eXtremeMAT

Laurent Capolungo

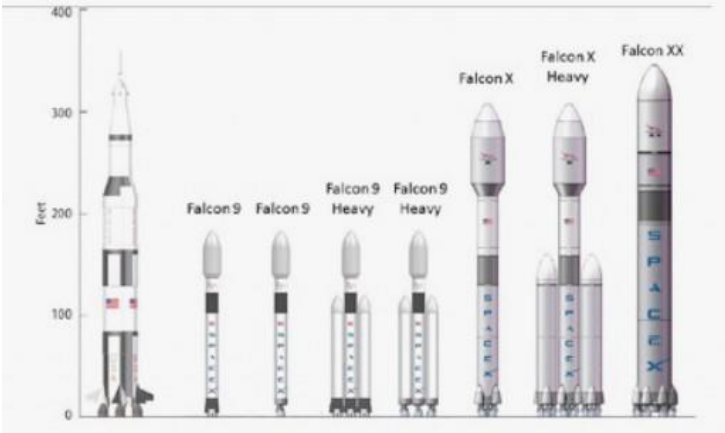
Acknowledgements

Jeff Hawk, Ram Devanathan
Edgar Lara Curzio, Michael Brady, Yuki Yamamoto, Brandon Wood, Mark Cawkwell, Romain Perriot, Arul Kumar, Aaron Kohnert, Richard LeSar, Youhai Wen, Ricardo Lebensohn, Nghiep Nguyen, Ben Spencer, Millicent Orondo, Brian Gleeson, Dave Alman, Edgar Lara Curzio, Jeff Hawk, Kelly Rose, Dongwon Shin, Rishi Pillai, Paul Jablonski, Tom Lograsso, Madison Wenzlick, Rui Fen, Valery Borovikov, Jennifer Bauer, Osman Mamum, Arun Sathanur

XMAT: Objectives and structure

eXtremeMAT
Accelerating the Development of Extreme Environment Materials
U.S. DEPARTMENT OF ENERGY

General scope: XMAT will develop, verify and validate research tools that help the US fossil energy industry in (i) assessing the failure of steel components subjected to complex non-monotonic loading, (ii) adopting emerging/new steels.



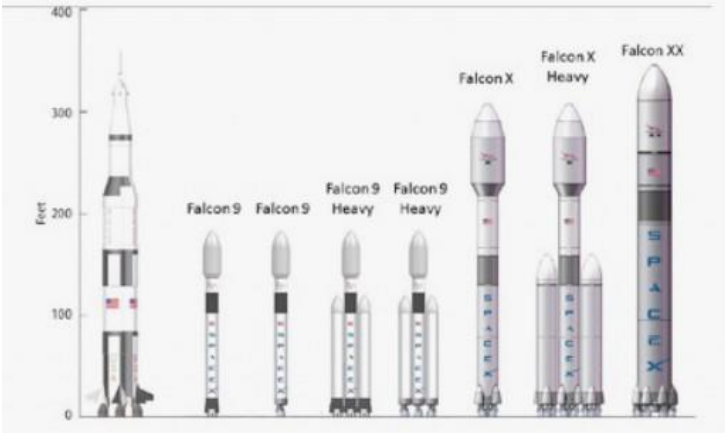
"I think it's very important to have a feedback loop, where you're constantly thinking about what you've done and how you could be doing it better." E. Musk

XMAT: Objectives and structure

eXtremeMAT
Accelerating the Development of Extreme Environment Materials
U.S. DEPARTMENT OF ENERGY

General scope: XMAT will develop, verify and validate research tools that help the US fossil energy industry in (i) assessing the failure of steel components subjected to complex non-monotonic loading, (ii) adopting emerging/new steels.

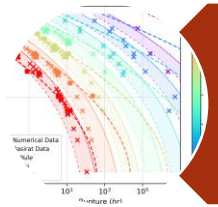
Applications to: conventional austenitic (**347H**, 316H) and ferritic steels (**P91**), **XMAT X351**..
Conditions: Temperatures from ~500 to 750C, Maximum stresses 100MPa, oxidation in air



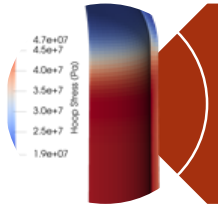
"I think it's very important to have a feedback loop, where you're constantly thinking about what you've done and how you could be doing it better." E. Musk

eXtremeMAT Thrusts

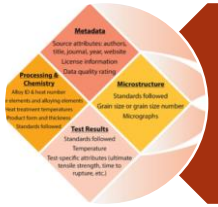
eXtremeMAT
Accelerating the Development of Extreme Environment Materials
U.S. DEPARTMENT OF ENERGY



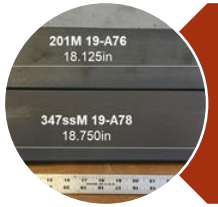
1. Material Lifetime & Performance Predictors



2. Component Lifetime & Performance Predictors



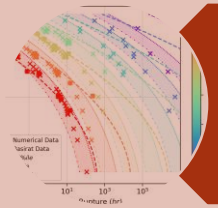
3. Data Science & Analysis Tools



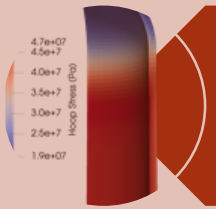
4. Guidelines for the Discovery of New Iron-Base Alumina Forming Alloys

eXtremeMAT Thrusts

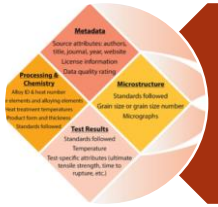
eXtremeMAT
Accelerating the Development of Extreme Environment Materials
U.S. DEPARTMENT OF ENERGY



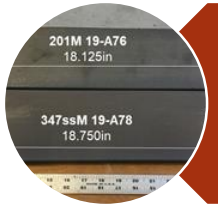
1. Material Lifetime & Performance Predictors



2. Component Lifetime & Performance Predictors



3. Data Science & Analysis Tools



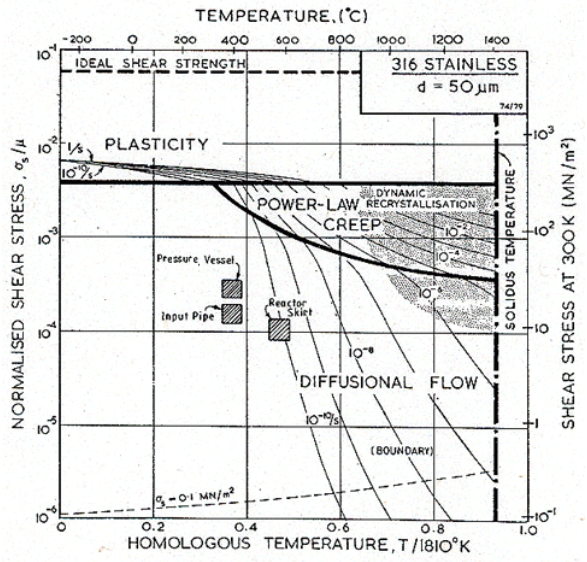
4. Guidelines for the Discovery of New Iron-Base Alumina Forming Alloys

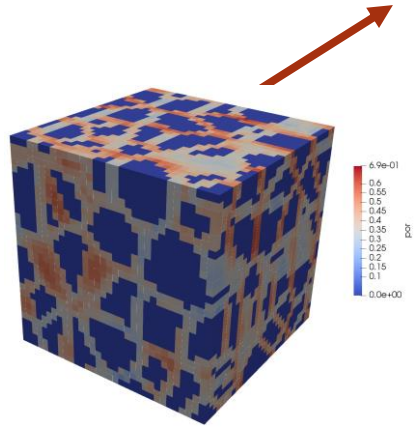
Capturing the effect of microstructure on contributing deformation mechanisms

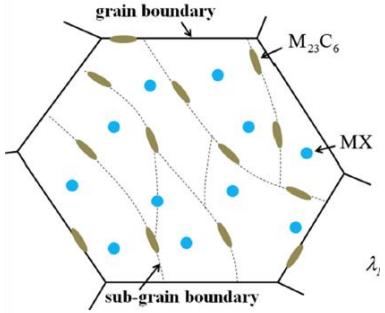
A mechanistic constitutive model was developped to account for the effects of microstructure, stress and temperature on the relative activity of different plastic deformation and damage mechanisms.

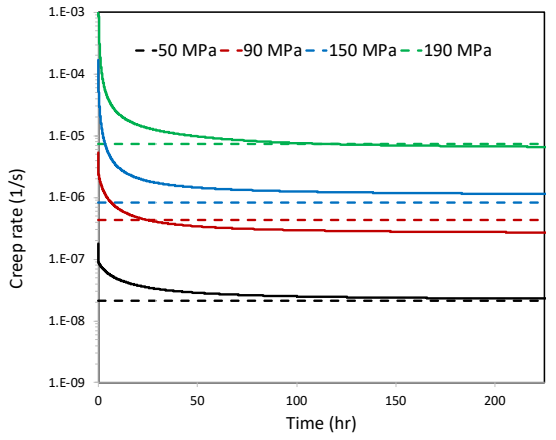
The model accounts for:

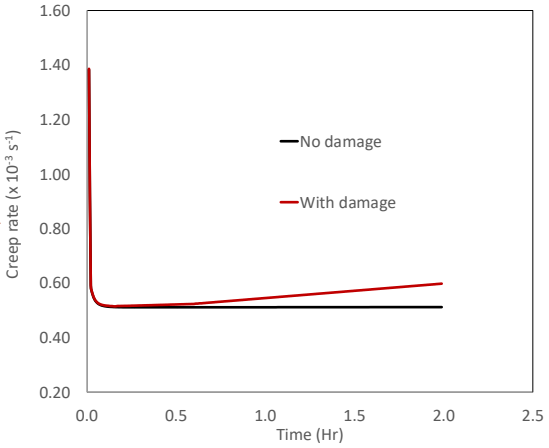
- Effects of precipitates (strengthening and weakening).
- Effects of dislocation content (cells, cell, walls).
- Point defect mediated plasticity (Coble creep, dislocation climb)
- Damage (nucleation, growth, coalescence)
- *Ageing (in progress)*









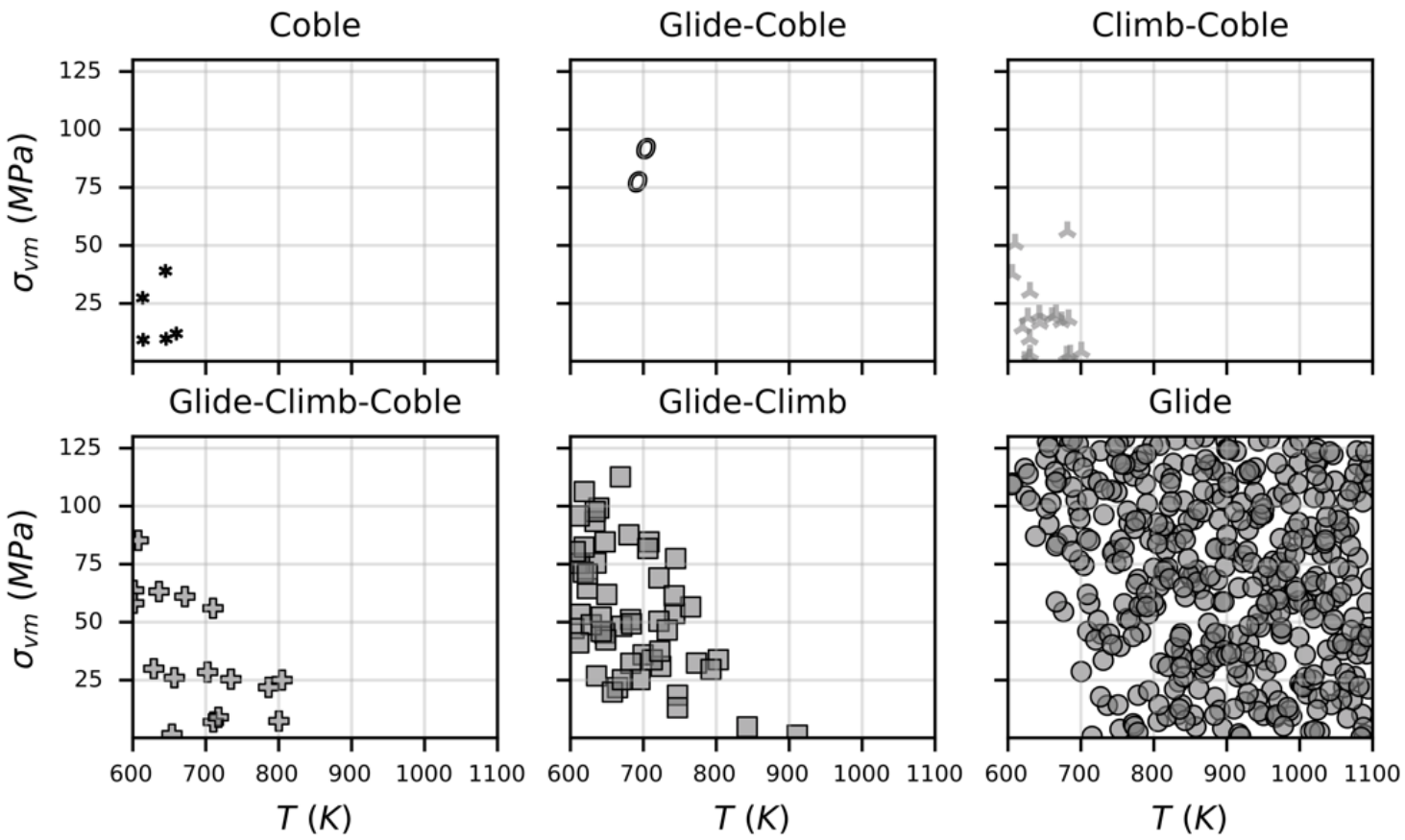


Capturing the effect of microstructure on contributing deformation mechanisms

A mechanistic constitutive model was developped to account for the effects of microstructure, stress and temperature on the relative activity of different plastic deformation and damage mechanisms.

The model accounts for:

- Effects of precipitates (strengthening and weakening).
- Effects of dislocation content (cells, cell, walls).
- Point defect mediated plasticity (Coble creep, dislocation climb)
- Damage (nucleation, growth, coalescence)
- *Ageing (in progress)*



Mechanistically derived creep rupture life predictors

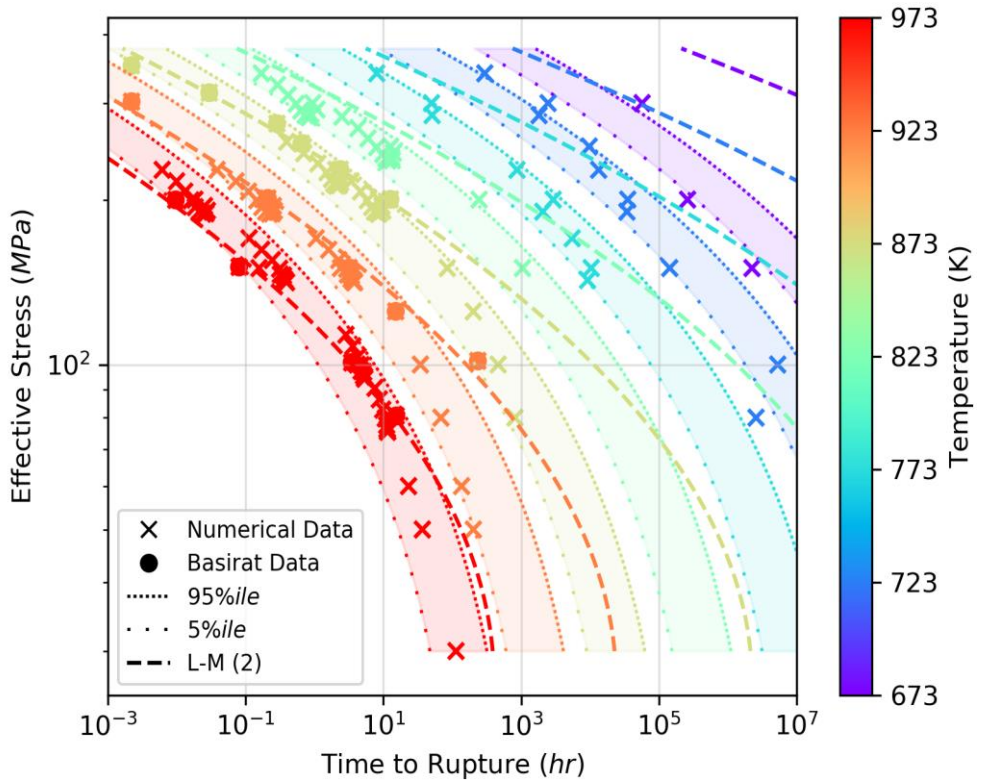
A mechanistic constitutive model was developped to account for the effects of microstructure, stress and temperature on the relative activity of different plastic deformation and damage mechanisms.

The model accounts for:

- Effects of precipitates (strengthening and weakening).
- Effects of dislocation content (cells, cell, walls).
- Point defect mediated plasticity (Coble creep, dislocation climb)
- Damage (nucleation, growth, coalescence)
- *Ageing (in progress)*

P91, 2D, FEM based, no aging, empirical damage nucleation model

N. Bieberdorf, V. Taupin, R. Lebensohn, L. Capolungo (in review)



A synthetic database of creep rupture life is generated and mined to derive a new rupture life criterion from a limited number of short term creep tests.

Towards an integrated approach to assess the performance of structural components

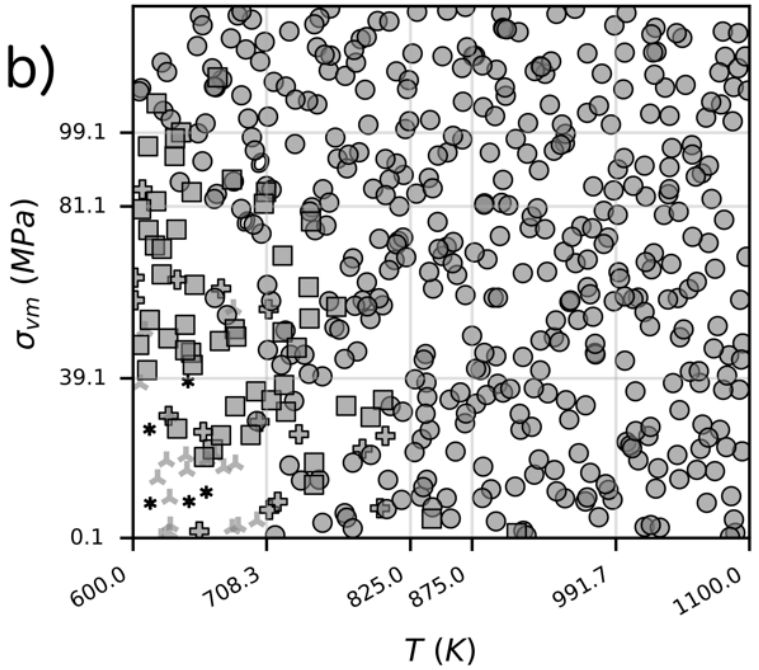
eXtremeMAT
Accelerating the Development of Extreme Environment Materials
U.S. DEPARTMENT OF ENERGY

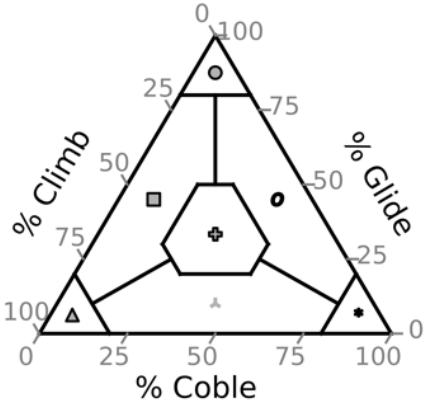
Edith Piaf
(not affiliated with extremeMat)

LaRomance

Los Alamos
Reduced Order Models for Advanced Nonlinear Constitutive Equations

Data driven constitutive models sensitive to dislocation content, cell structures, precipitate content.

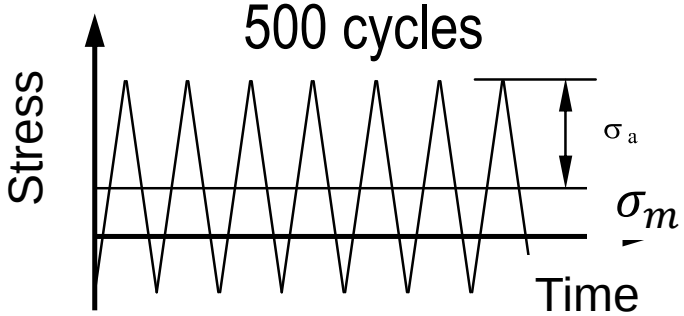


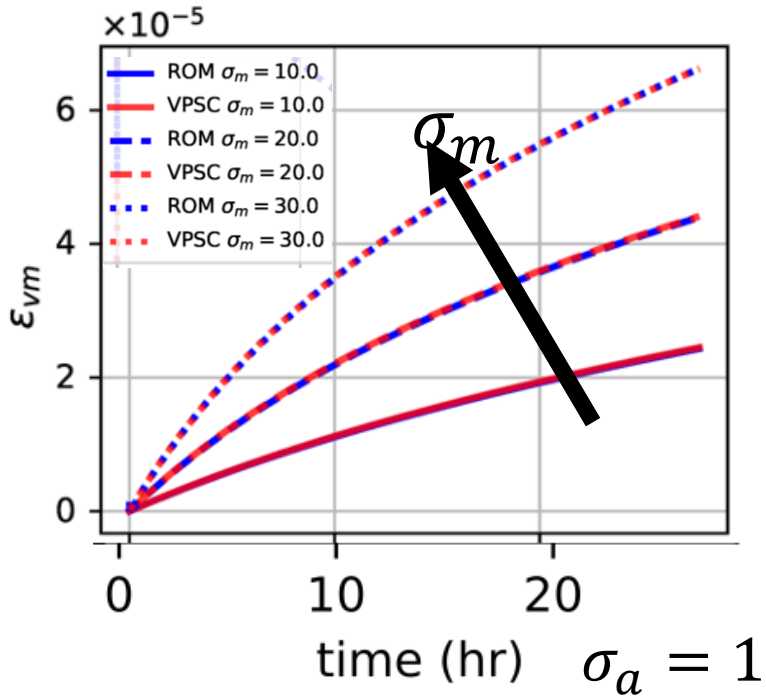


$$\dot{\varepsilon}_{vm}(\bar{\rho}_{cell}, \bar{\rho}_w, \varepsilon_{vm}, \sigma_{vm}, T) \sim \sum_{c,w,\varepsilon,\sigma,T=0}^{degree} \alpha_{cw\varepsilon\sigma T} P_c(\bar{\rho}_{cell}) P_w(\bar{\rho}_w) P_\varepsilon(\varepsilon_{vm}) P_\sigma(\sigma_{vm}) P_T(T)$$

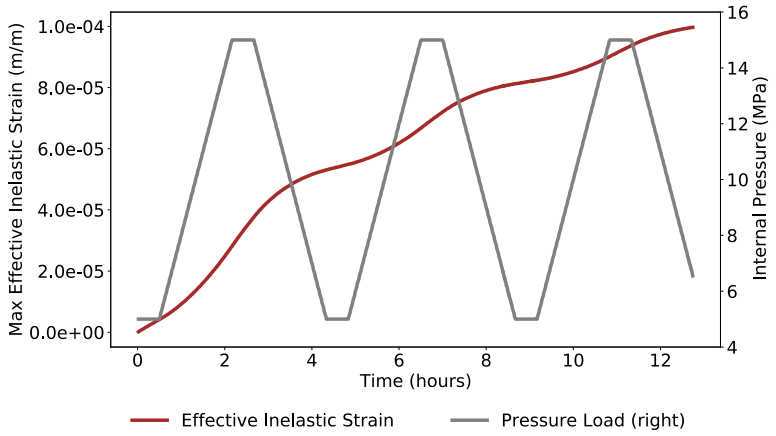
- *A database of more than 30000 creep simulations is generated.*
- *Strain increments as a function of stress and materials state are recorded (>10^6 datapoints).*
- *The database is mined to derive a constitutive model that can be used in finite element simulations*

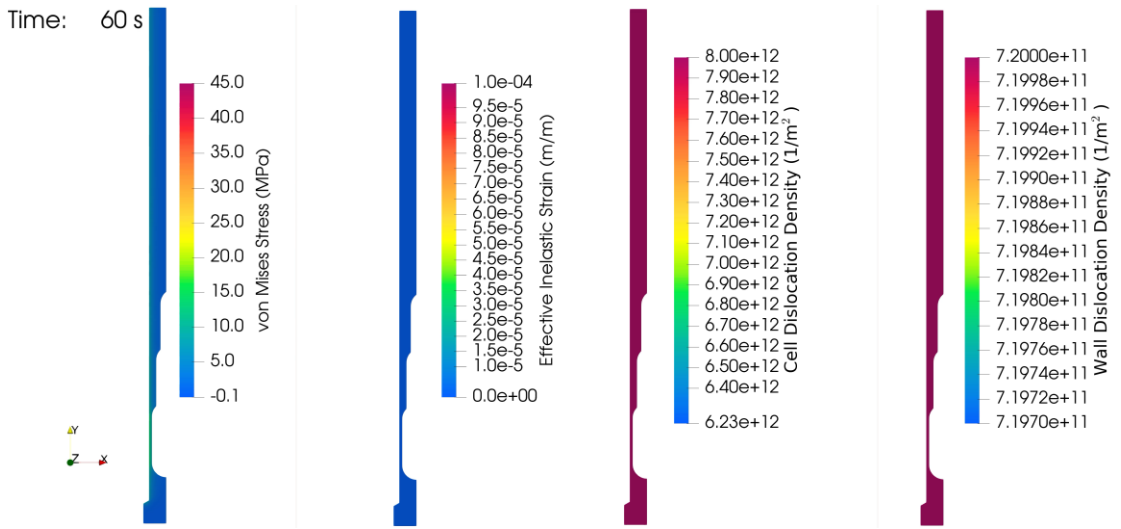
Predictive capability and integration of surrogate models





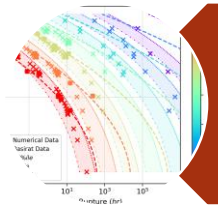
$\sigma_a = 15\ MPa$



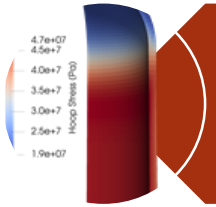


eXtremeMAT

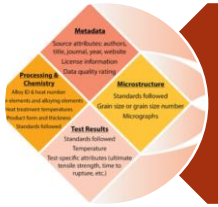
eXtremeMAT
Accelerating the Development of Extreme Environment Materials
U.S. DEPARTMENT OF ENERGY



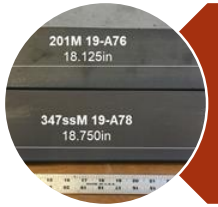
1. Material Lifetime & Performance Predictors



2. Component Lifetime & Performance Predictors



3. Data Science & Analysis Tools



4. Guidelines for the Discovery of New Iron-Base Alumina Forming Alloys

NATIONAL ENERGY TECHNOLOGY LABORATORY
AMES LABORATORY Creating Materials & Energy Solutions U.S. DEPARTMENT OF ENERGY
INL Idaho National Laboratory
Lawrence Livermore National Laboratory
Los Alamos NATIONAL LABORATORY EST. 1943
OAK RIDGE National Laboratory
Pacific Northwest NATIONAL LABORATORY