatics Strategy - Citrination

PLATFORM FEATURES

Data extraction from documents

Our data extraction pipeline turns technical documents containing crucial data into a structured, searchable database. Data from figures, tables, and text appear in your private instance of the Citrine platform.

Big data analytics built for manufacturing companies

Citrine's machine learning isn't one-size-fits-all—it's specifically tailored to mine large-scale materials and chemical datasets and help solve the greatest challenges at manufacturing companies.

World's largest collection of physical data

We are consolidating the universe of published materials and chemicals data, which our platform mines to augment your organization's own internal knowledge. Citrination, our public data resource, is trusted by users at nearly 2,000 industrial, academic, and government institutions worldwide.

Modern, scalable data infrastructure

We have built the leading materials data system of record so you don't have to—harness this powerful infrastructure inside your organization, so you can focus on making great products and avoid IT headaches.

Citrine Example – Thermoelectric Discovery

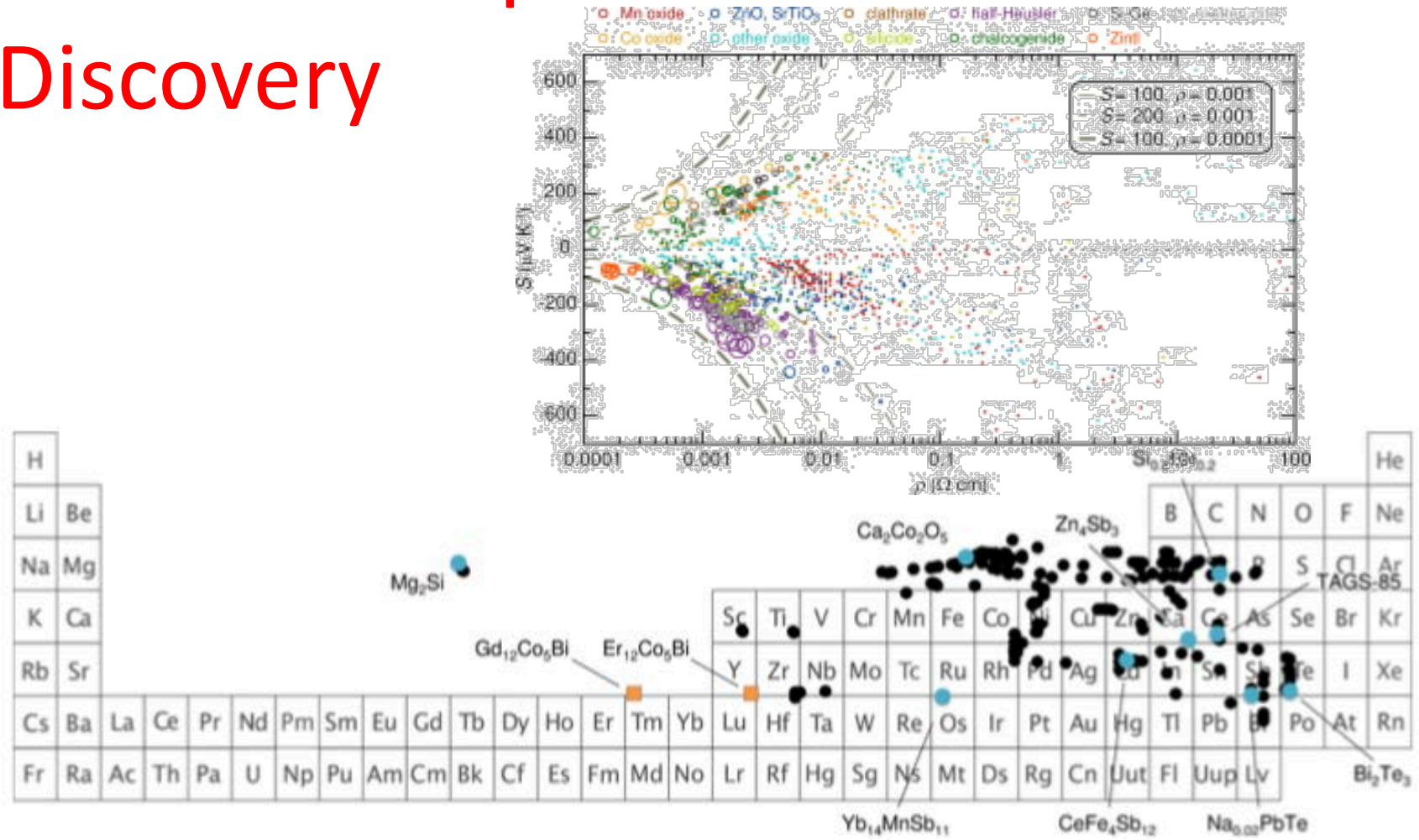


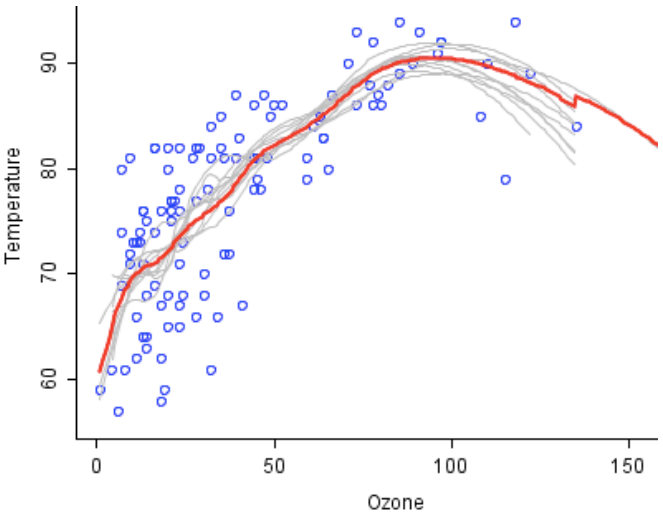
FIG. 1. Most known thermoelectric materials lie in a tight cluster in composition space (black and blue dots; blue dots have chemical formulae explicitly labelled). The recommendation engine presented here allows the identification of new thermoelectric materials families that are well outside the existing composition space of common systems in the Gaultois *et al.* database.[6] In particular, we report the characterization of $RE_{12}Co_5Bi$ (RE = Gd, Er; orange squares), which are chemically and structurally distinct from known thermoelectrics.

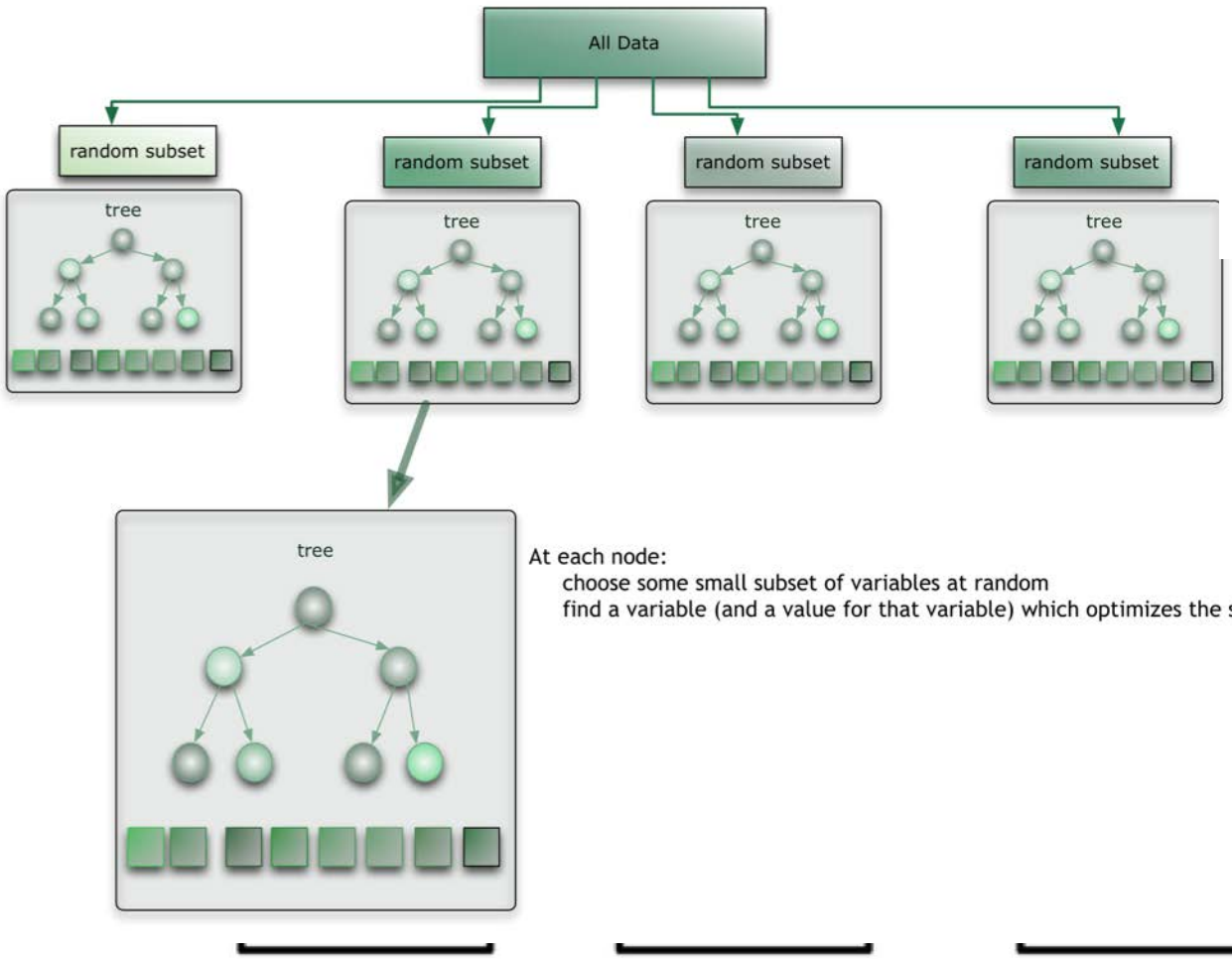
Approach

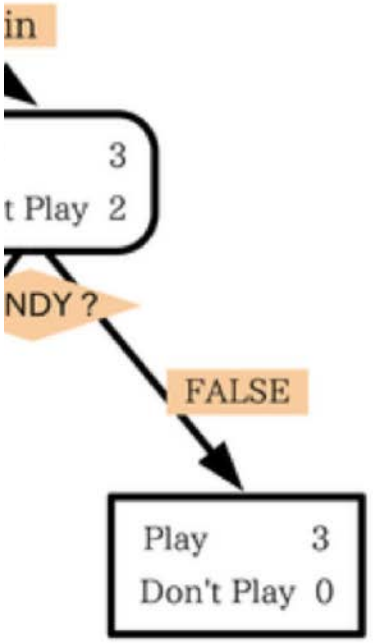
- Training data
  - Materials Data API (http://www.materialsproject.org/open)
  - NIMS Materials Database (http://mits.nims.go.jp/index_en.html)
  - Contains: Seebeck coefficients, thermal conductivities, electrical conductivities, and band gaps measured for thousands of materials as a function of temperature and a variety of other metadata conditions.
- Data Algorithm
  - Random Forest

Random Forests??

- Decision Tree -> Random Forest







https://citizennet.com/blog/2012/11/10/random-forests-ensembles-and-performance-metrics/

Case Study - Results

	Seebeck coefficient	Electrical resistivity	Thermal conductivity	Band gap
$MnCo_2Ga$				
$MnCu_2In$				
$MnNi_2Ga$				
$MnNi_2In$				
$TiNi_2Ga$				
VCo_2Ga				
$TiRu_2Ga$				
$TiRu_2In$				
$MnRu_2In$				

Try it out!

http://thermoelectrics.citrination.com/#/

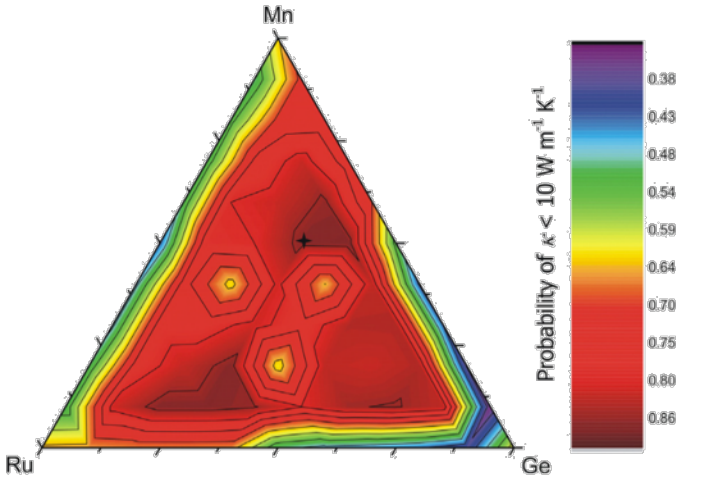


Figure 4. Probability of low thermal conductivity ($\kappa < 10\,Wm^{-1}\,K^{-1}$) as a function of theoretical composition.

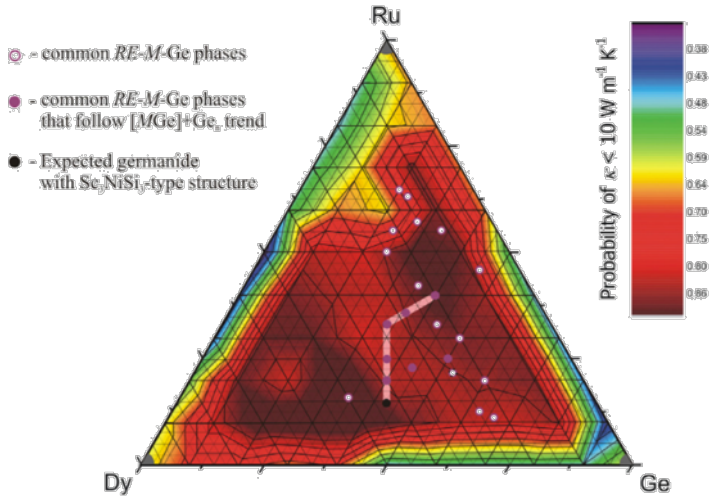
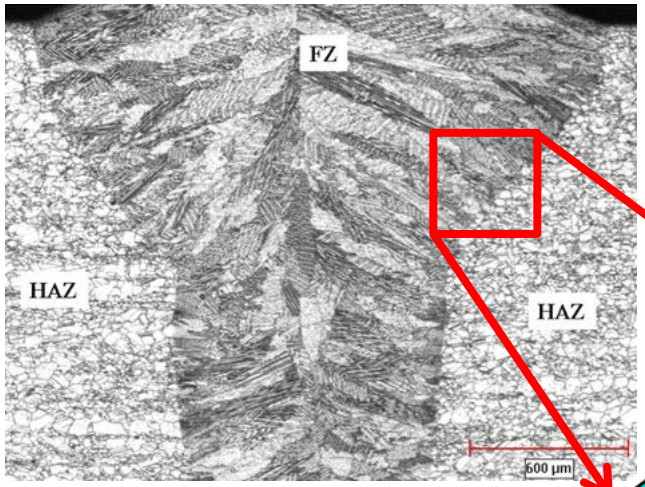


Figure 5. *RE*–*M*–Ge composition diagram with common ternary structure types and predicted thermal conductivity mapped on the Dy–Ru–Ge diagram.

A “3M” Creep Model of Ni-base Superalloys

Multiscale, Microstructure-Sensitive, Mechanism-Informed

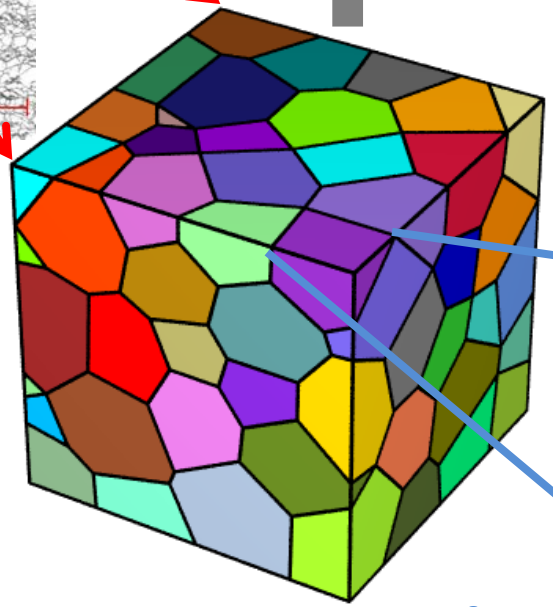


Polycrystal creep: homogenization model (3D, heterogeneous deformation at grains)

Up-scale

- Full creep curves
- Creep life prediction
- …

Single-crystal creep: integration of phase-field and FFT-CP (image-based, full-field

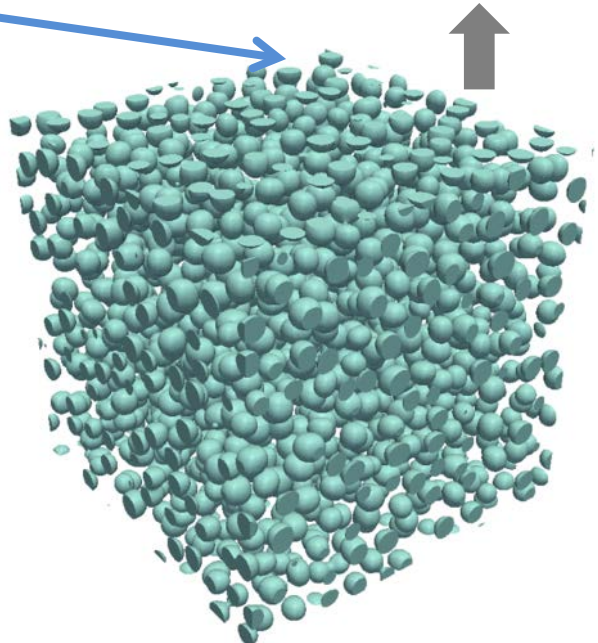


Reconstruction of statistically equivalent representative volume element (RVE) capturing structural heterogeneities

Down-scale

- Structural heterogeneities
- Statistical analysis
- …

Reconstruction of RVE for γ/γ' two-phase microstructure quantified by experimental characterization



3D Full-Field Model of Single Crystal Creep

What experiments has revealed:

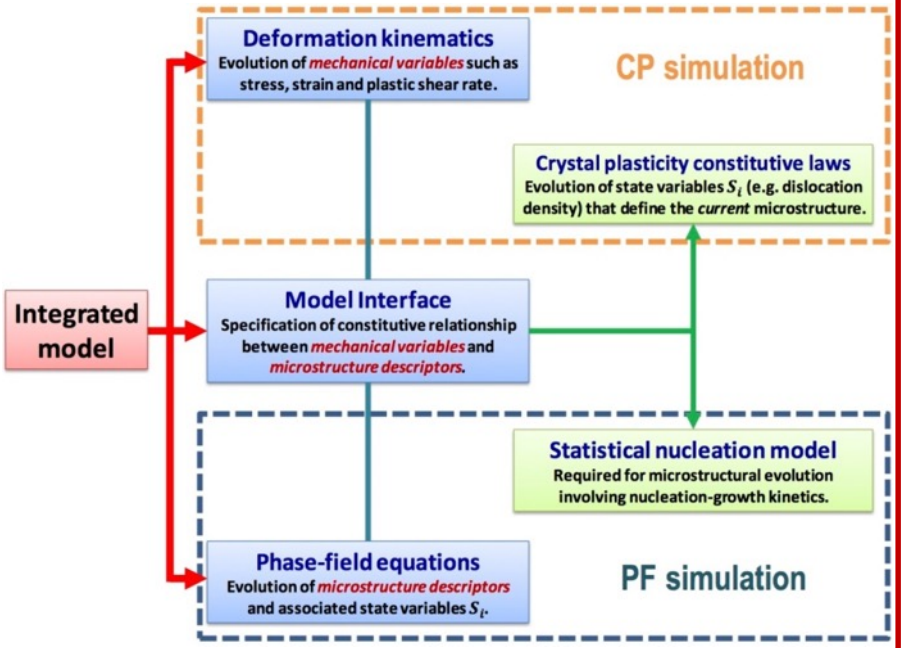
Micromechanical evolution

- Plastic deformation of γ/γ' two-phase structure at sub-grain level
- Heterogeneous: stress/strain concentration vs γ' morphology
- Spatial distribution of dislocations and time evolution

Microstructural evolution

- Coarsening of γ' particles
- Dissolution of γ' particles
- Rafting
- …

What we have developed:



What we will do:

- Incorporating ***experimentally identified creep mechanisms*** via dislocation-based crystal plasticity model
- ***Dynamic coupling*** between crystal plasticity model and phase-field

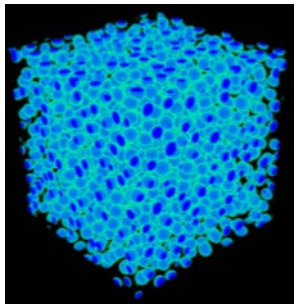
FFT elasto-viscoplastic (FFT-EVP) formulation

$$\boldsymbol{\sigma}^{t+\Delta t}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}^{e,t+\Delta t}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \left[\boldsymbol{\varepsilon}^{t+\Delta t}(\mathbf{x}) - \boldsymbol{\varepsilon}^{p,t}(\mathbf{x}) - \dot{\boldsymbol{\varepsilon}}^{p,t+\Delta t}\left(\mathbf{x}, \boldsymbol{\sigma}^{t+\Delta t}\right)\Delta t\right]$$

$$\dot{\boldsymbol{\varepsilon}}^{p}(\mathbf{x}) = \sum_{\alpha=1}^{\mathcal{N}} \mathbf{m}^{\alpha}(\mathbf{x})\, \dot{\gamma}^{\alpha}(\mathbf{x})$$

- Small-strain framework is adopted.
- Implicit Euler treatment requires numerical iteration.
- Periodic boundary condition (PBC) must be satisfied.

Phase-field/experimental obtained γ/γ' microstructure



Direct sampling on the microstructure image

FFT-EVP simulations

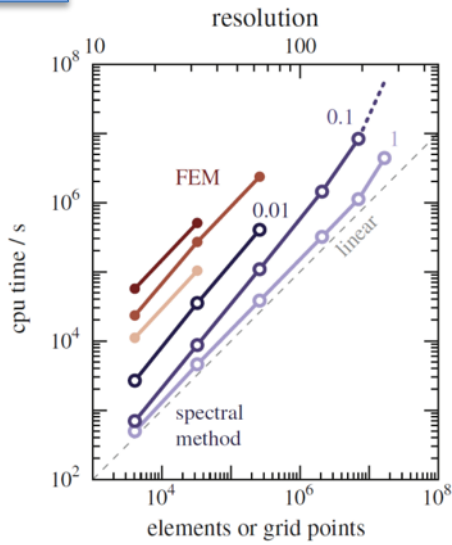
"image-based" approaches

Spectral (FFT) method

- Fields are approximated by a Fourier series
- Strong stress equilibrium is required at every discretization point

Finite element method

- Fields are approximated by low-order piecewise shape-functions
- Weak stress equilibrium is required in a volume-average



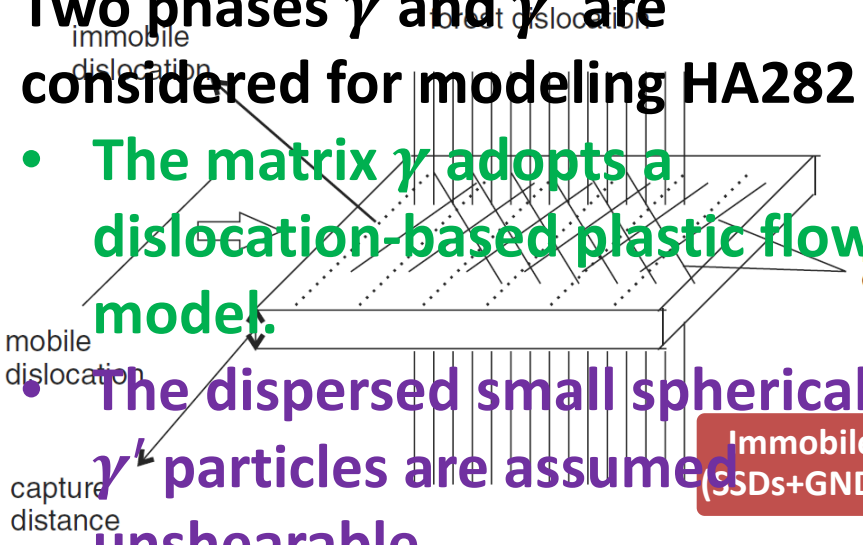
Lebensohn, R. A., et al. (2012). *Int. J. Plast.*, *32*, 59-69.

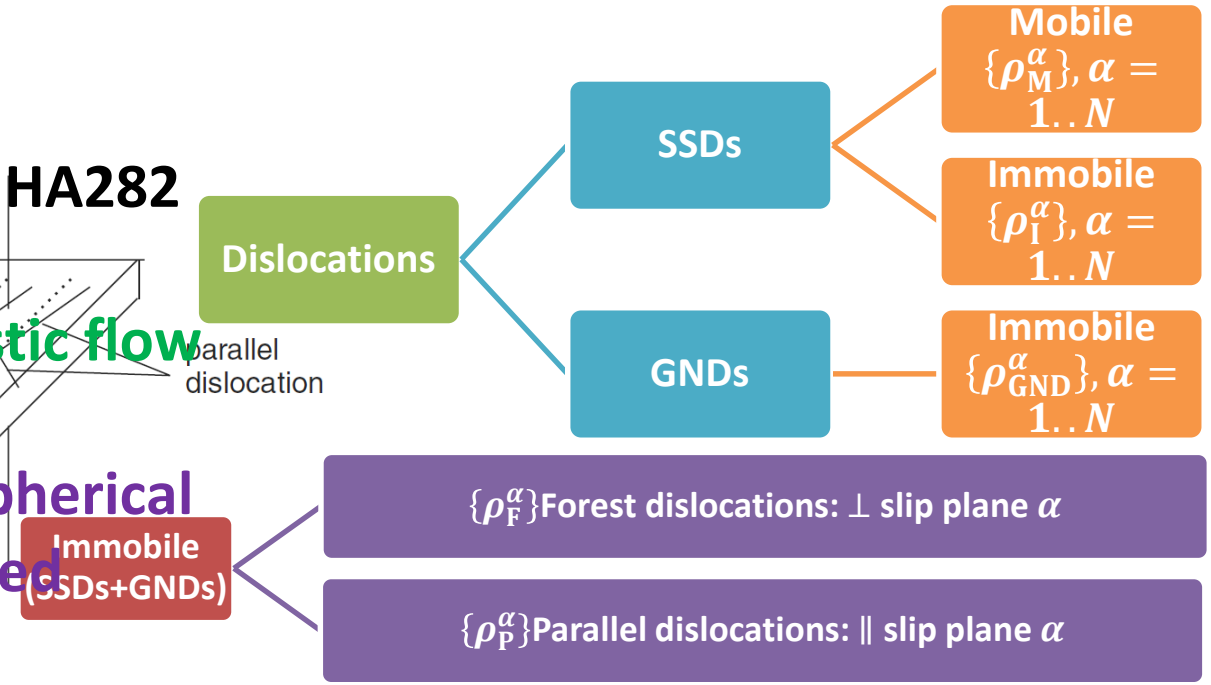
Eisenlohr, P., et al. (2013). *Int. J. Plast.*, 46, 37-53.

A dislocation-based constitutive model

Two phases γ and γ' are considered for modeling HA282

- **The matrix γ adopts a dislocation-based plastic flow model.**
- **The dispersed small spherical γ' particles are assumed unshearable.**





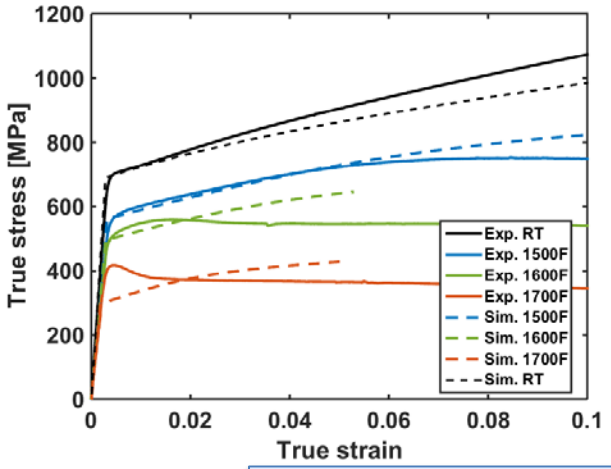
Orowan-type ($\dot{\gamma} = \rho v b$) kinetic equation:

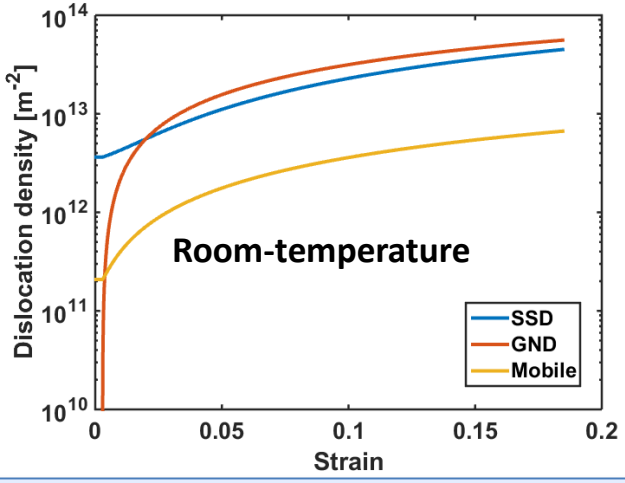
$$\dot{\gamma}^\alpha = \begin{cases} 0, & |\tau^\alpha| \le \tau_{\text{pass}}^\alpha \\ \dot{\gamma}_0^\alpha \exp\left[-\dfrac{Q_{\text{slip}}}{k_B T}\right] \sinh\left[\dfrac{|\tau^\alpha| - \tau_{\text{pass}}^\alpha - \tau_{\text{oro}}^\alpha}{\tau_{\text{cut}}^\alpha}\right] \text{sign}(\tau^\alpha), & |\tau^\alpha| > \tau_{\text{pass}}^\alpha \end{cases}$$

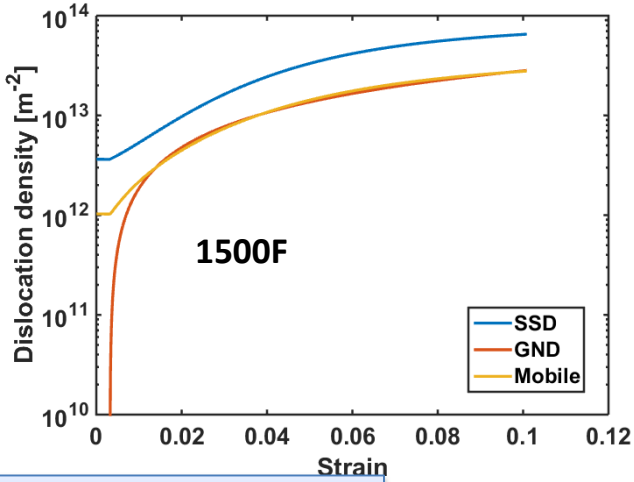
- The $\tau_{\text{pass}}^\alpha$ and τ_{cut}^α are due to the immobile dislocations serving as obstacles for mobile dislocation to shear.
- The τ_{oro}^α are due to the presence of dispersed particles and its calculation can rely on the microstructural information such as volume fraction, particle size, and channel width.

Ma, A., Roters, F., & Raabe, D. (2006). Acta Mater., 54(8), 2169-2179.

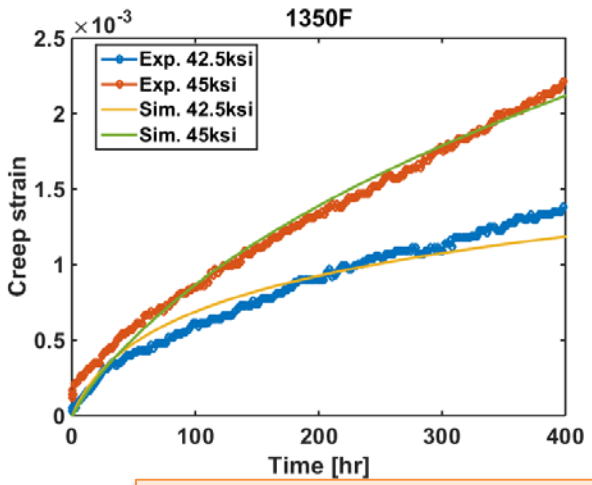
FFT-EVP in simulating static γ/γ'

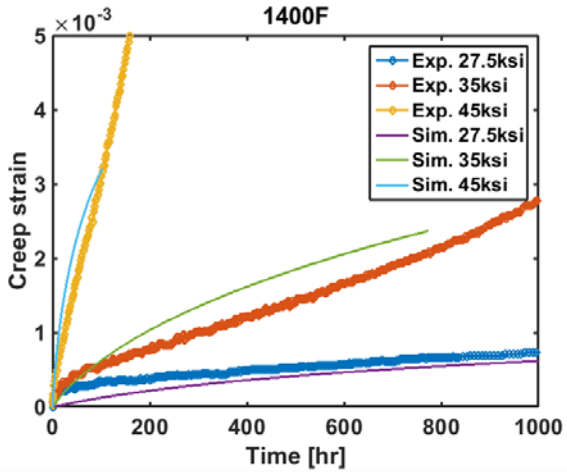


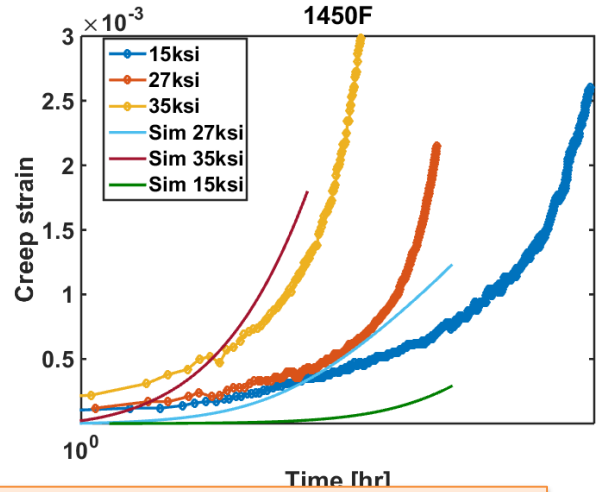




Comparison between simulated and experimental tensile tests, and simulation predicted dislocation density evolution during the test.

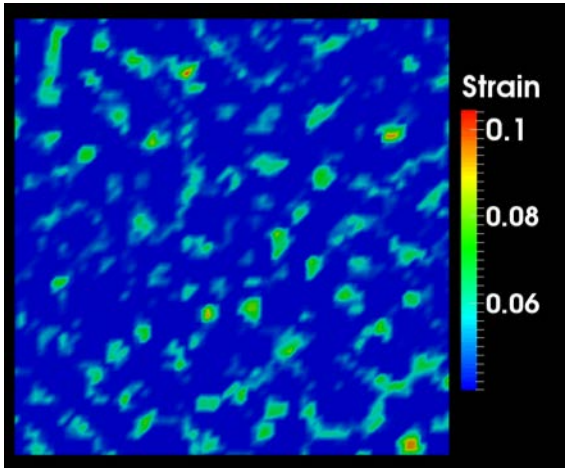




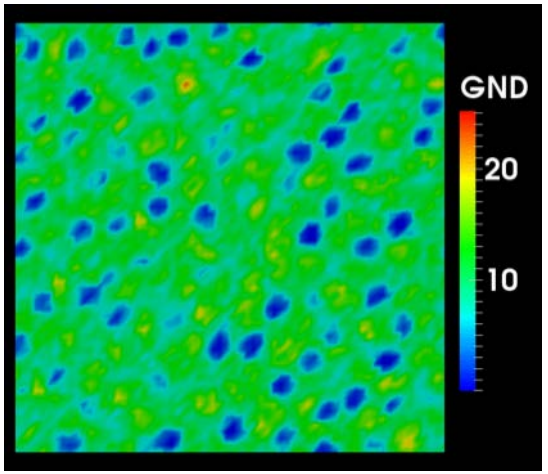


Comparison between simulated and experimental creep tests. The simulation can currently capture the initial and the transition up to early stages of secondary creep.

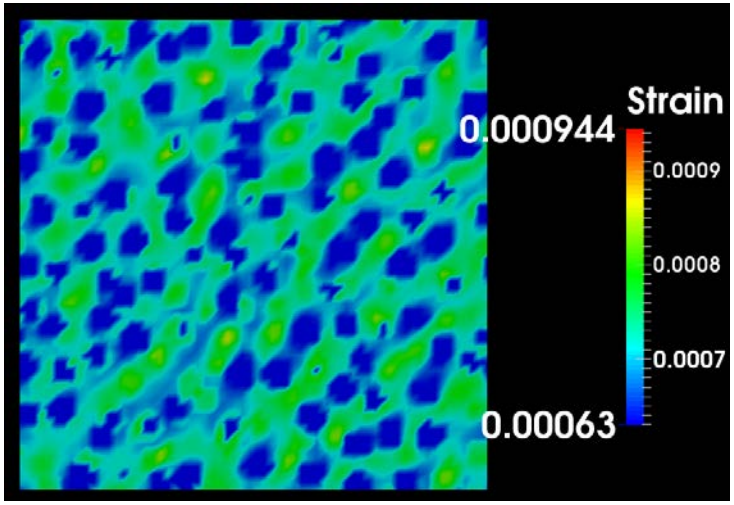
Heterogeneous deformation from simulation



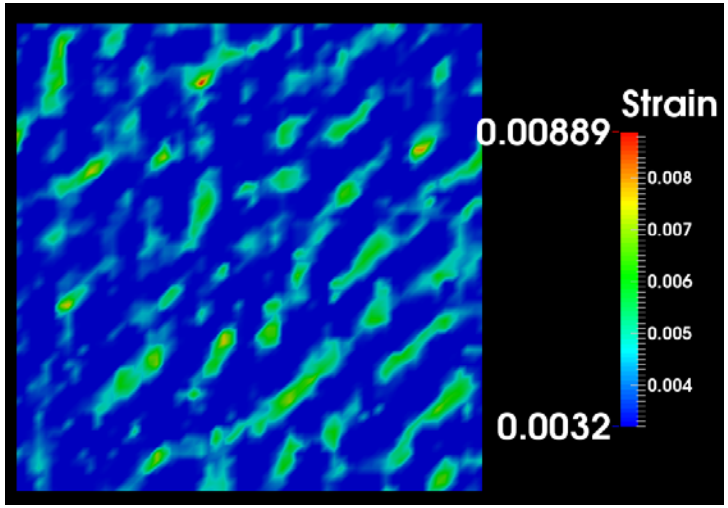
ε_{33} distribution during tensile (macro strain=3.5%), RT



GND distribution during tensile (macro strain=3.5%), RT

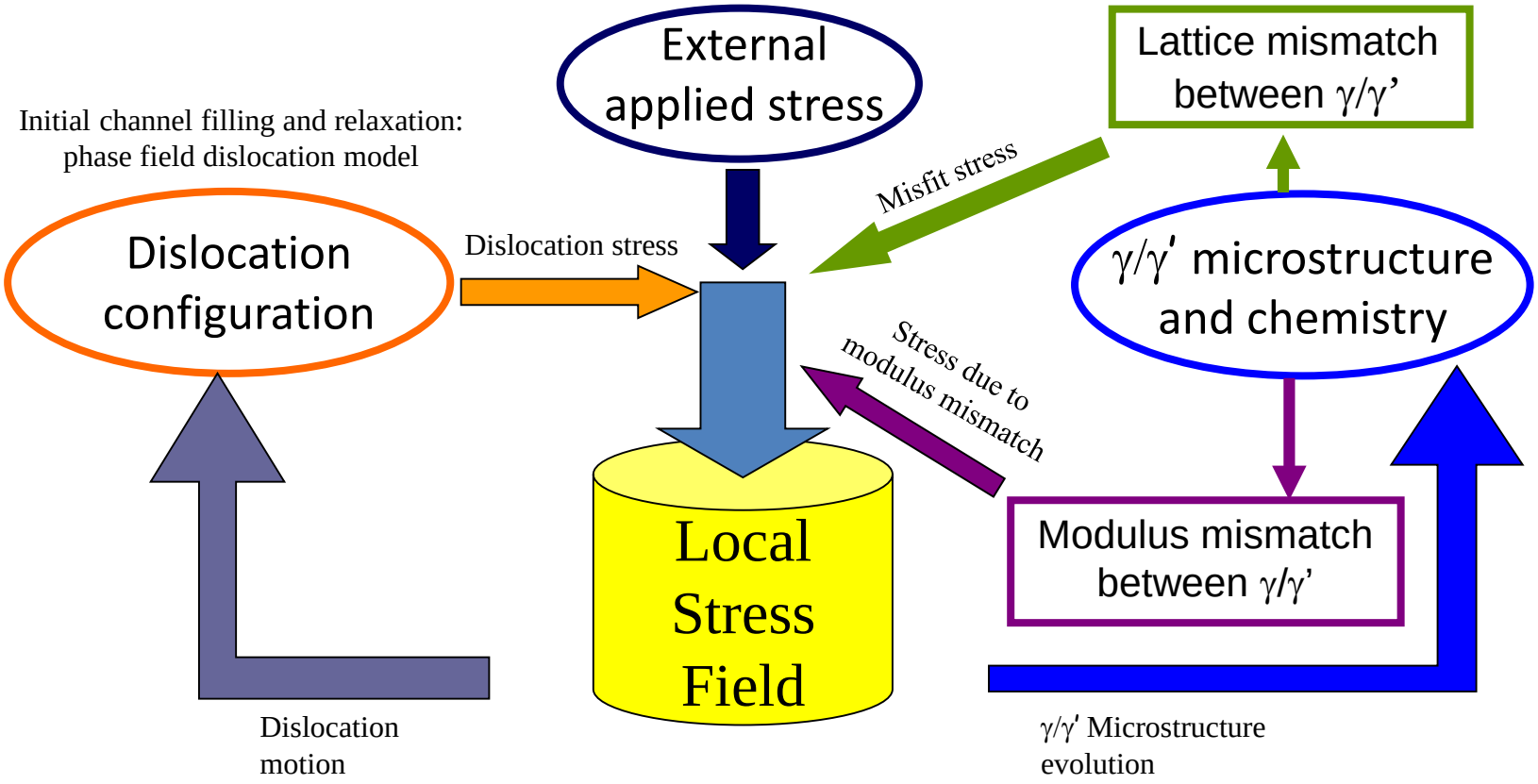


Creep, 27.5ksi, average strain=0.00063, 1400F



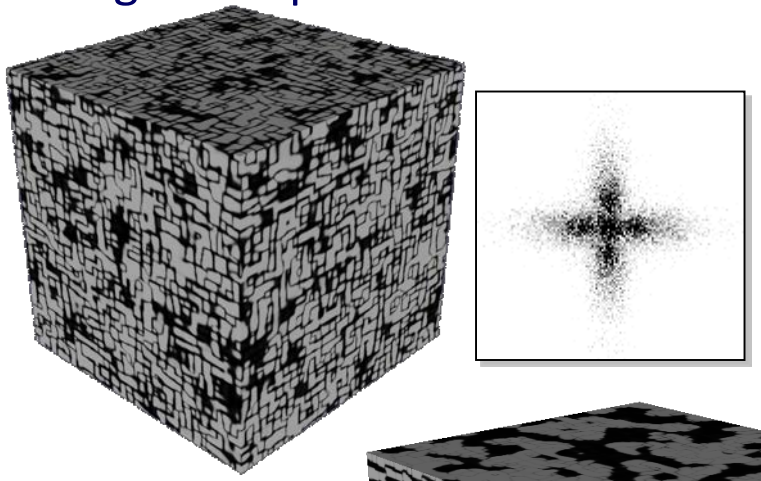
Creep, 45ksi, average strain=0.0032, 1400F

Microscopic phase-field modeling of rafting mechanisms

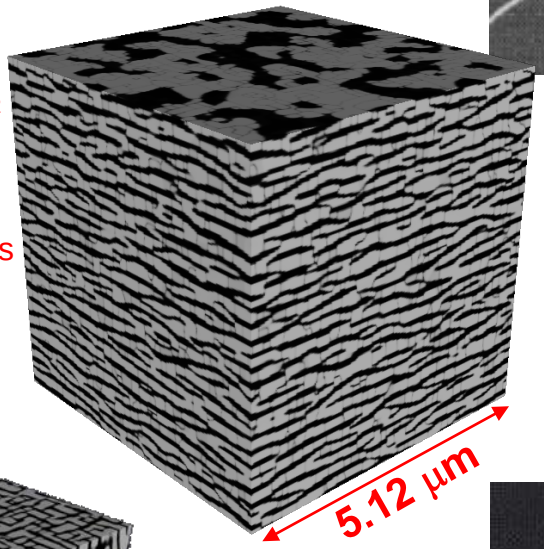


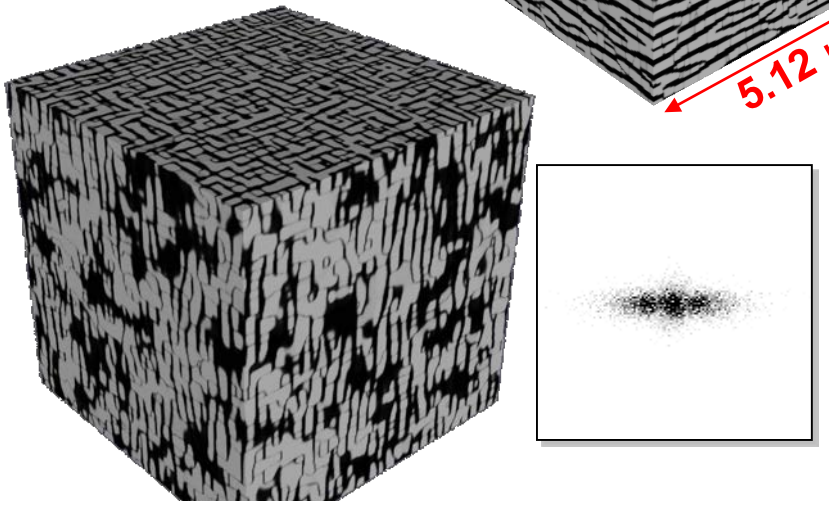
- Rafting caused by channel plasticity under homogeneous modulus assumption
- Rafting caused by modulus inhomogeneity without considering channel plasticity
- Rafting under combined effect of channel plasticity and modulus inhomogeneity

Coarse-grained phase field simulations



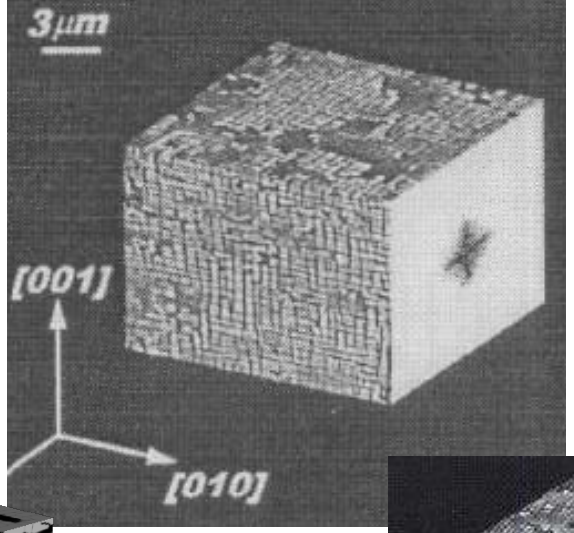
Interfacial energy: 14 mJ/m^2
Applied stress: 152Mpa
Temperature: 1300K
Effective diffusivity: 10^{-16}m^2/s
Volume fraction of γ': 60%
Lattice misfit: -0.3%
Aging time: 5.67 hours



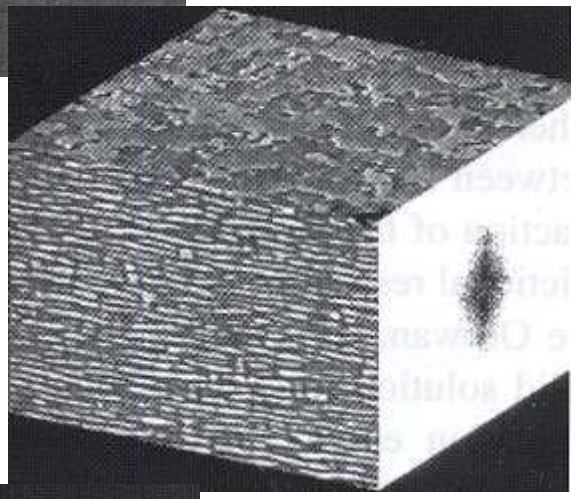


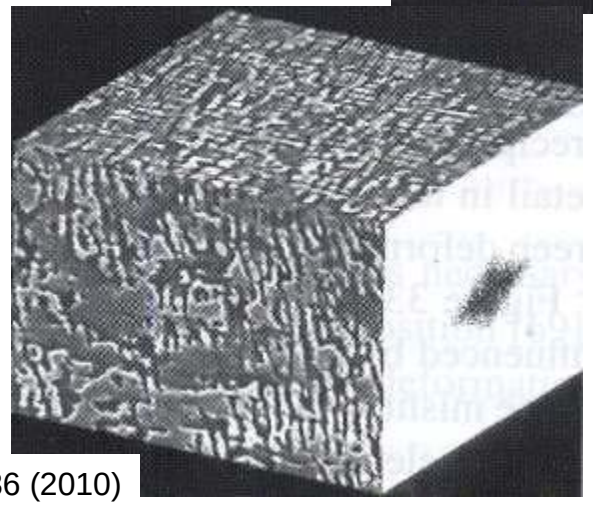
N. Zhou, C. Shen, MJ.Mills and Y. Wang, ***Phil. Mag.*** **90**:405-436 (2010)

Experimental observations



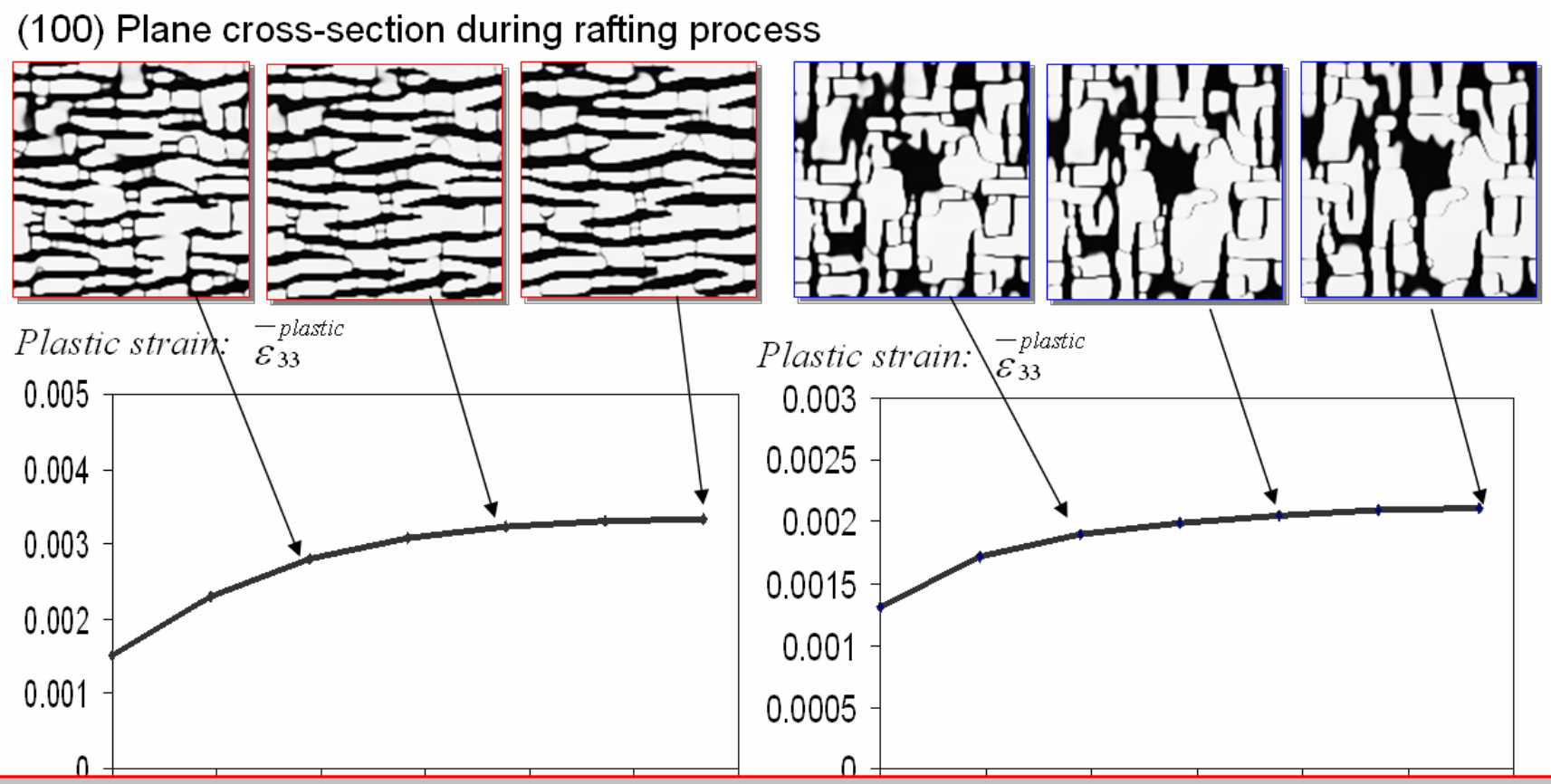
Misfit: -0.5%
Applied stress: 130MPa
Temperature: 1050^{o}C
Aging time: 8 hrs.





M. Fahrmann, W. Hermann, E. Fahrmann, A. Boegli, and T. Pollock, Materials Science and Engineering, A260, 212–221 (1999).

Creep strain vs. time

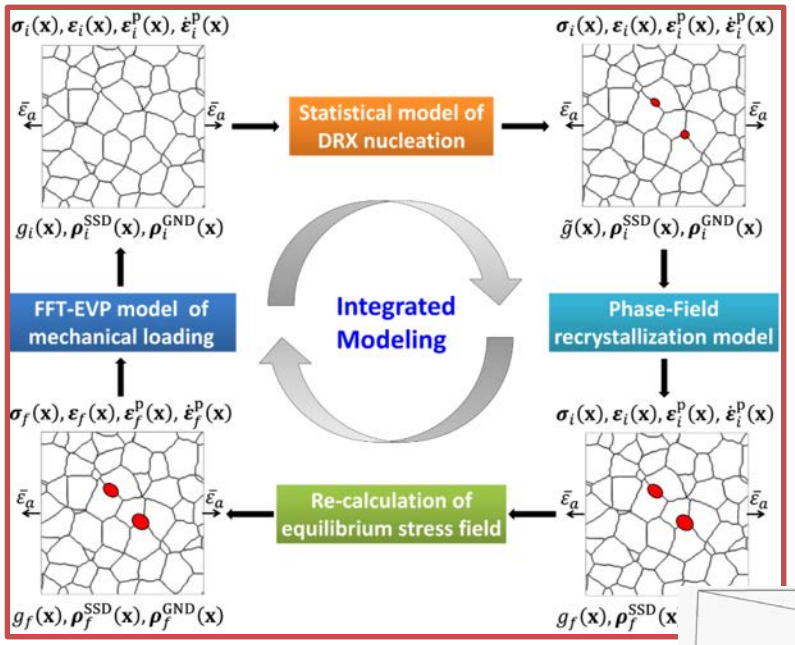


The coarse-grained model could be used in the optimization of existing alloys and development of new alloys such as Co-base superalloys **if properly informed and validated**.

N. Zhou, C. Shen, MJ.Mills and Y. Wang, ***Phil. Mag.*** **90**:405-436 (2010)

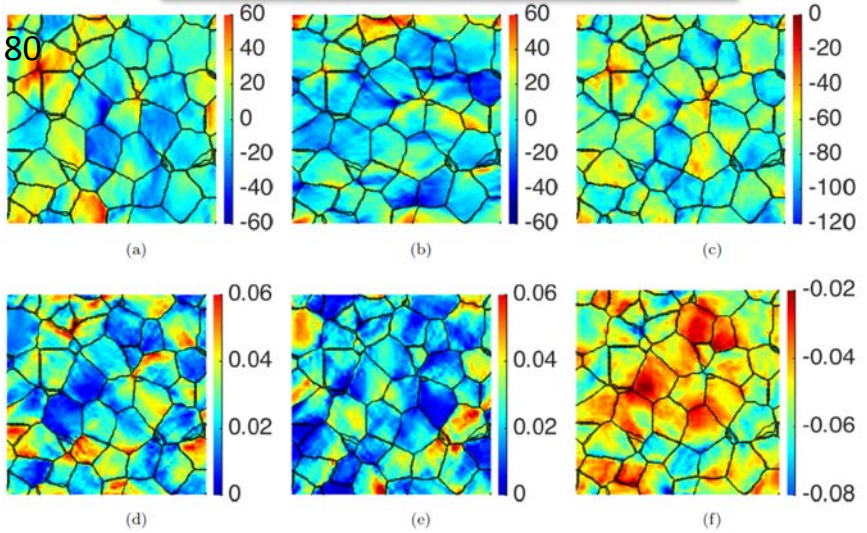
Demonstration of Integrated Modeling

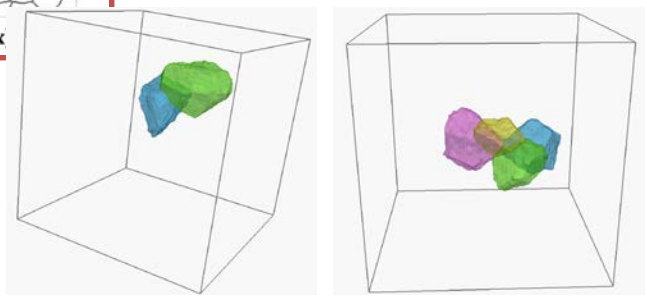
A model of dynamic recrystallization

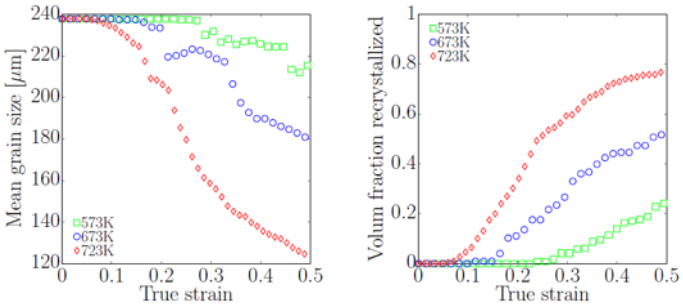


P Zhao, TSE Low, Y Wang, SR Niezgoda. *IJP* 80 (2016): 38-55.

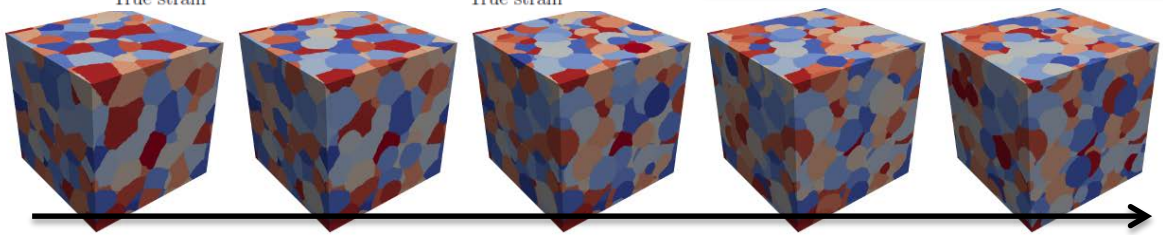
Micromechanical output





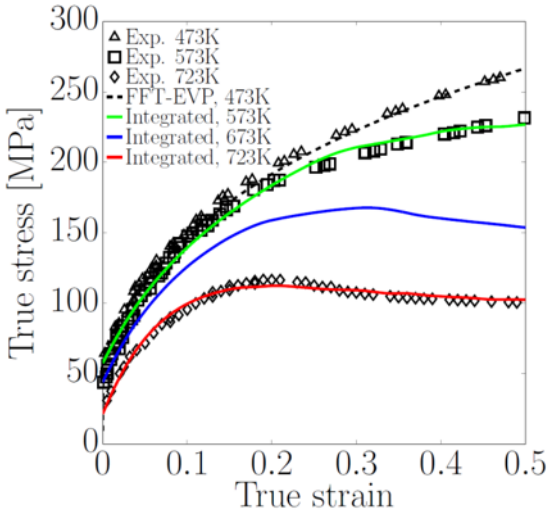


Microstructural output



Increasing deformation at elevated temperature

Stress-strain output



Homogenized Polycrystalline Creep Model

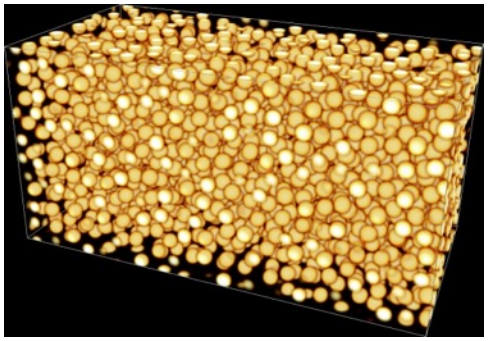
Key morphological parameters to be employed:

- γ‘ volume fraction f
- Average γ‘ radius r_p

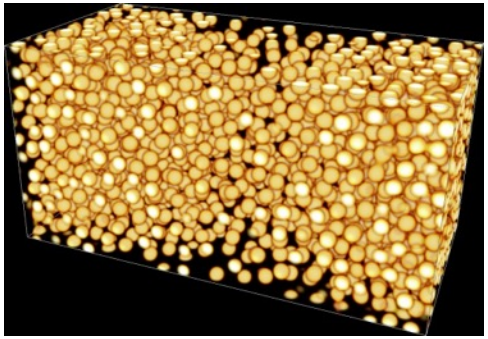
→ ***Mean-field*** descriptors

- Inter-particle spacing L_p → ***Local*** information

→ **Describing the constitutive behavior of a "homogenized" grain**



e.g., non-uniform γ' distribution with same vol.%



Two approaches for L_p:

1. Analytical expression based on average volume fraction f and mean particle size r_p:

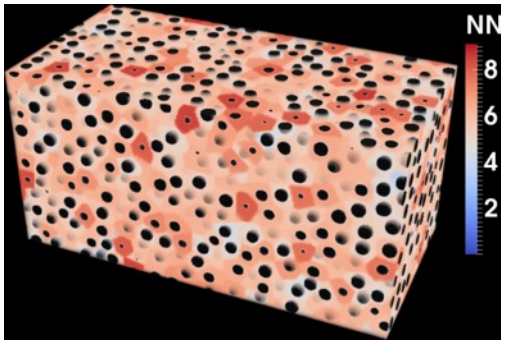
$$L_p = 1.6 r_p \left[\sqrt{\frac{\pi}{4f}} - 1 \right],$$

which has NO local information

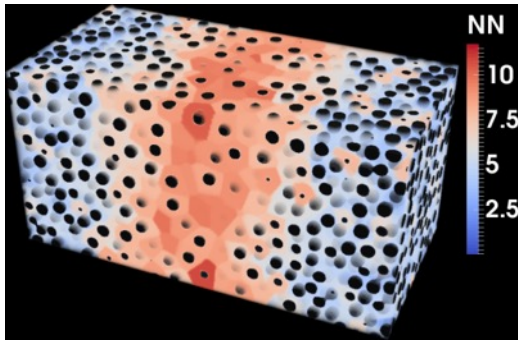
2. The nearest-neighbor (NN) distance $d_{\mathrm{NN}}(\mathbf{x})$ that represents the *local* "channel width". Then

$$L_p = \langle d_{\mathrm{NN}}(\mathbf{x}) \rangle_{\mathbf{x}}$$

The *microstructure-sensitivity* of L_p depends on the way of evaluation



Local $d_{\mathrm{NN}}(\mathbf{x})$ defined using nearest-neighbor distance



Homogenized Polycrystalline Creep Model

- **Thermally-Activated Deformation Theory** : $\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \exp\left[-\frac{\Delta G(\tau)}{k_B T}\right]$

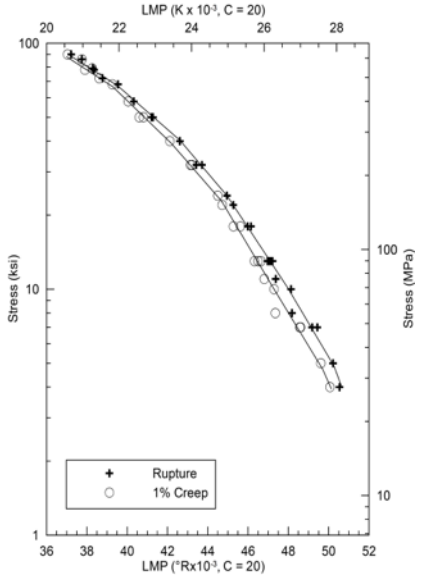
  where $\dot{\gamma}^{\alpha}$ is the plastic shear rate on slip system α, $\dot{\gamma}_0^{\alpha}$ is the reference shear rate, k_B is the Boltzmann constant, T is the temperature.
- The activation energy barrier $\Delta G(\tau)$ is formulated using the **mechanical threshold stress** (MTS) model: $\Delta G(\tau) = \mathrm{Q}_0 \left[1 - \left(\frac{\tau - \hat{\tau}_a}{\hat{\tau}_t}\right)^p\right]^q$ where τ is the shear stress, p and q are constants ($0 \le p \le 1, 1 \le q \le 2$). The $\hat{\tau}_a$ and $\hat{\tau}_t$ are respectively the athermal and thermal mechanical threshold strength:
- Evolution of threshold strengths:
  - Athermal $\hat{\tau}_a$ depends on grain size and follows **Hall-Patch** relationship
  - Thermal $\hat{\tau}_t$ follows a **Voce-like hardening law**: $\frac{d\hat{\tau}_t}{d\gamma^{\alpha}} = \theta_0 \cdot \frac{\mu}{\mu_0}\left[1 - \frac{\hat{\tau}_t}{\hat{\tau}_{ts}(\dot{\gamma},T)}\right]^{\kappa}$

- This grain-level constitutive model will be **calibrated against the full-field single crystal creep model**
- Pre-determined analytical or more sophisticated dependence of the *three key microstructure descriptors* will be employed for calibration to **encode the sub-grain microstructure-sensitivity as well as underlying mechanisms**

Model Validation and Creep Lifing Prediction

- **The developed grain-level creep model will be calibrated using experimental data**
  - Model input: Statistically equivalent, experimentally informed synthetic polycrystals will be generated using DREAM3D
  - Model output:
    - Creep curves, as well as other mechanical responses
    - Stress, strain, plastic shear rate distribution over the grain aggregate
- **Model predictions on other temperature/stress range will be used to directly compare with experimental data as the model validation**
  - Since no creep cavitation is considered, the comparison will be restricted to the primary and secondary creep stage.
  - Failure-related properties are also excluded in the comparison.

- **Creep lifing prediction will be made on the Larson-Miller vs a target creep strain, e.g. 1%**



Larson-Miller plot of rupture and 1% creep for Haynes 282 alloy

- **Correlation of microstructure descriptors and creep mechanisms with creep performance will be revealed via our multiscale modeling**

Who's Doing What

- Niezgoda & Wang – Project PIs
- Pengyang Zhao (Research Associate) and Supriyo Chakroborty (Ph.D. Student)
  - The actual work
- Bryce Meredig and Greg Mulholland (Citrine) support in inputing data into Citrination and development of machine learning operations
- Chen Shen (GE GRC) assisting in agglomerating all pre-competitive data on creep in Haynes 282 and Inconel 740

Task List

- Task 1 - Project Management and Planning
  - Develop and maintain a comprehensive project management plan to ensure team interactions and collaborations with the industrial participants, track deliverables, minimize risk and find alternatives, interface with DOE, and report progress and financials in accordance with the requirements set forth in the award document.
- Task 2 - Data Assessment, Database Development and Informatics
  - Collect, analyze and assess existing data from creep tests on the selected alloy. In collaboration with Citrine Informatics, the data will be entered into Citrination for analysis. Statistical assessment of the data will be performed to determine where the data are insufficient or contradictory, and develop relationships between the effects of alloy composition and processing (microstructure) on creep.
- Task 3- Assessment of Predictive Accuracy of Current Models
  - The PIs will evaluate existing models to ascertain confidence on creep-life predictions and determine which if any provide a statistically adequate fit to the data and safe extrapolation of the data to 300,000 hours of operation.

Task List

- Task 4 - Development of Multiscale Physics-based Creep Model for Ni-base Superalloys
  - **Subtask 4.1 Full-field Modeling of Single Crystal Creep:** Develop a 3D full-field modeling framework using a combination of phase field method (PFM) for precipitate microstructure evolution and FFT-based crystal plasticity (FFT-CP) modeling for dislocation density evolution, integrated in a unified framework through a *two-way-coupling* model-interface. This PFM + FFT-CP modeling framework will focus on intragrannular or single crystal creep behavior where details of dislocation-precipitate interaction will be considered explicitly
  - **Subtask 4.2 Homogenized Polycrystalline Creep Model:** The PIs will develop a polycrystalline level homogenized CP model that will allow for simulating creep behavior of large grain aggregates so that direct comparison between model predictions and experimental data can be made.
- Task 5 - Effect of Microstructure Inhomogeneity on Creep
  - Demonstrate a proof-of-concept study the effect of inhomogeneity in microstructure (such as precipitate volume fraction and grain size) on long-term creep behavior of weldments and large components using the homogenized polycrystalline CP model.

Missing Task!!!!!

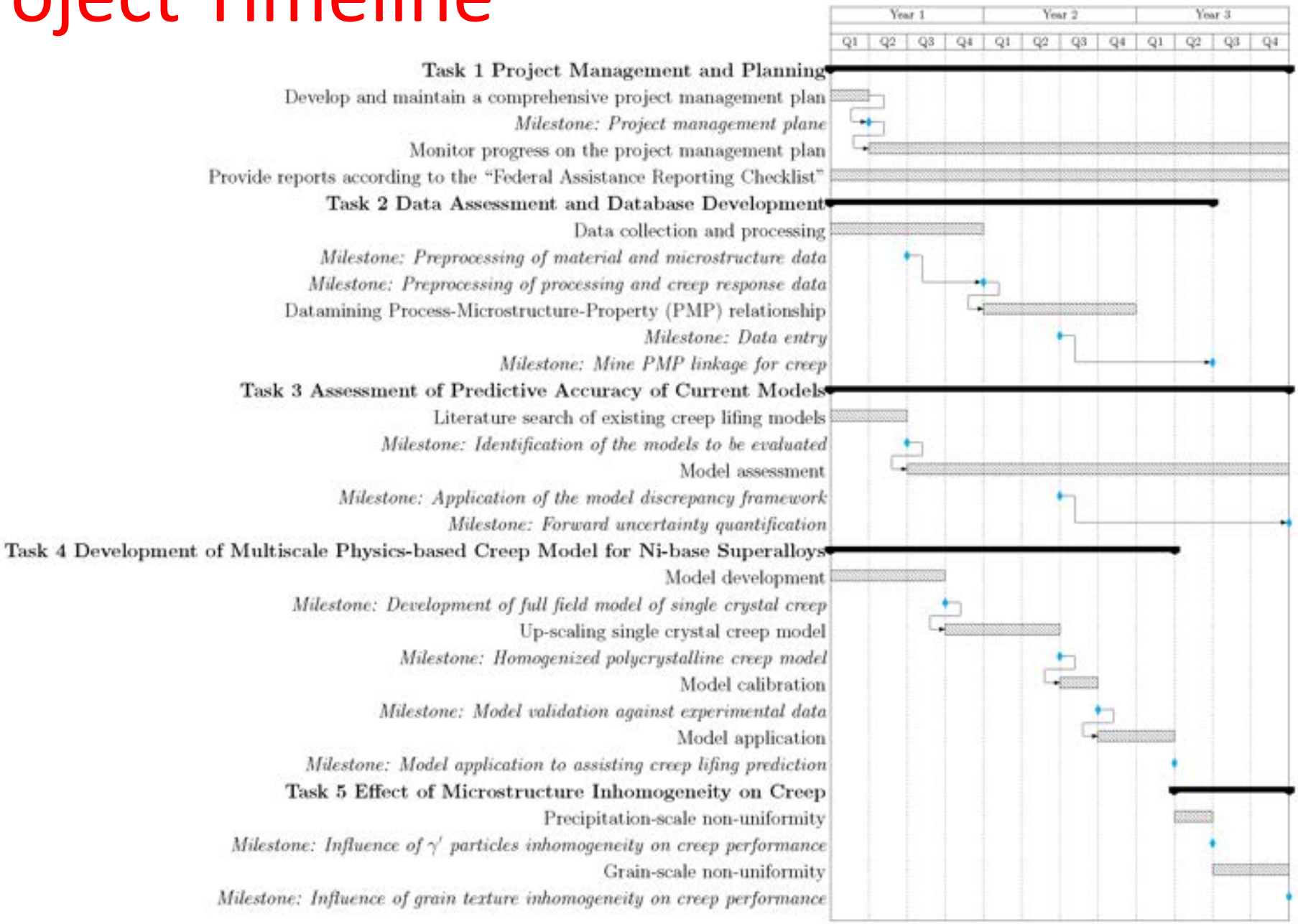
- Feedback to Citrination
  - Bring modeling and simulation results back to machine leaning database for future design and product optimization use.

Milestone Log

Table 2: Program milestone log.

Budget period	Milestone Title	Completion Date
1	Project Management and Planning (Task 1)	Y1Q1
1	Preprocessing of Material and Microstructure Data (Task 2)	Y1Q2
1	Preprocessing of Processing and Creep Response Data (Task 2)	Y1Q4
2	Data Entry (Task 2)	Y2Q2
2	Mine PMP Linkages for Creep (Task 2)	Y3Q2
2	Identification of the Models to be Evaluated (Task 3)	Y1Q2
3	Application of the Model Discrepancy Framework (Task 3)	Y2Q2
3	Forward Uncertainty Quantification (Task 3)	Y3Q4
1	Development of Full Field Model of Single Crystal Creep (Task 4)	Y1Q3
2	Homogenized Polycrystalline Creep Model (Task 4)	Y2Q2
2	Model Validation against Experimental Data (Task 4)	Y2Q3
3	Model Application to Assisting Creep Lifing Prediction (Task 4)	Y3Q1
3	Influence of γ' particles inhomogeneity on creep performance (Task 5)	Y3Q2
3	Influence of grain texture inhomogeneity on creep performance (Task 5)	Y3Q4

Project Timeline



Clear as Mud?