Accelerating the Development of Extreme Environment Materials

eXtremeMAT

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Acknowledgements

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XMAT: Objectives and structure

**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
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**Applications to:** conventional austenitic (347H, 316H) and ferritic steels (P91), XMAT X351..

**Conditions:** Temperatures from ~500 to 750°C, Maximum stresses 100 MPa, oxidation in air

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eXtremeMAT Thrusts

1. Material Lifetime & Performance Predictors
2. Component Lifetime & Performance Predictors
3. Data Science & Analysis Tools
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Capturing the effect of microstructure on contributing deformation mechanisms

A mechanistic constitutive model was developed 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)
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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

**LaRomance**

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Los Alamos

Reduced Order Models for Advanced Nonlinear Constitutive Equations

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

\[
\dot{\varepsilon}_{vm}(\rho_{cell}, \rho_w, \varepsilon_{vm}, \sigma_{vm}, T) \sim \sum_{c,w,e,o,T=0}^{\text{degree}} \alpha_{cweot} P_c(\rho_{cell})P_w(\rho_w)P_e(\varepsilon_{vm})P_o(\sigma_{vm})P_T(T)
\]

- 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

\[ \sigma_a = 15 \text{ MPa} \]
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