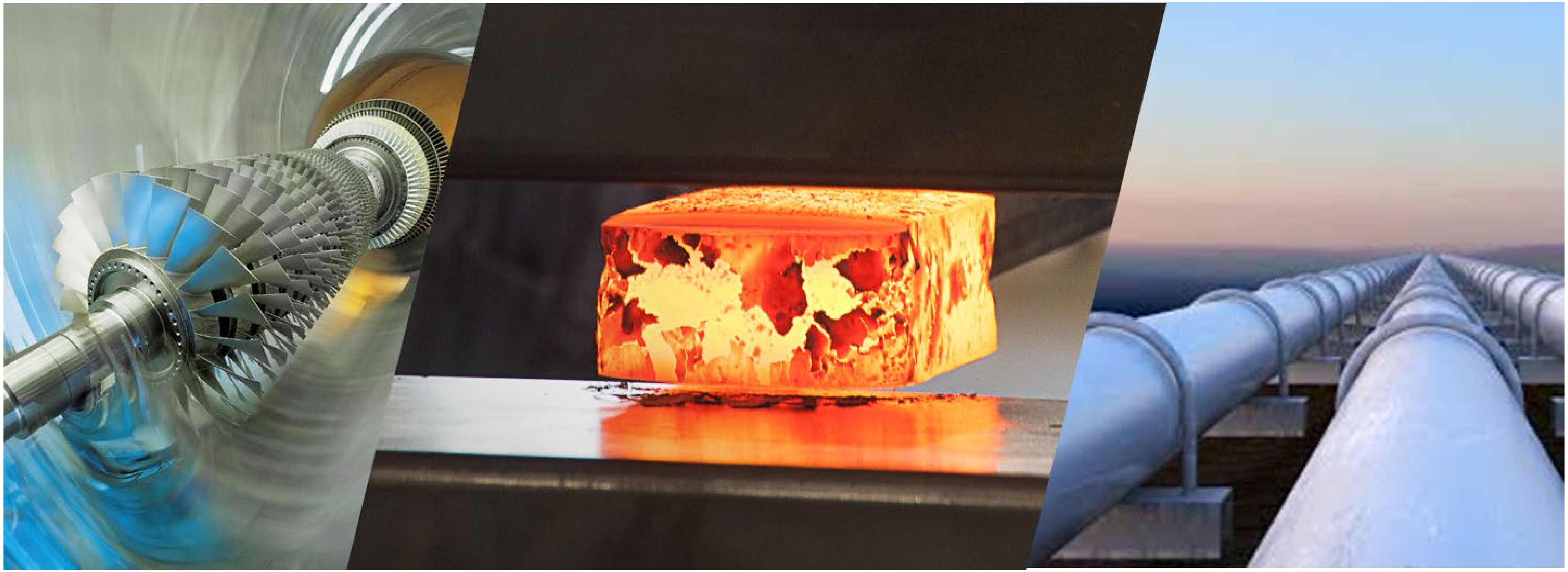
eXtremeMAT

U.S. DEPARTMENT OF ENERGY

eXtremeMAT Progress Summary & eXtremeMAT-H_2 Kickoff



Laurent Capolungo & David Alman

October 18, 2022

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OAK RIDGE National Laboratory
Pacific Northwest NATIONAL LABORATORY

eXtremeMAT Team

Team: M. A Kumar, M. Detrois, P. Jablonski, Y. Yamamoto, M. Gao, Q.Q. Ren, R. Lebensohn, A. Chakraborty, M. Glazoff, A. Rovinelli, A. Talapatra, A. Kohnert, M. Wenzlick

- Leadership Team: D. Alman, E. Cerreta, M. Kramer, G. Ilebvare, E. Lara Curzio

eXtremeMAT Approach & Progress

eXtremeMAT
Accelerating the Development of Extreme Environment Materials

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APPROACH | **BENEFIT**

Reduce the time & cost for alloy development, qualification & certification

High–Fidelity Constitutive Model Capturing effects of **alloy microstructure** and deformation & damage processes

Database of responses with experimental data and ***synthetic data*** generated over wide range of conditions

Surrogate (reduced order) models.

Data Driven Alloy Life Predictors

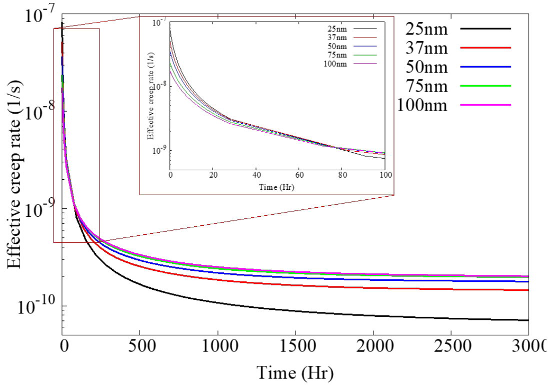
Engineering Models for embedding in FEM packages

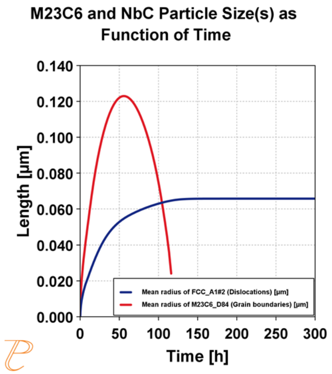
Improved physics-based mechanistic models

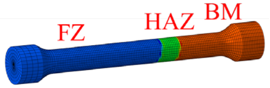
Improved component design, eliminate over design, enable predictive maintenance

Incorporated Microstructure into Simulation for 347H

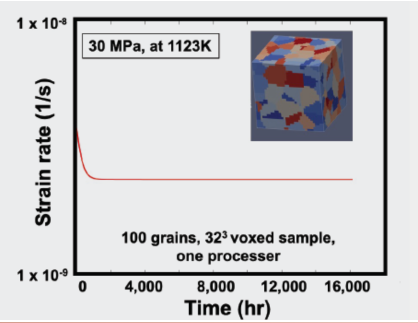
- Precipitate Coarsening (NbC, $M_{23}C_6$, Sigma),
- Effect of B and N
- Impact of ageing on creep behavior

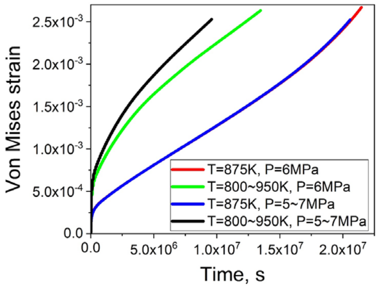




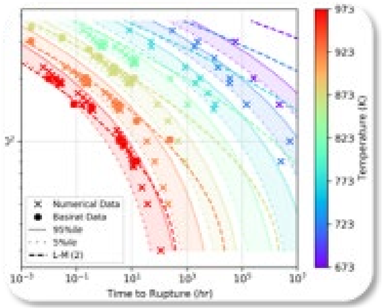


Mechanistic model can simulate 10 years of creep behavior in ~5 hours



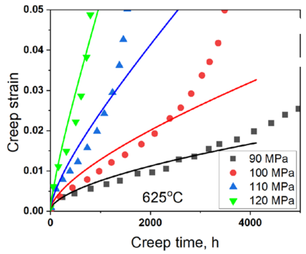


Simulate cyclical loading



Accurately predict creep life from a limited number of short-term

Models for the oxidation within a multi-phase multi-component framework.



Framework for predicting the performance of welds

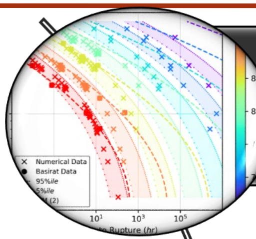
eXtremeMAT: original objectives

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

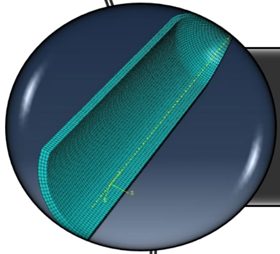
Applications to: conventional austenitic (**347H**, 316H) and ferritic steels (**P91**), XMAT X351..

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

Impact: Reduce the time and cost for alloy qualification and certification.

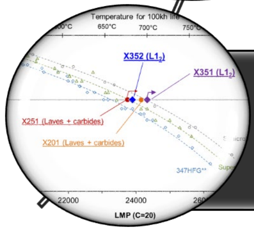


Material lifetime assessment models



Integrated constitutive models

Materials database and analysis tools



Guidelines for the discovery of new alumina forming alloys

Microstructure and composition-aware constitutive model can be used to reduce uncertainty in materials performance

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Lifetime predictors: state of the art

a. No account for the materials' microstructure.
b. Effect of composition (B)
c. Cannot be used for extrapolation
d. No account for multiaxial loading effects..

$$P_{LM}(\sigma) = [C_{LM} + \log_{10}(t_R)]T$$

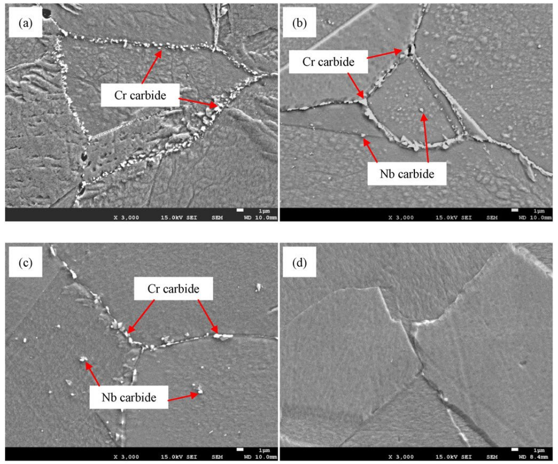
(Larson Miller law)

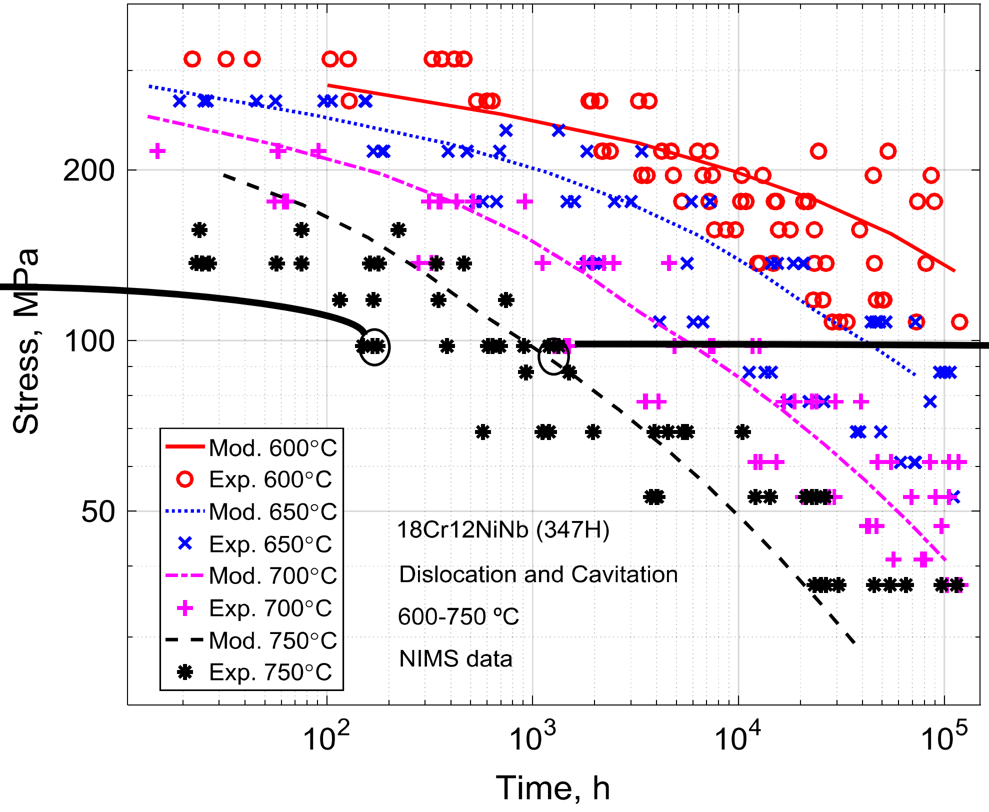
P_{LM}: stress function
C_{LM}: constant
σ: effective stress
T: temperature
t_R: time to rupture

Uncertainty associated with performance of metals:

Model form
Parametric
Epistemic (composition, microstructure).
Experimental conditions

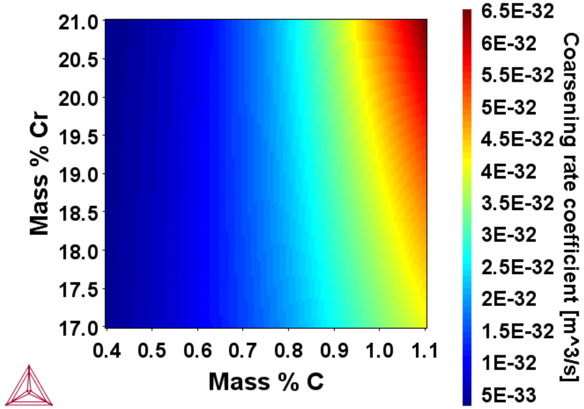
Microstructure?





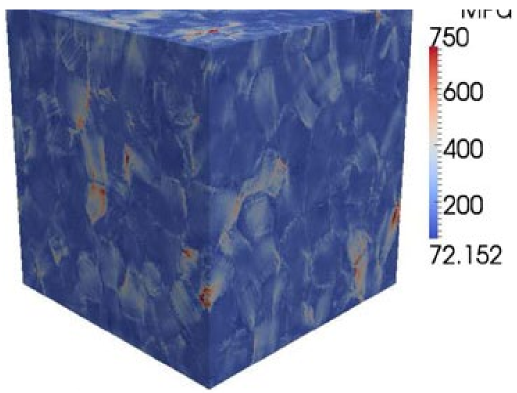
Composition?

(Nb,Cr)C coarsening rate as a function of [C] and [Cr] - steel 347H



Mechanistic models can be used to relate composition, microstructure and creep response

A polycrystal model for the creep response of austenitic and ferritic steels can be used to assess the effects of microstructure on performance



(b) Von mises effective stress

Classical Norton-Bailey model, $\dot{\boldsymbol{\varepsilon}}^{ss} = A \exp\left(-\frac{Q}{kT}\right) \sigma^n$

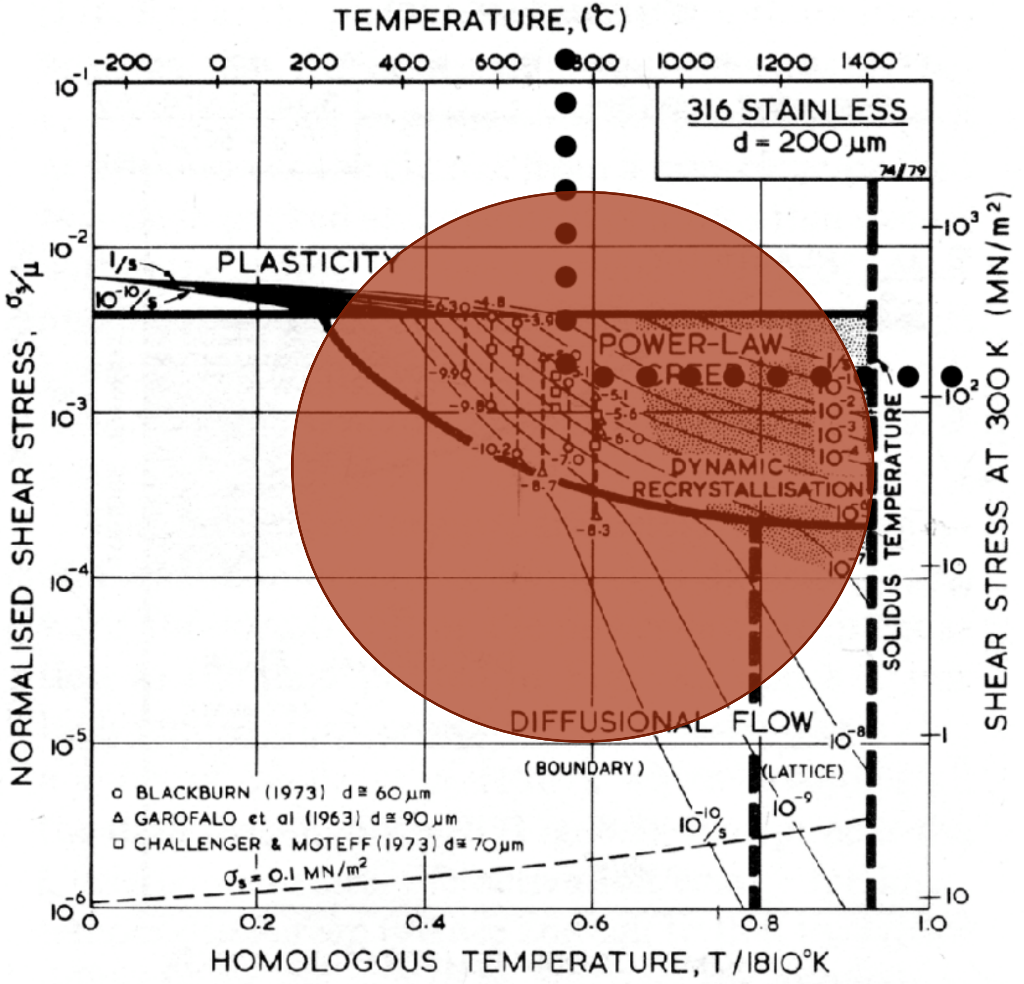
Modified BMD model: $\dot{\epsilon}^{ss} = \frac{DEb}{kT}\left(\frac{\sigma - \sigma^{th}}{E}\right)^n \left(\frac{b}{d}\right)^p$

G. Potirniche et al., NEUP project 09-835, final report (2009)

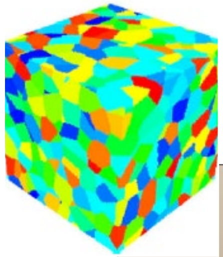
Creep model accounts solutes and precipitates

$$\dot{\epsilon}^{ss} = \frac{\pi \Omega k T}{(\alpha G M)^2} \sigma^3 \left(A(\sigma - \sigma_P)^2 + B(\sigma - \sigma_P) + C\right) \times \left[\frac{D_{sol} D_L}{2\pi c_0 \ln\left(\frac{r_2}{r_1}\right) D_L + (bkT)^2 \ln\left(\frac{c^*}{c_0}\right) D_{sol}}\right]$$

Fernandez et al., Advanced Engg Mater, 22 (2020) 1901355

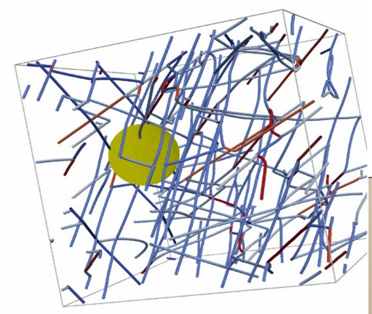


Scientific gaps in relating microstructure composition and performance



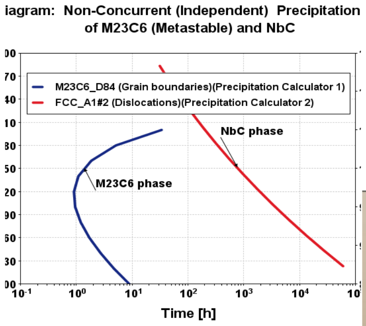
Plasticity

- Dislocation glide
- *Solute vs precipitate strengthening*
- Dislocation climb
- *Vacancy mediated*



Damage

- *Cavity nucleation*
- Cavity growth
- Cavity coalescence



Aging

- *Second phase evolution*
- *Effect on plastic response and damage*

Effects of **microstructure** (grain size, texture, precipitates, dislocation content,solutes), **stress** (3D, time evolution), **temperature** (time evolution) on material performance

eXtremeMAT's experimental and computational framework aims to bridge the gap between fundamental materials science and outstanding engineering challenges

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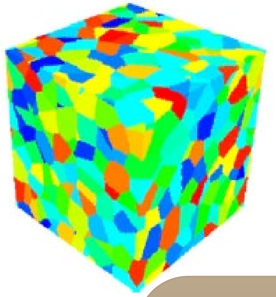
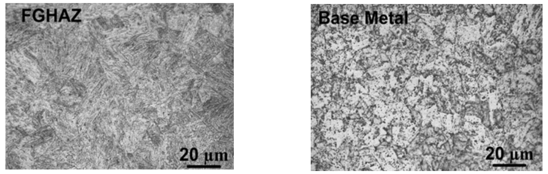
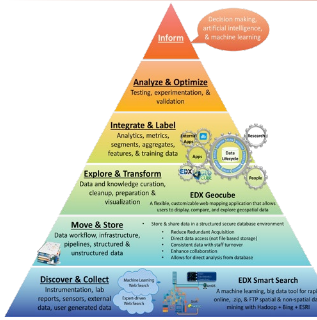


Polycrystal simulations (VPSC, EVP-FFT)

Mechanical tests and microstructure characterization, making new materials

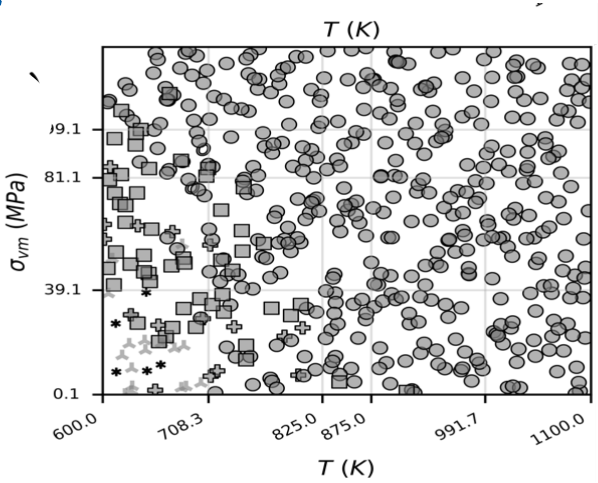


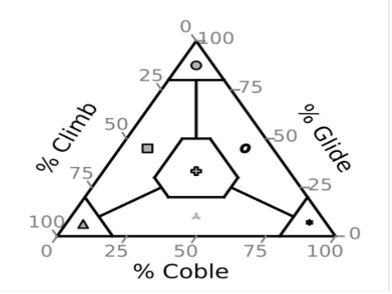
Pandey et al., Arch Civil Mech Eng, 19 (2019) 297-310



Database generation

Surrogate r

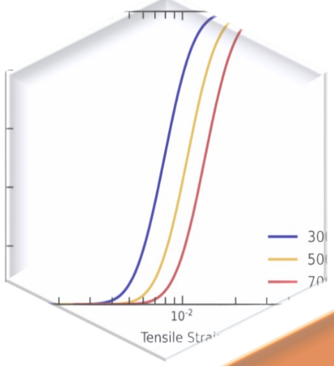




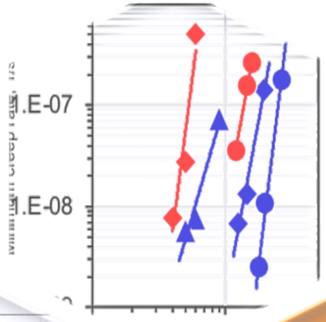
$$\dot{\varepsilon}_{vm}(\bar{\rho}_{cell}, \bar{\rho}_w, \varepsilon_{vm}$$

$$\sum_{c,w,\varepsilon,\sigma,T,\varphi=0}^{degree} \alpha_{cw\varepsilon\sigma T\varphi} P_c(\bar{\rho}_{cell}) P_w($$

Scientific advances allowing to relate microstructure, composition and performance



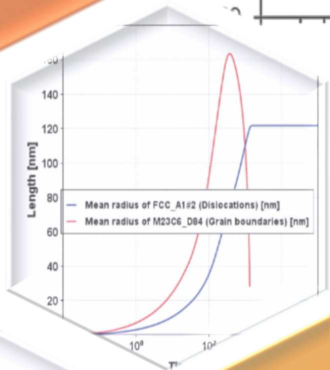
Cavity nucleation model: mechanism and microstructure sensitivity



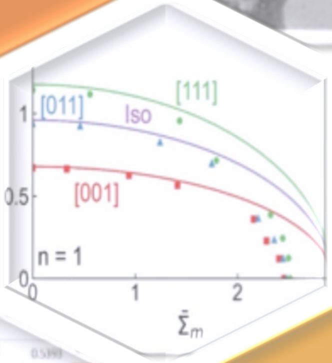
Processed and characterized 12 alloys

Characterized precipitate formation during anneal as a function of composition

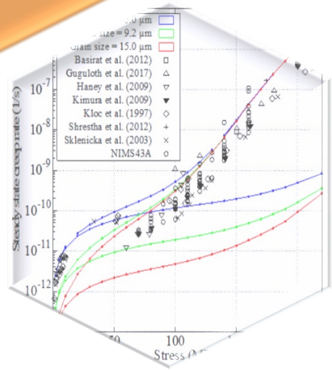
Predicted the kinetics of concurrent precipitation and dissolution from DFT and TC-Prisma

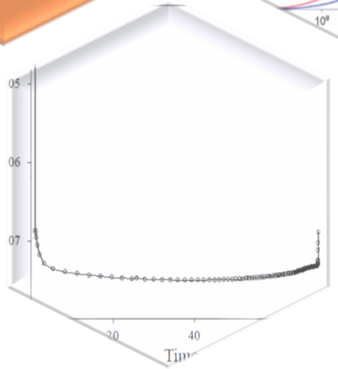


Cavity growth: growth rate under viscoplastic flow

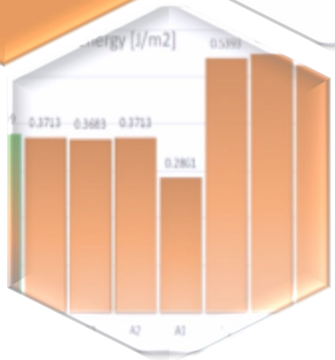


Quantified the role of microstructure onm the steady primary and secondary creep response of Gr91





3D model predicting the primary secondary and tertiary creep response of BCC and FCC steels



Quantified on the basis of DFT the role of trace elements

eXtremeMAT's tools help bridge the gap between materials science and engineering designs

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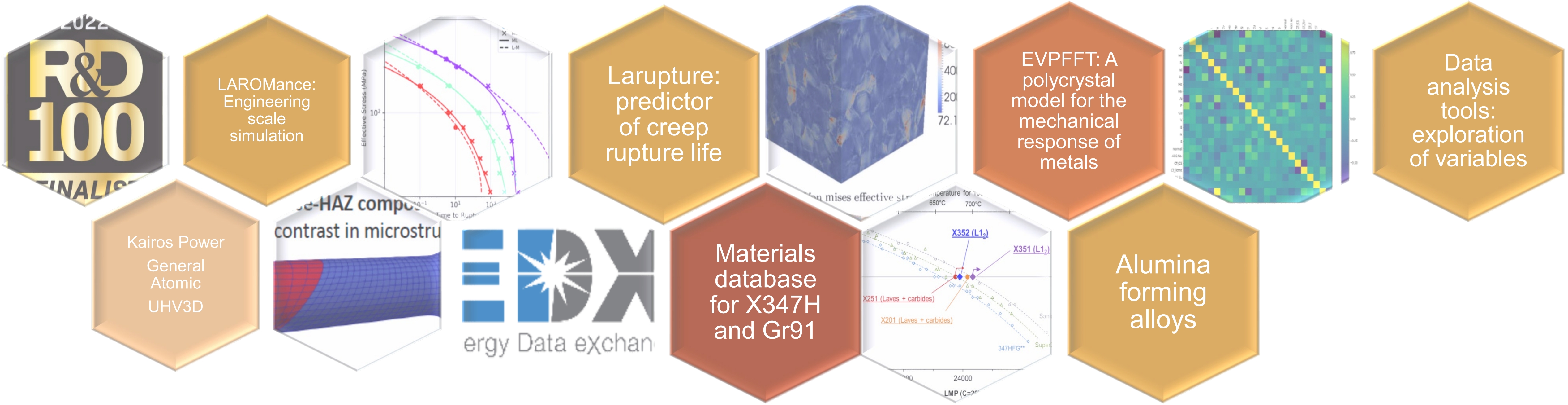
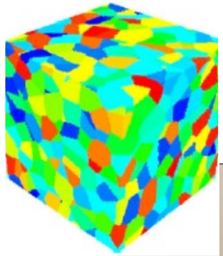


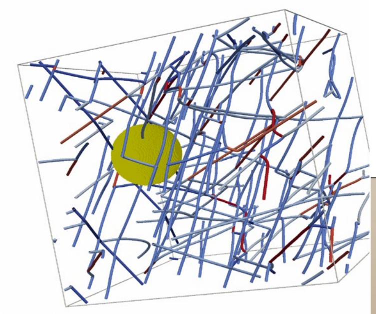
https://www.youtube.com/watch?v=Y1A8ZiPQ5no

Scientific gaps in relating microstructure composition and performance



Plasticity

- Dislocation glide
- *Solute vs precipitate strengthening*
- Dislocation climb
- *Vacancy mediated*



Damage

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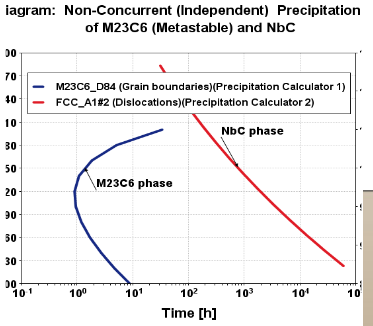
- Cavity growth
- Cavity coalescence



Aging

- *Second phase evolution*
- *Effect on plastic response and damage*

Effects of **microstructure** (grain size, texture, precipitates, dislocation content,solutes), **stress** (3D, time evolution), **temperature** (time evolution) on material performance

ExtremeMAT proposed the first comprehensive model that captures the coupling between all diffusive mechanisms as a function of microstructure

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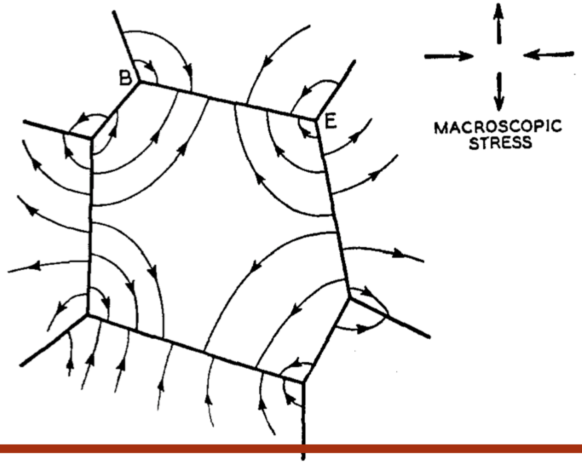
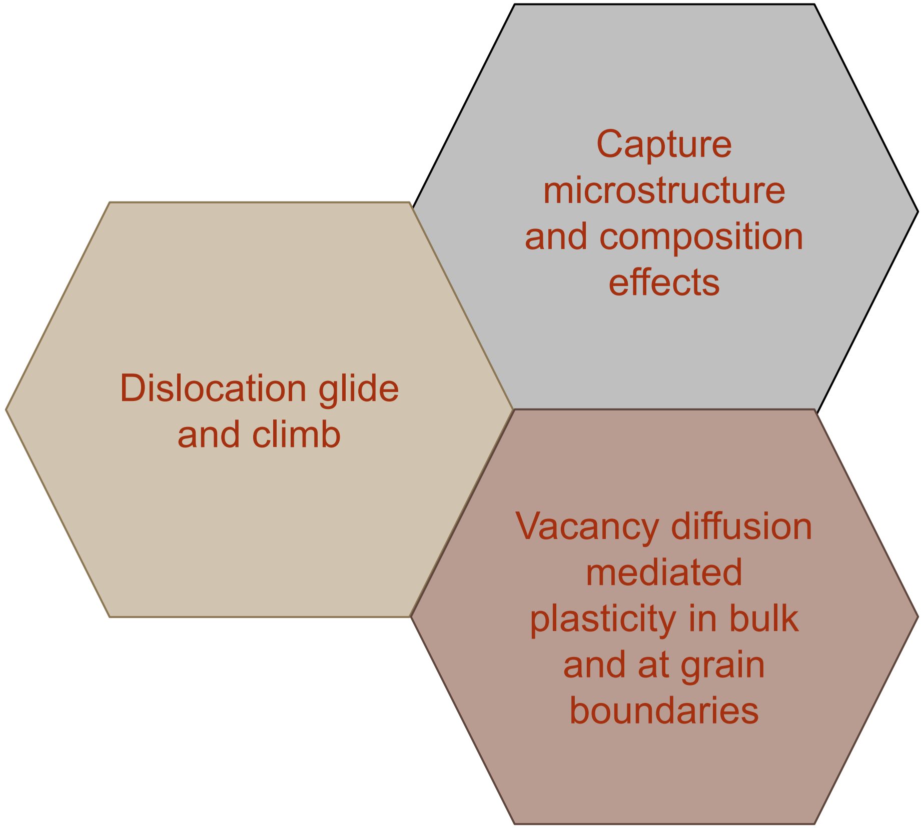
Current models for vacancy mediated plasticity

- No consideration of vacancy field evolution thereby neglecting local effects.
- No Coupling with dislocation climb (i.e. no effects of initial dislocation content due to processing).
- No relation with damage.



$$\dot{\varepsilon}_{NH}^{diff} = \frac{A D_{bulk} \Omega_0 \sigma}{k d^2 T}$$

ExtremeMAT's approach:
Chemo-mechanical plasticity solver



Multi-national laboratory consortium

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ExtremeMAT proposed the first comprehensive chemo-mechanical model that captures the coupling between all diffusive mechanisms as a function of microstructure

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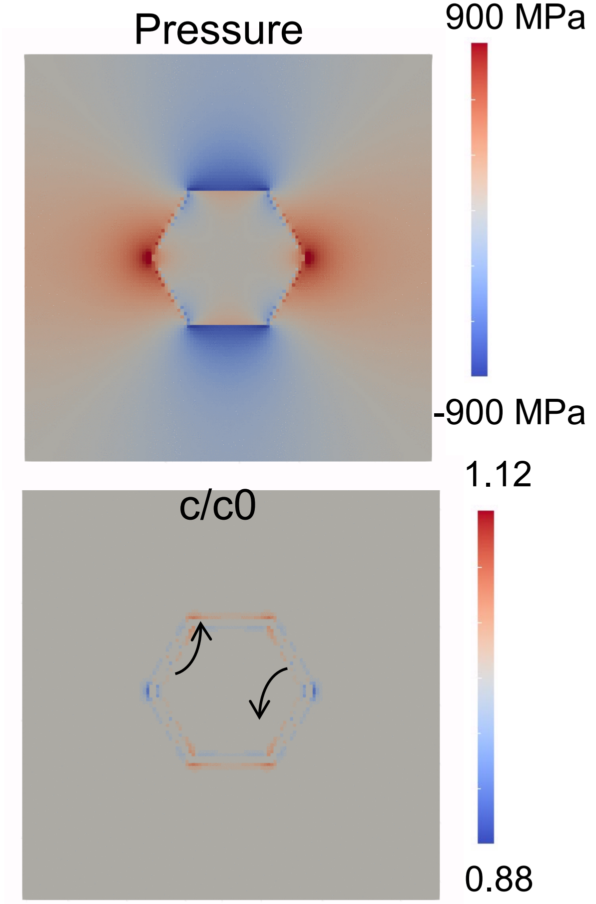
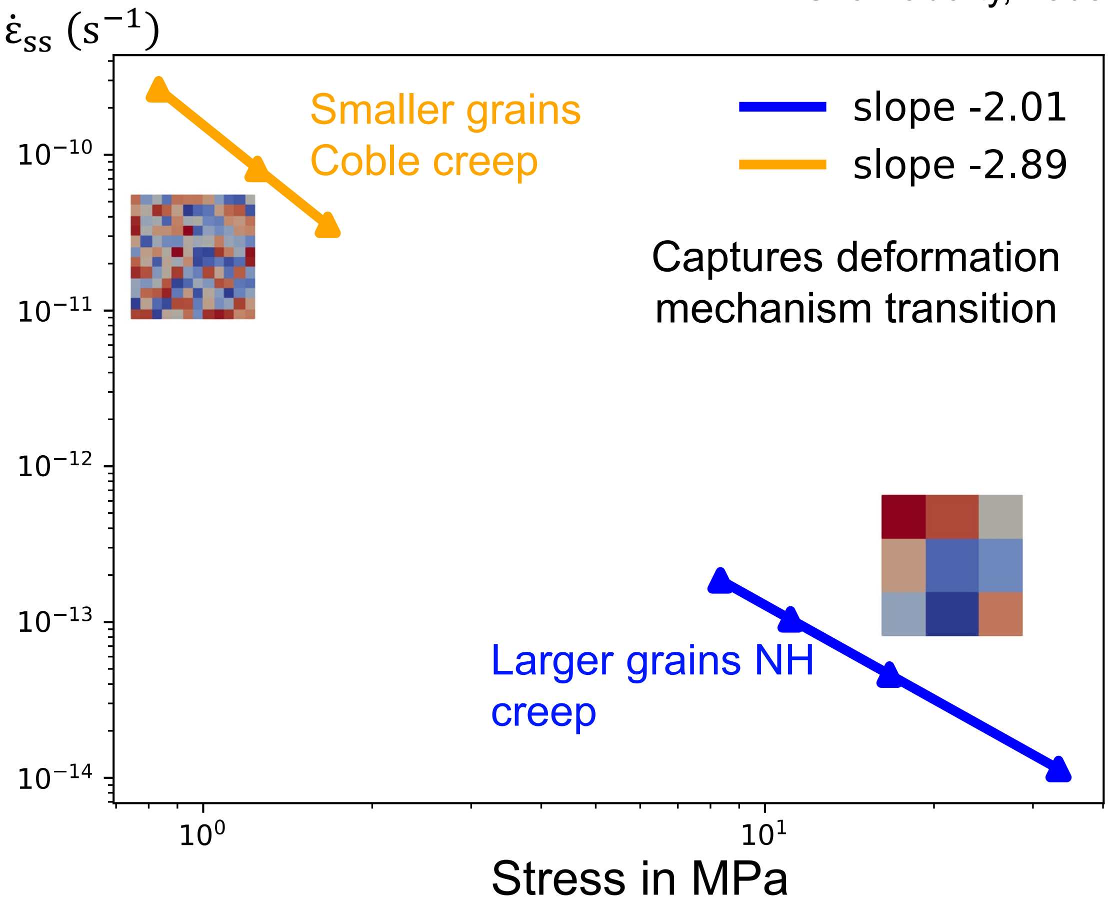
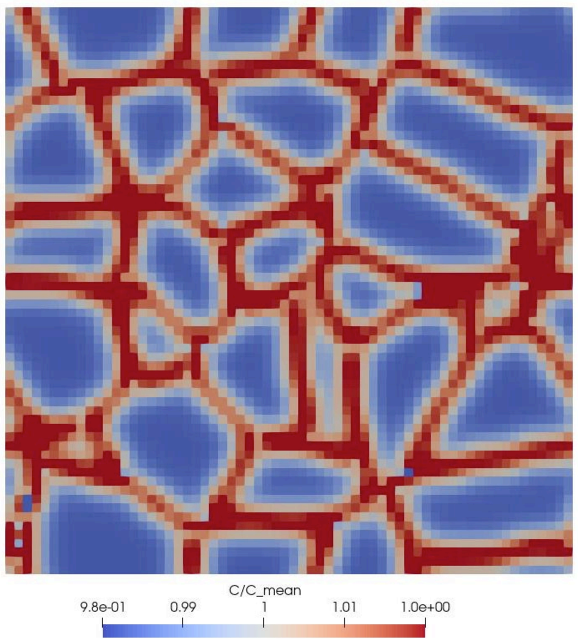
Chakraborty, Lebensohn, Capolungo, submitted to JMPS 2022



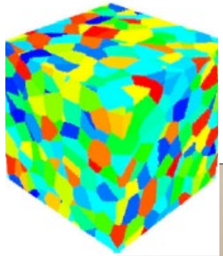
Captures kinetics of vacancy flow





Can possibly predict damage nucleation sites

Scientific gaps in relating microstructure composition and performance



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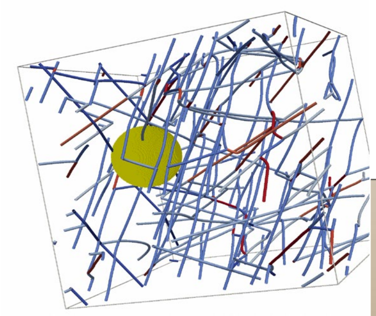

Damage

- *Cavity nucleation*
- Cavity growth
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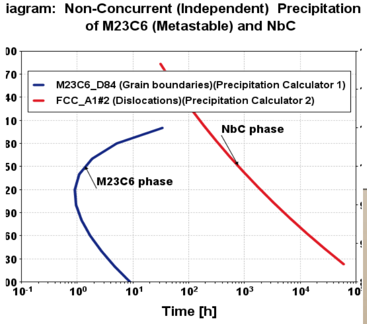

Aging

- *Second phase evolution*
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Effects of **microstructure** (grain size, texture, precipitates, dislocation content,solutes), **stress** (3D, time evolution), **temperature** (time evolution) on material performance

ExtremeMAT proposed the first comprehensive model that predicts cavity nucleation as a function of local microstructure state

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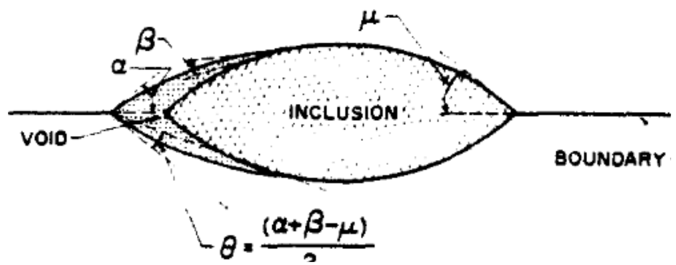
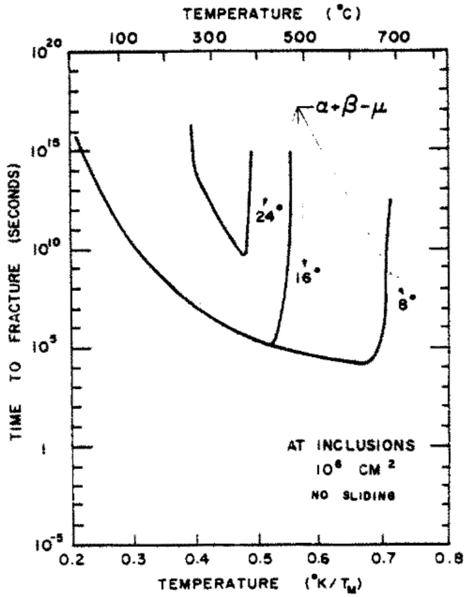
Most models for cavity nucleation rely on grain boundary sliding

- **Cannot explain cavities on boundaries normal to the tensile axis (which are common) or in alloys which are stabilized against sliding**
- **For this reason, empirical models are usually used instead**



(e) The time-to-rupture curves have been obtained for the case when a polycrystal is deformed at a constant strain-rate at different temperatures. When no sliding of the boundaries is allowed then void nucleation is possible only when interface energies are comparable to the total surface energy of the void being created. These conditions may be met at non-wetting or almost non-wetting inclusions.



Empirical models

For void nucleation, the criterion from Chu and Needleman is used:

$$\dot{\tilde{n}}_{0\to a} = F_\varepsilon(\boldsymbol{\varepsilon}^p)\dot{\varepsilon}^{p}_{eq}$$

} Assumption: Voids nucleate by a distribution of local strain

With,

$$F_\varepsilon(\boldsymbol{\varepsilon}^p) = \frac{\dot{n}_{sat}}{\sqrt{2\pi V_\varepsilon}} \exp\left(\frac{-(\varepsilon^p_{eq} - \varepsilon_c)^2}{2V_\varepsilon}\right)$$

$\dot{n}_{sat}$: saturation number density of voids
ε_c : is the mean critical magnitude for nucleation strain
V_ε: statistical variance in critical nucleation strain and stress

R Raj and MF Ashby, Acta Metallurgica 23 (1975) 653

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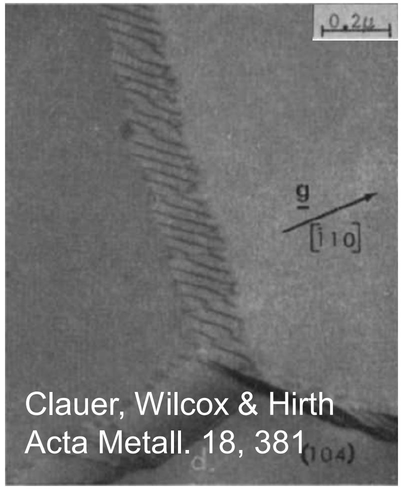
Analytical Models

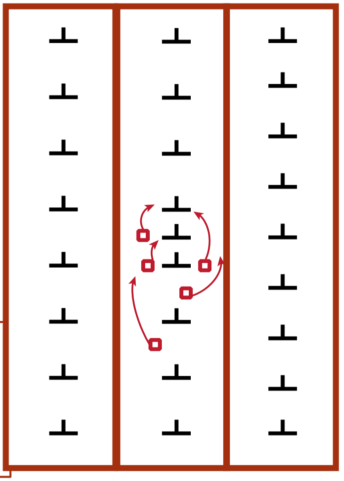


Clauer, Wilcox & Hirth
Acta Metall. 18, 381

TEM micrograph of tilt wall formed during creep

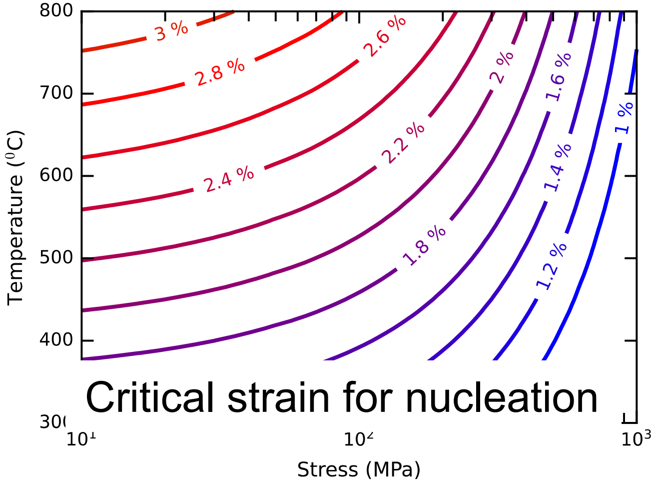
Calculate vacancy supersaturations generated when dislocations are added to the creep sub-structure

Vacancies emitted to equilibrate array when new dislocations are added



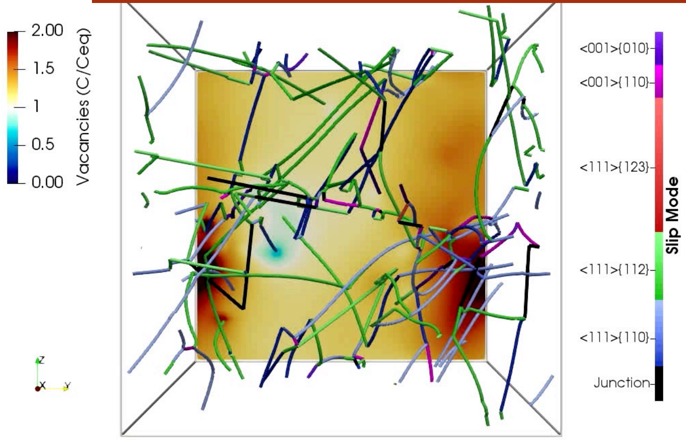
-Vacancy density in the sub-structure increases with strain

-Sufficient to nucleate cavities past ~1-2% strain



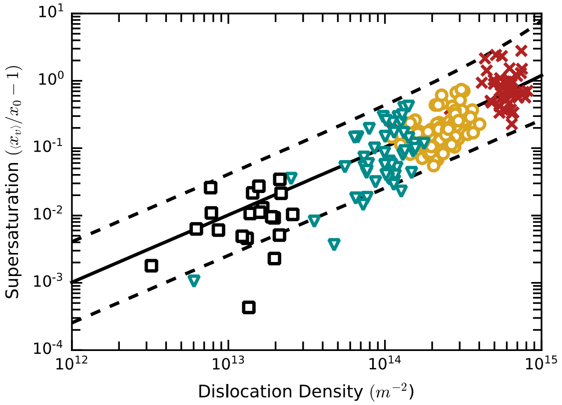
Vacancy supersaturations in dense regions of the substructure lead to cavity formation even at low stress

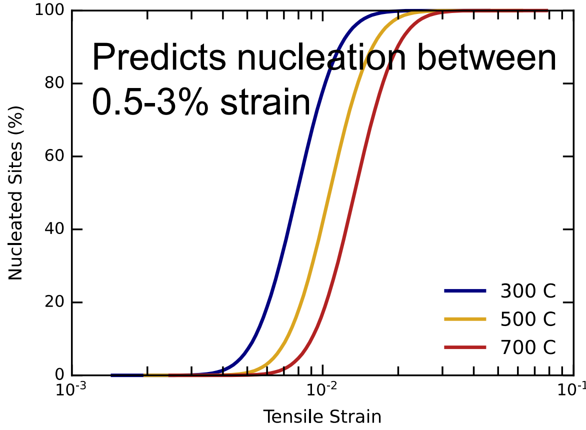
DDD Simulations



Vacancy concentration around a dislocation network

Supersaturation as a function of dislocation density





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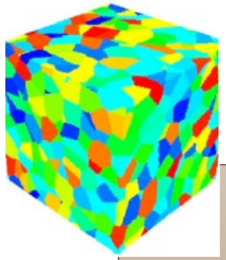
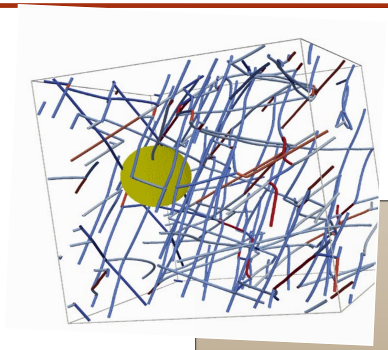
Scientific gaps in relating microstructure composition and performance



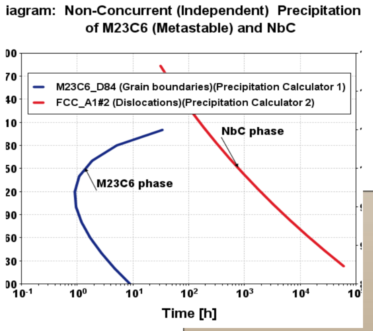
Plasticity

- Dislocation glide
- *Solute vs precipitate strengthening*
- Dislocation climb
- *Vacancy mediated*



Damage

- *Cavity nucleation*
- Cavity growth
- Cavity coalescence



Aging

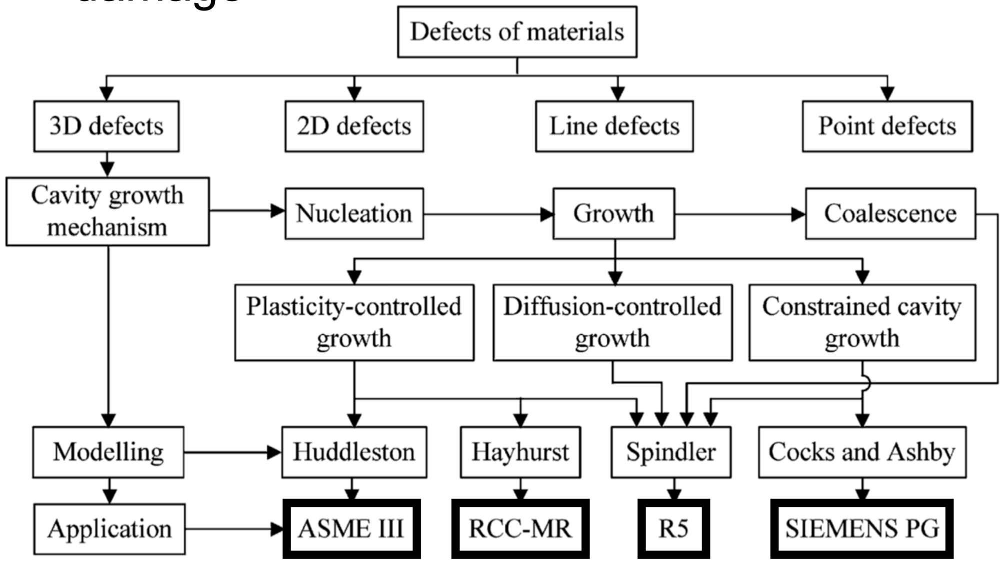
- *Second phase evolution*
- *Effect on plastic response and damage*

Effects of **microstructure** (grain size, texture, precipitates, dislocation content,solutes), **stress** (3D, time evolution), **temperature** (time evolution) on material performance

ExtremeMAT proposed the first mechanistic tertiary creep damage model sensitive to microstructure and to crystal structure.

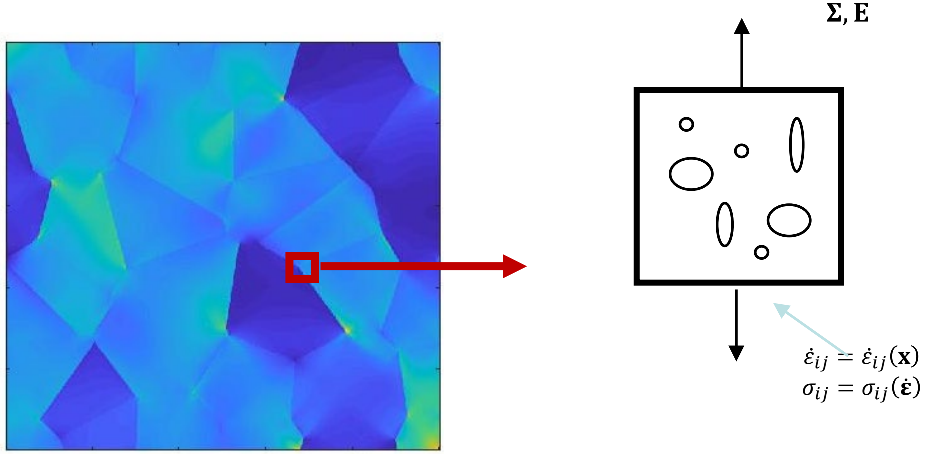
Current damage evolution models are:

- Empirical (e.g. Chaboche) or limited to macroscale with isotropic plastic response
- Independent of microstructure
- Do not account for all modes of growth of damage



eXtremeMAT:

Mechanistic model for damage growth mediated by all likely deformation modes



CP-glide

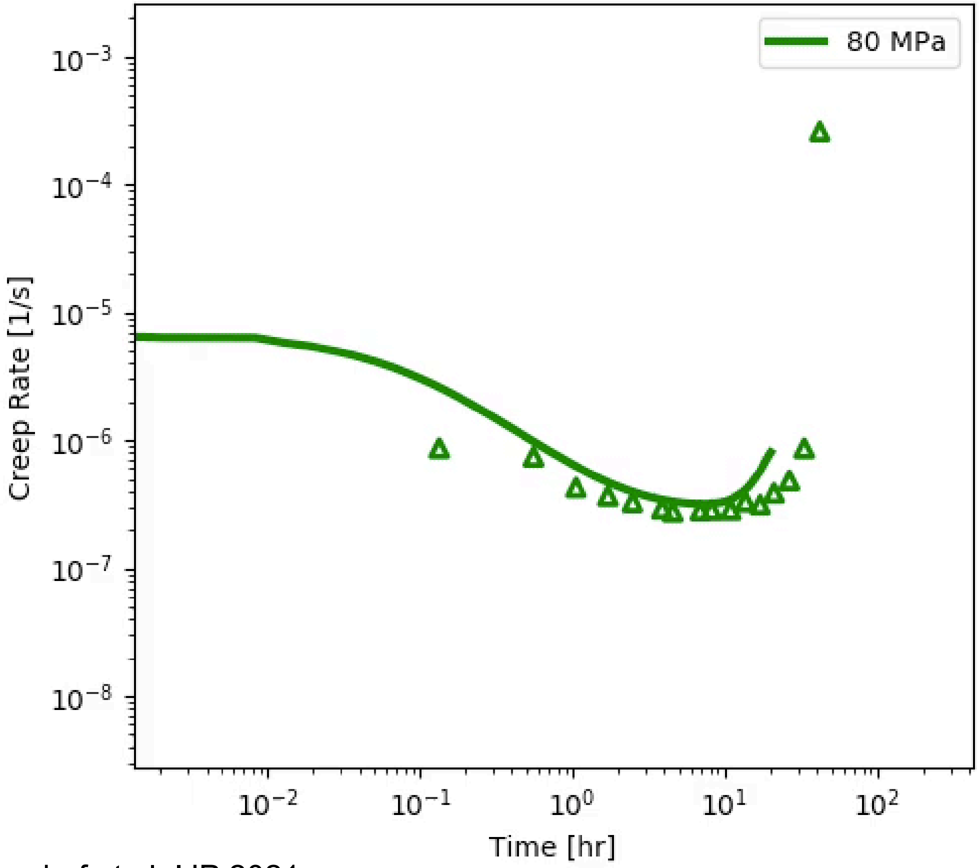
$$\Psi^s = \frac{\dot\epsilon_0\sigma_0}{n+1}\left(\frac{|\Lambda^s|}{\sigma_0}\right)^{n+1}$$

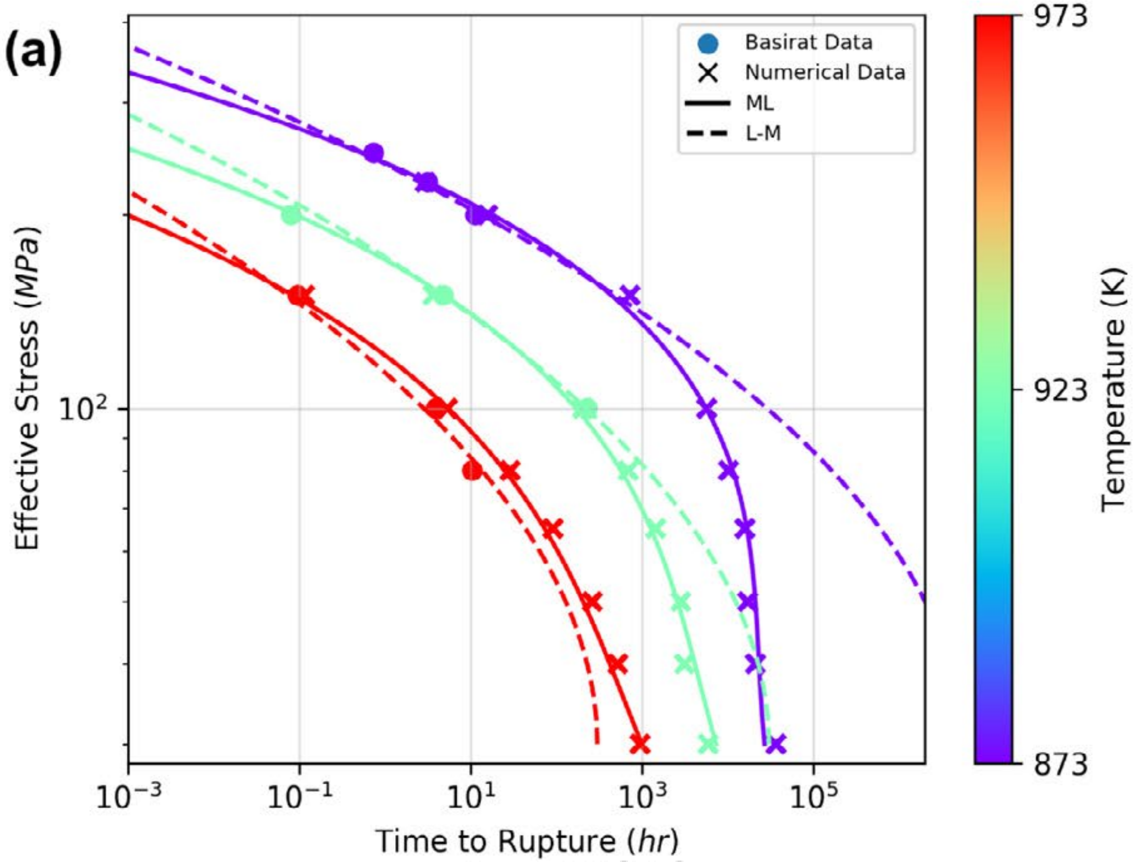
$$\dot\varepsilon_i = \sum_{s=1}^{S} \frac{\partial\Psi^s}{\partial\sigma_i} = \frac{\partial\Psi^s}{\partial\Lambda^s}\frac{\partial\Lambda^s}{\partial\sigma_i} = \sum_{s=1}^{S} \underbrace{\dot\gamma_0^s\left(\frac{|\Lambda^s|}{\sigma_0}\right)^{n} \mathrm{sign}(\Lambda^s)}_{\text{magnitude}}\underbrace{\frac{\partial\Lambda^s}{\partial\sigma_i}}_{\text{direction}}$$

$$Q^s = \left(\frac{\tau^s}{\Lambda^s}\right)^2$$

ExtremeMAT proposed the first mechanistic tertiary creep damage model sensitive to microstructure

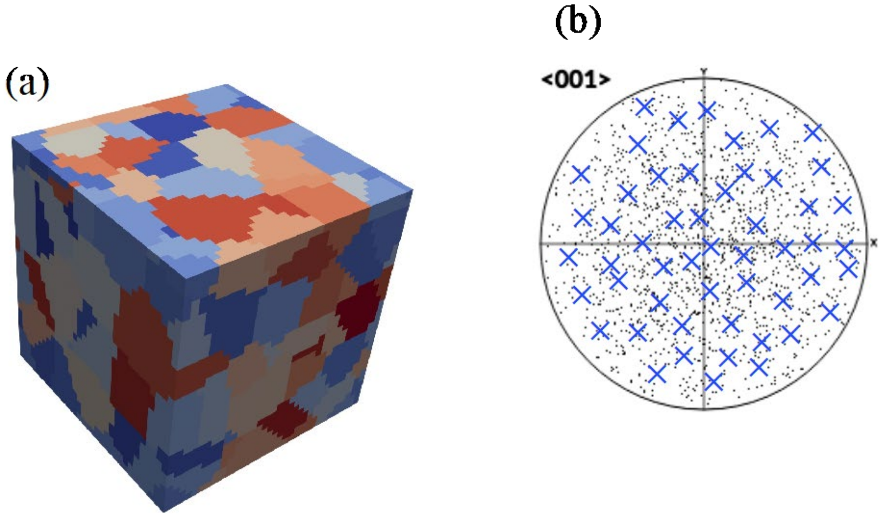
Temperature = 973 K
Stress = 80 MPa



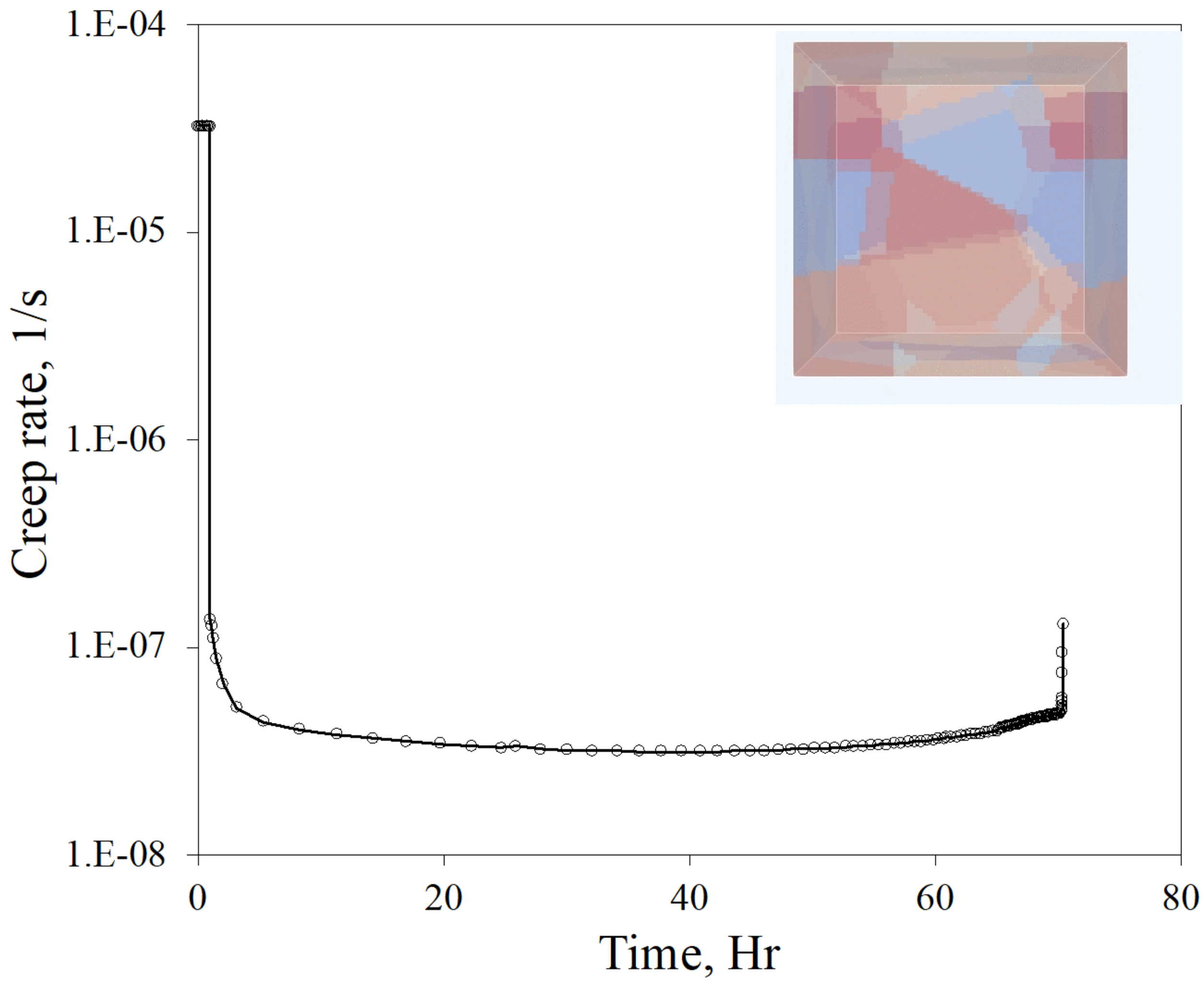


(*) N. Bieberdorf et al. IJP 2021.

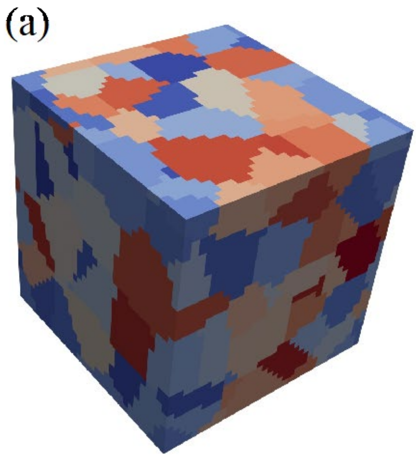
3D EVPFFT application

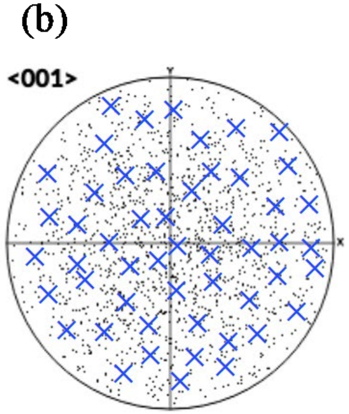


- Polycrystal simulation of the mechanical response of Gr91
- 50 Grains
- 64x64x64 Fourier grid

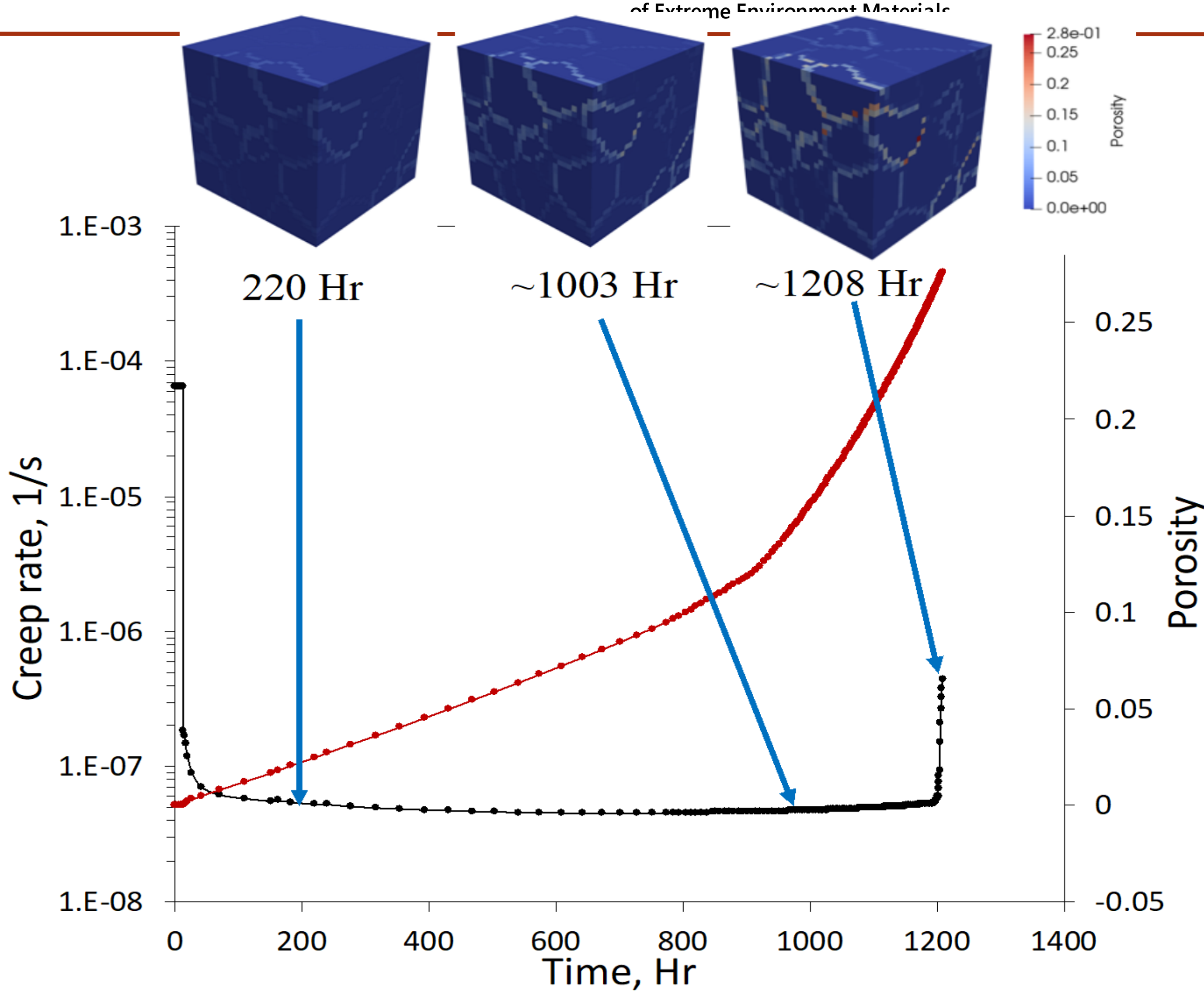


3D EVPFFT application



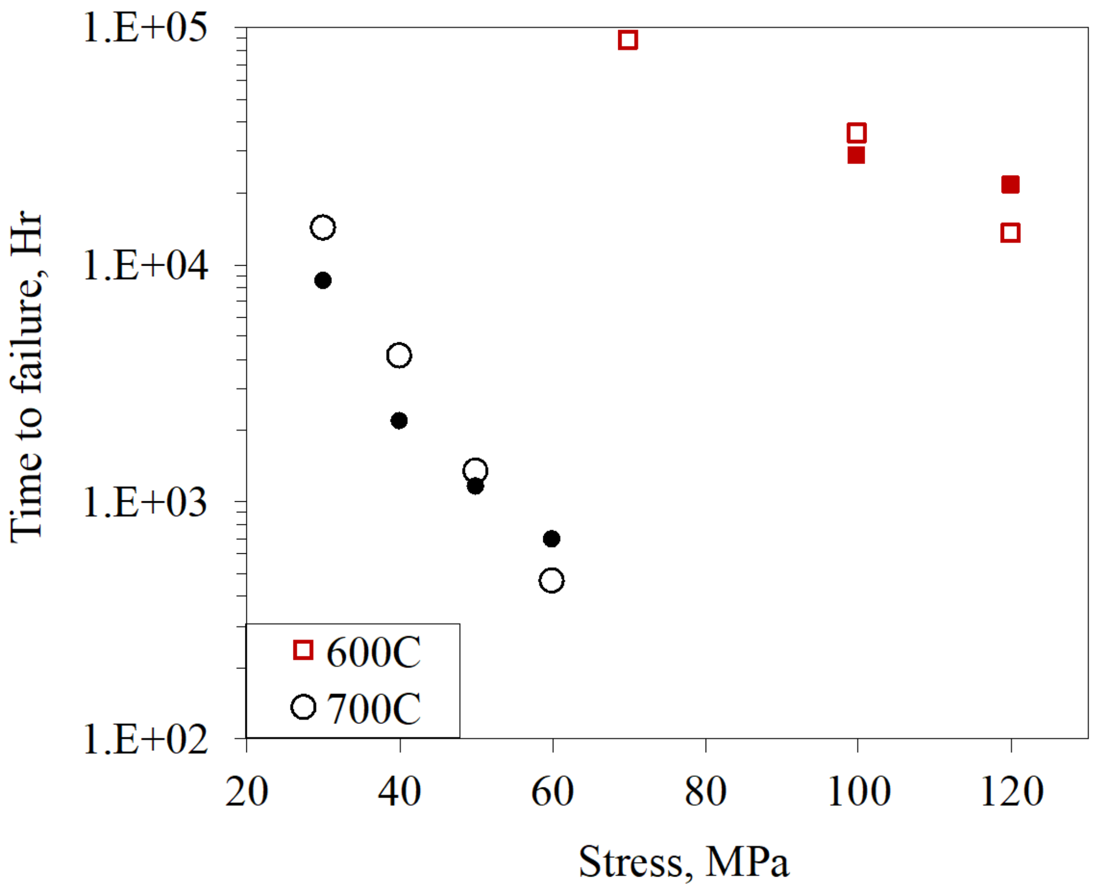


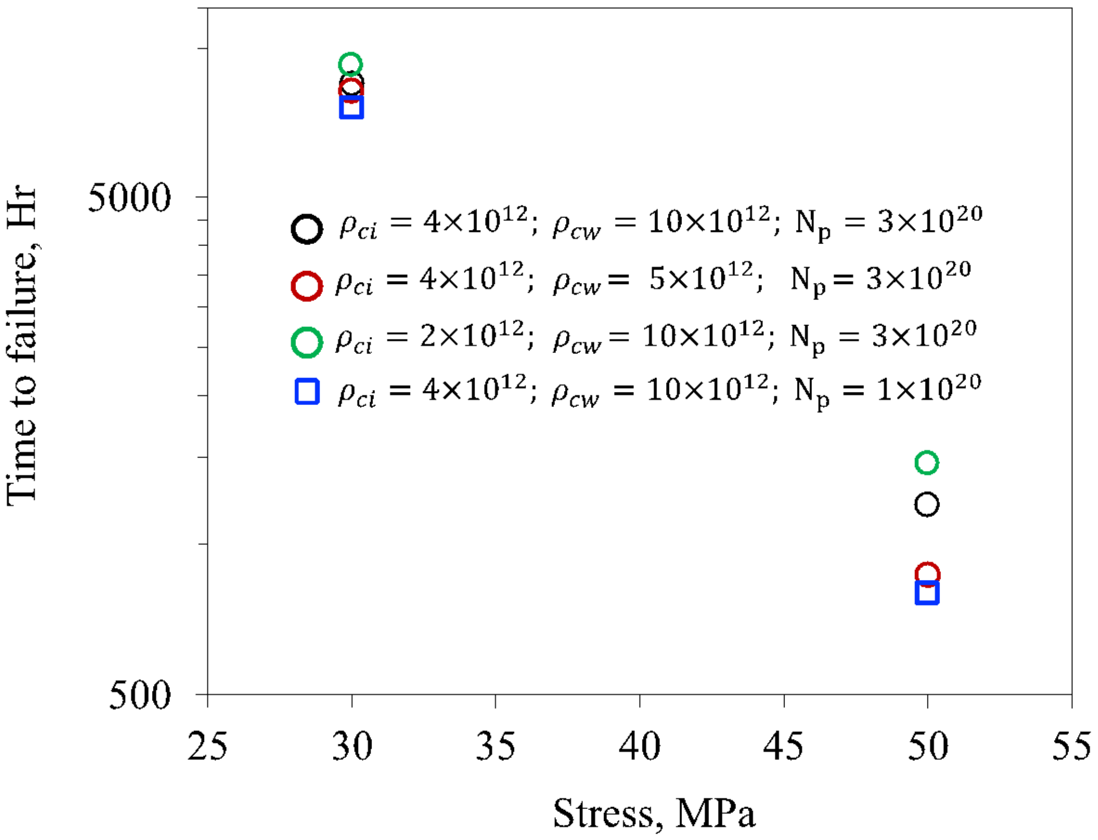
- Polycrystal simulation of the mechanical response of Gr91 subjected to creep loading at 700K
- 50 Grains
- 64x64x64 Fourier grid



ExtremeMAT proposed the first mechanistic tertiary creep damage model sensitive to microstructure: 3D EVPFFT application

Open symbols: Experiment; Filled symbols: Model

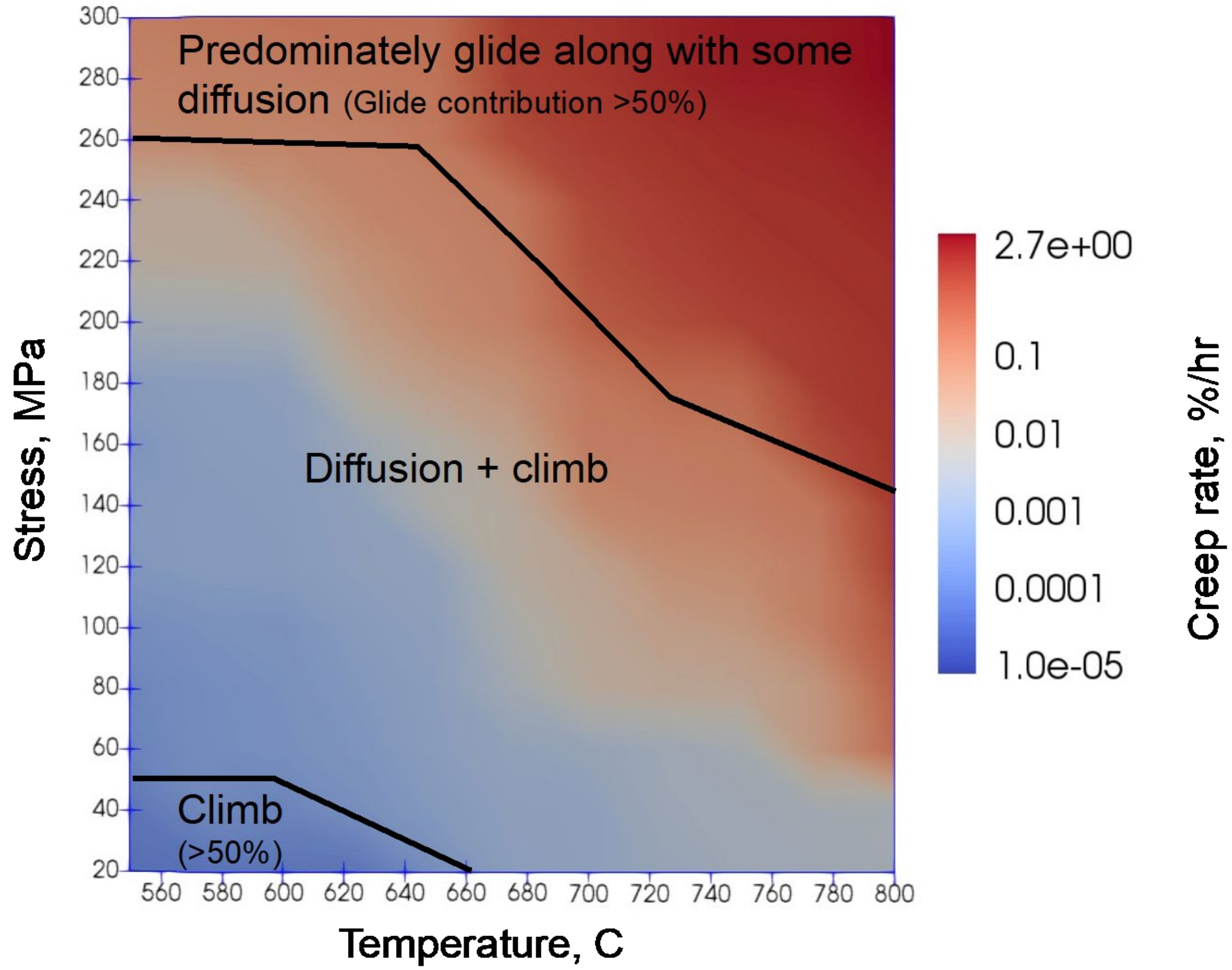


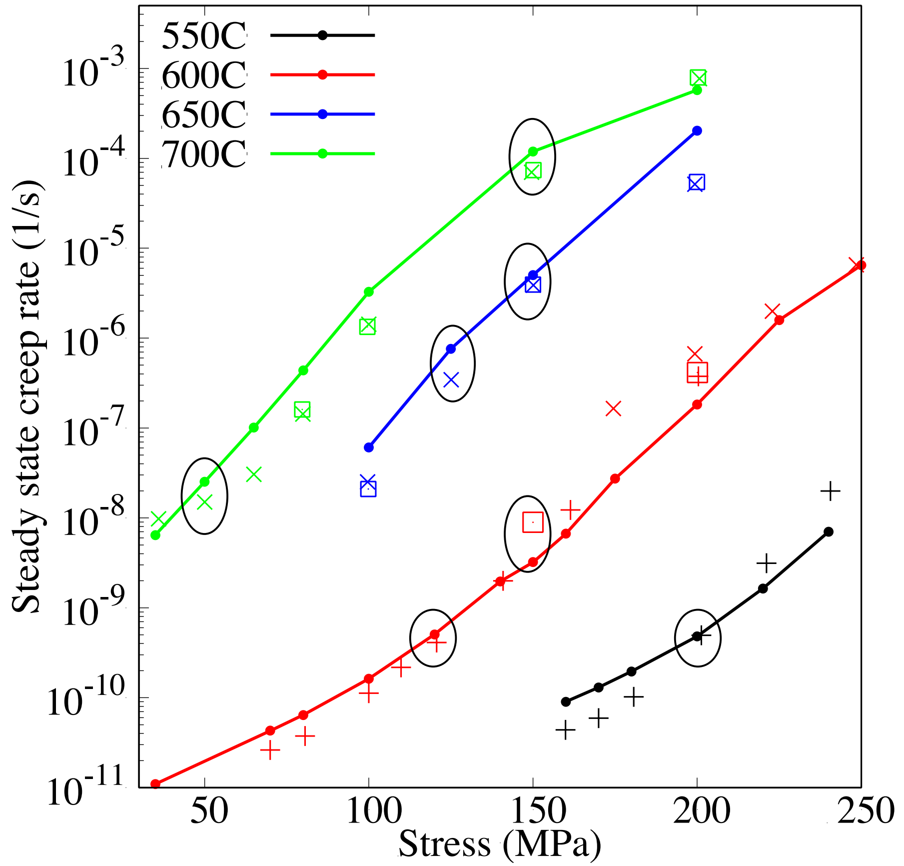


ExtremeMAT's model can predict how the time to rupture in arbitrary loading scenarios is affected by stress, temperature and microstructure

Quantifying the effects of microstructure on plastic response

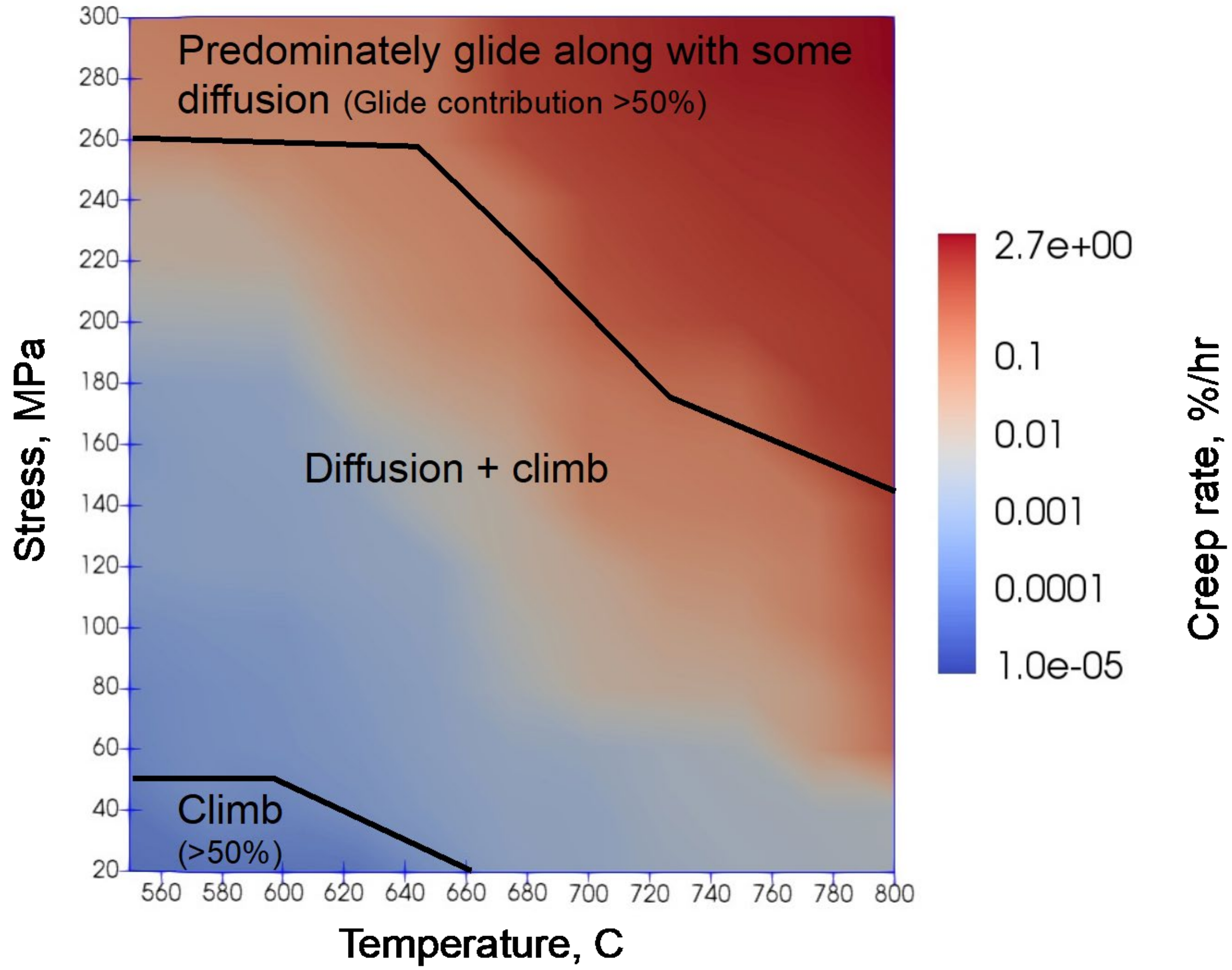
Quantifying the effects of microstructure on plastic response

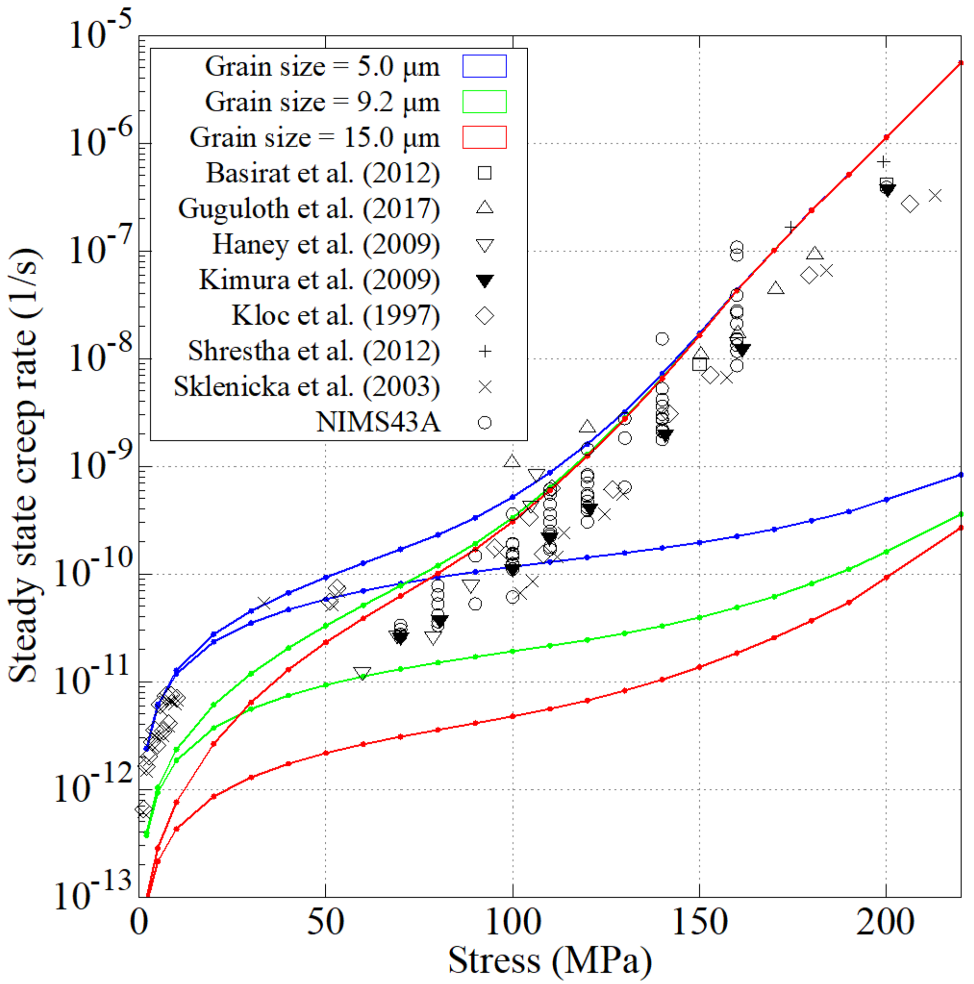




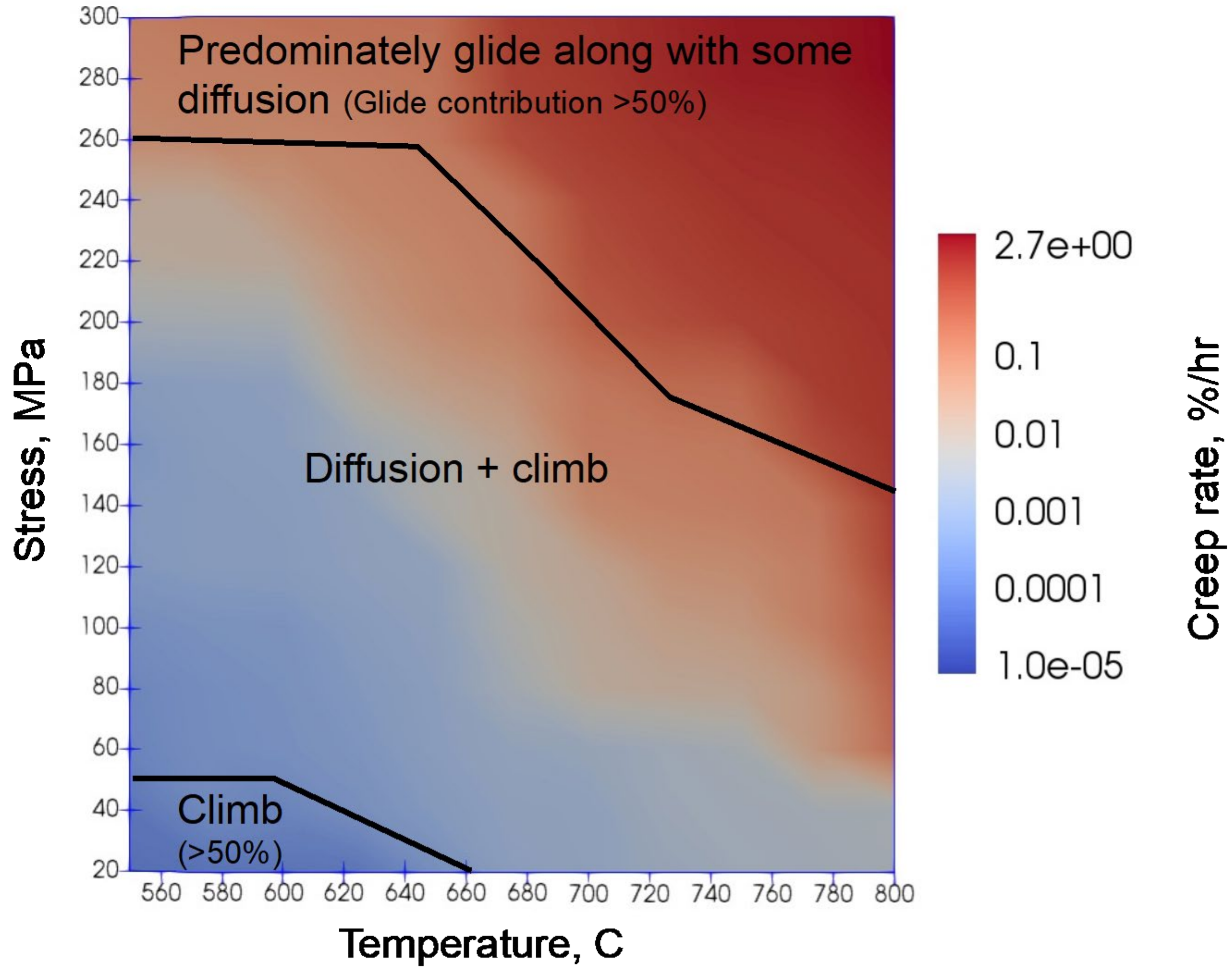
□: Basirat et al. (2012) ×: Shrestha et al. (2012)
+: Kimura et al. (2009) –●–: Model

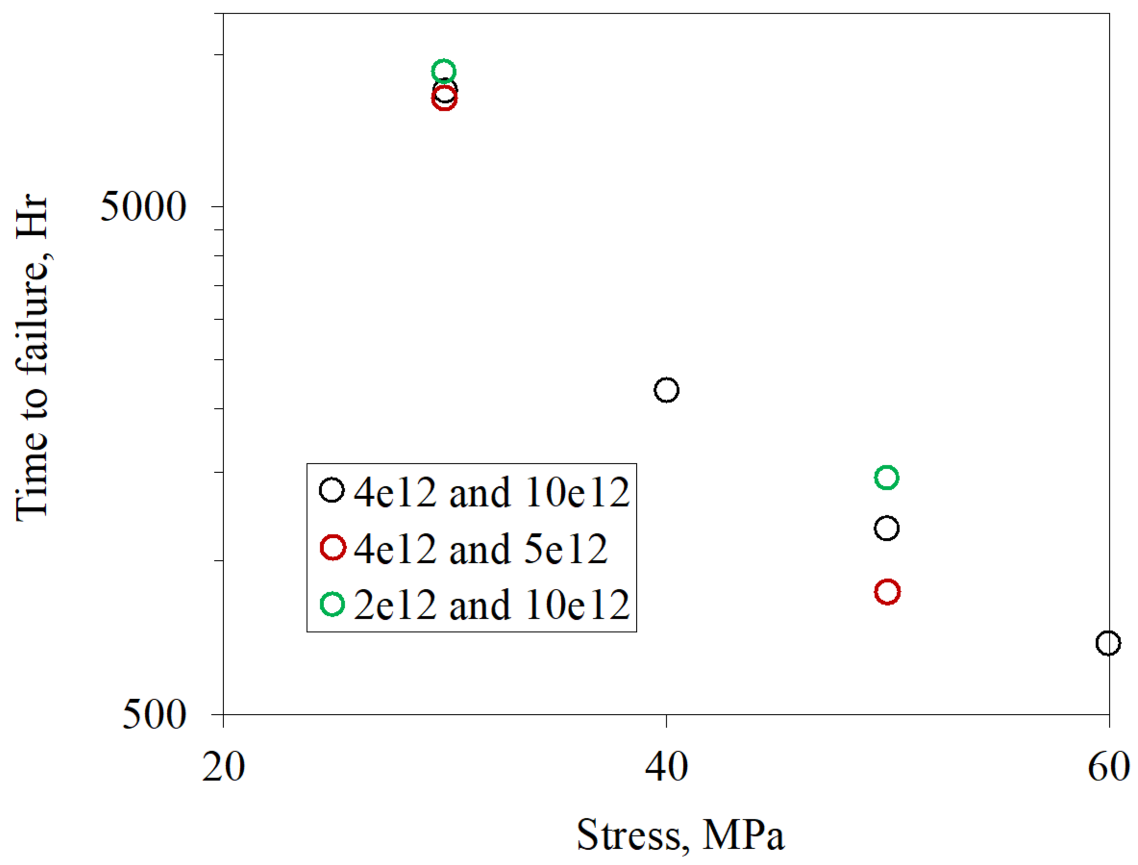
Quantifying the effects of microstructure on plastic response





Quantifying the effects of microstructure on plastic response





Quantifying the effects of aging on materials response and proposing routes for material design

Precipitate strengthening

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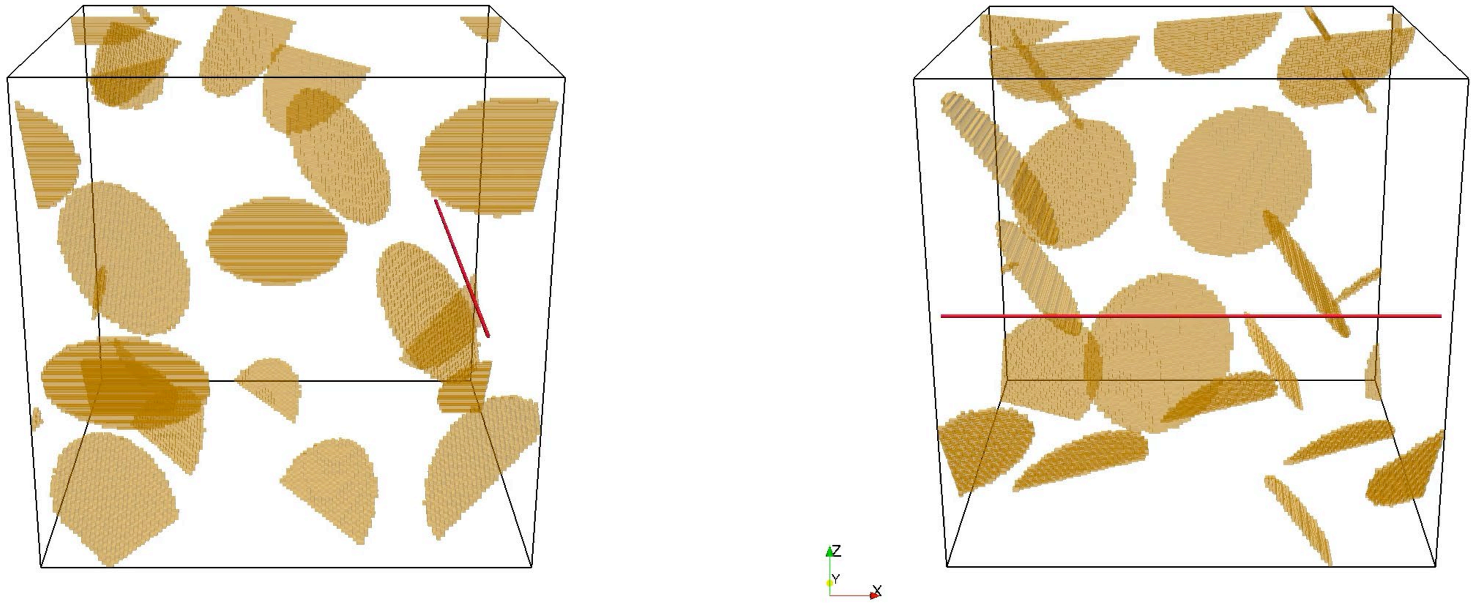

Precipitates are overwhelmingly seen as strengtheners

R. Santos-Guemes et al. JMPS 2021

Dispersed Barrier Hardening: based on mean spacing between defects.

$$\Delta\sigma = \alpha\mu b\sqrt{Nd}$$

Friedel-Kroupa-Hirsch:
based on elastic interactions between SIA loops and straight dislocations.

$$\Delta\sigma = \alpha\frac{\mu b^{0} R N^{\frac{3}{2}}}{8}$$

Bacon-Kocks-Scattergood: based on random array of spherical obstacles.
Includes elastic self-interaction.

$$\Delta\sigma = \alpha\frac{\mu b}{2\pi L}\left[\ln\left(\frac{L}{b}\right)\right]^{1/2}\left[\ln\left(\frac{d'}{b}\right)+0.7\right]^{3/2}$$

Processing, aging and testing different grades of 347H steels to separate solute vs strengthening and trace elements effects

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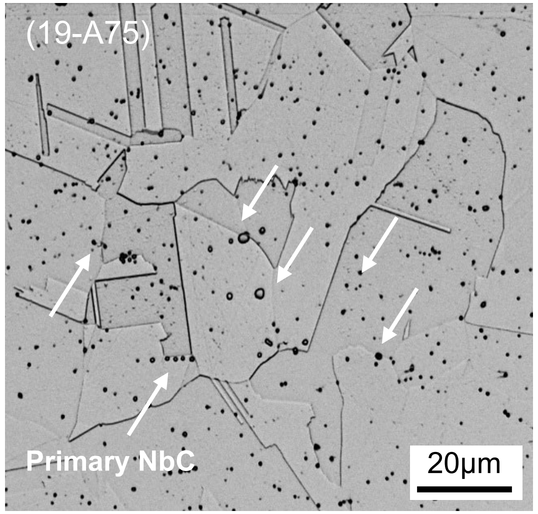
A 347H plate delivered



As-received microstructure (OM)

Heat ID	Alloy name	Analyzed chemistry, wt.% (B and N: wppm)								Remarks
		C	Cr	Mn	Nb	Ni	Si	B	N	
19-A75	347H	0.0508	18.52	0.98	0.39	11.03	0.5	<5	22	High purity, creep tested at ORNL
19-A92	347H	0.0561	18.23	0.91	0.52	10.92	0.44	<5	56	High purity, for tube creep tests
20-A2	347H	0.0541	18.72	0.98	0.3	10.84	0.44	<10	8	High purity, tensile and creep at NETL
20-A18	347H	0.0545	18.36	0.93	0.54	11.02	0.45	<5	11	Additional high purity 347H
19-A93	347H-N	0.056	18.38	0.91	0.53	11.06	0.4	<5	184	N added, for tube creep tests
20-A19	347H-N	0.0531	18.37	0.93	0.51	10.97	0.42	<5	163	N added, tensile and creep tests
20-A20	347H-N+B	0.0553	18.38	0.92	0.57	10.97	0.46	11	168	B + N added, tensile and creep tests
NIMS-CDS (28B)	Max.	0.07	18.05	1.82	0.82	12.55	0.88	27	284	Available at https://smds.nims.go.jp/creep/en/
	Min.	0.05	17.26	1.66	0.49	12	0.72	3	160	

3 similar alloys with varying N and B content are tested under creep and tensile loads, stress jump tests.

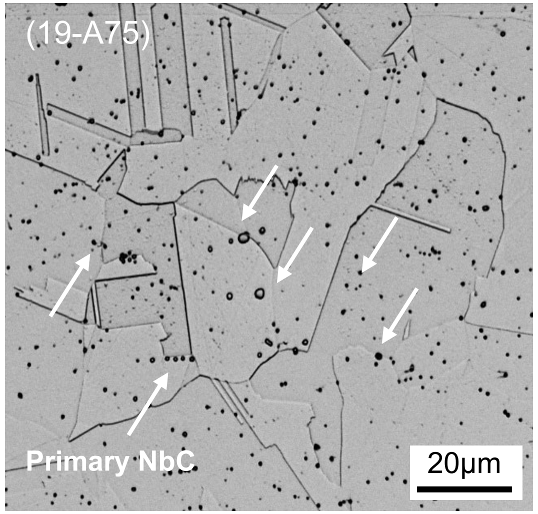
The material systems will be tested in an as received and after aging (750C 336h).

Tests are replicated in different laboratories to ensure consistency of the data.

Materials microstructure will be aged to assess thermodynamics and kinetic databases

Processing, aging and testing different grades of 347H steels to separate solute vs strengthening and trace elements effects

A 347H plate delivered



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Aging increases the creep rates, N+B reduce the creep rate

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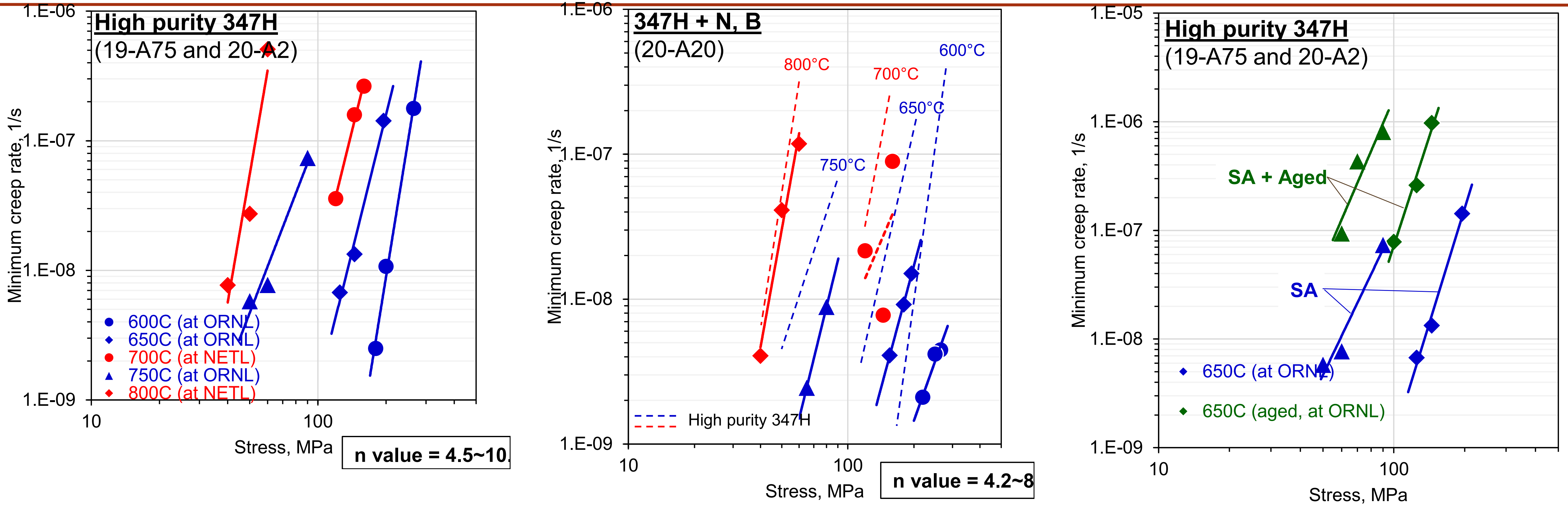
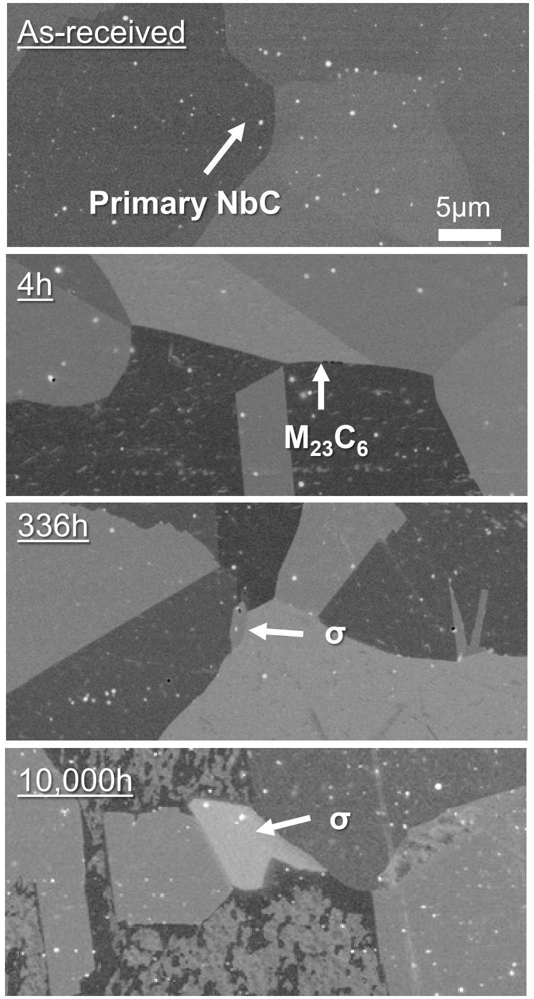


The addition of N + B consistently reduces the creep rate by up to an order of magnitude. Materials aged for 336h at 750C prior to loading exhibit significantly higher creep rates (why? see presentation 1t).

Aging of 347H leads to the formation of secondary NbC, and Sigma phase. N and B stabilize the metastable M23C6 phase

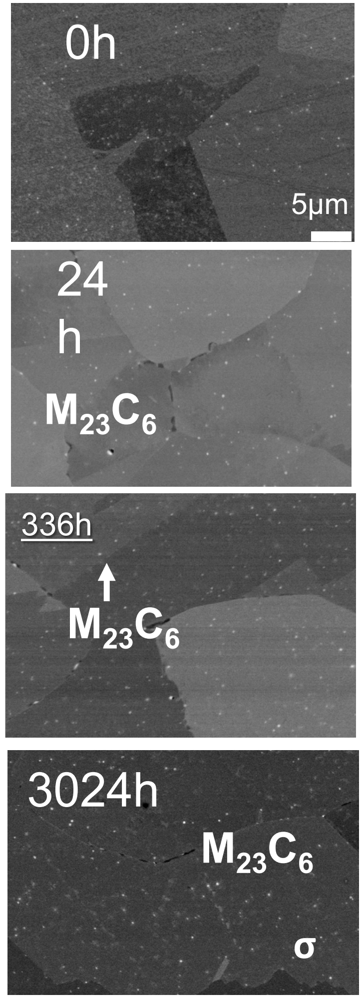


Aged at 750°C
(High purity 347H)

Timeline

AR	**Primary NbC**
4h, 26h, 168h	**NbC + $M_{23}C_6$**
	NbC + $M_{23}C_6$ + σ
336h, 482h, 1008h, 3024h, 10000h	**NbC + σ**

Note; $M_{23}C_6$ was observed only between 4h and 168h



Aged at 750°C
(347H_NB, NETL 20-A20)

Timeline

AR	**Primary NbC**
4h, 26h, 168h, 336h, 482h, 1008h, 3024h	**NbC + $M_{23}C_6$**
10000h	**NbC + $M_{23}C_6$ + σ**

Ren et al. JOM 2022

Aging of 347H leads to the formation of secondary NbC, and Sigma phase. N and B stabilize the metastable M23C6 phase

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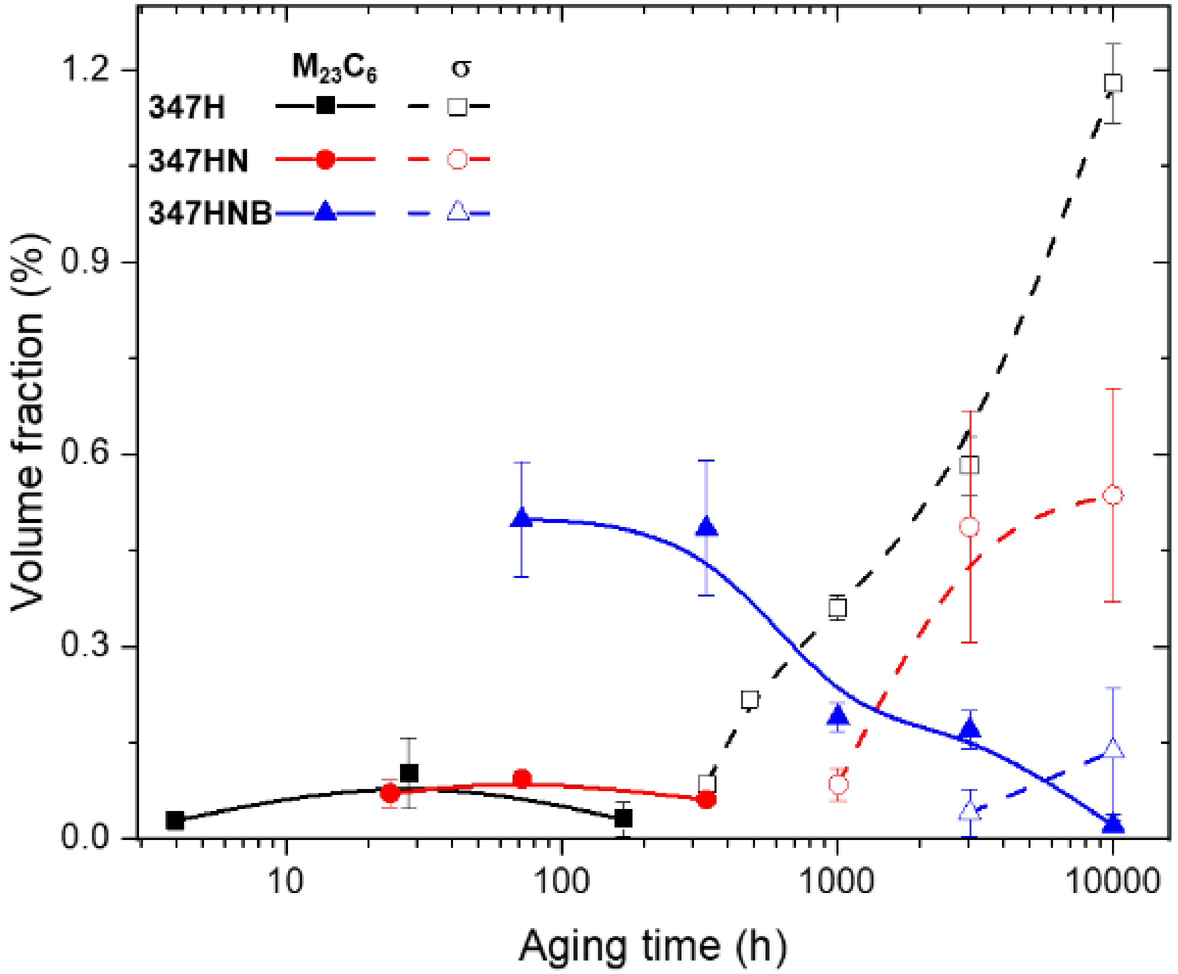


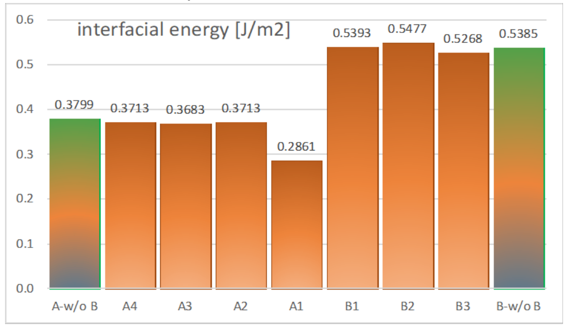
Enhancing thermodynamics databases with DFT simulations to consider elastic energy and trace elements

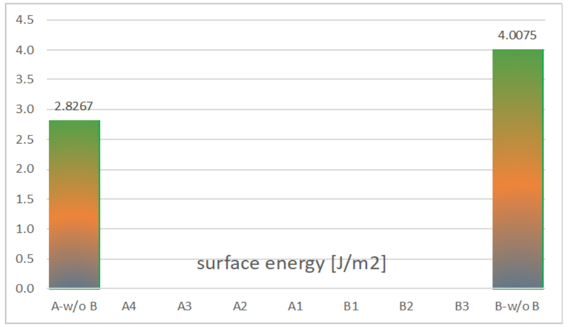
- **Boron decreases interfacial energy of fcc-Fe/$M_{23}C_6$ interface** by ~ **0.0938 J/m²**,a very significant value ***Boron*** prefers to substitute ***Carbon*** in A-type $Cr_{23}C_6$

- **B** prefers to **bond with both Fe and Cr, increasing ordering of interface and its stability.** This makes diffusion of C and Cr along/across interface more complicated, **preventing coarsening of $M_{23}C_6$ particles**

- The interfacial energy without B doping for **A-type** is **0.3799 J/m²** (8 C atoms are at the interface neighboring with both Fe and Cr)
- It is lower than B-type (zero C atoms are at the interface), **0.5385 J/m².**

- With B, the **lowest interfacial energy is (A1) 0.2861 J**

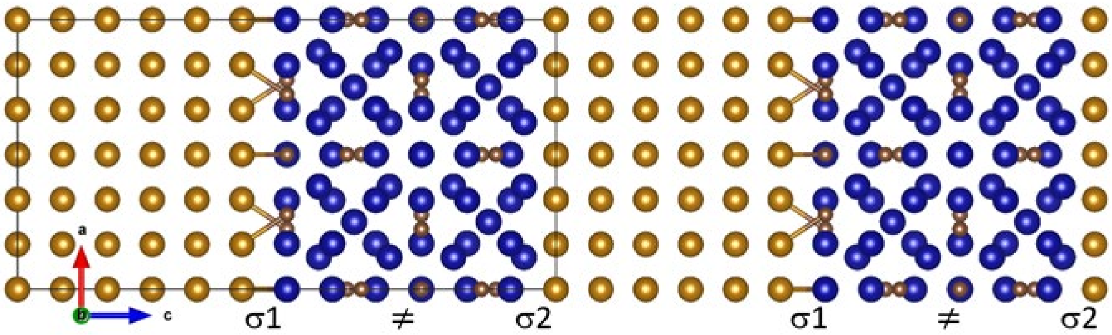


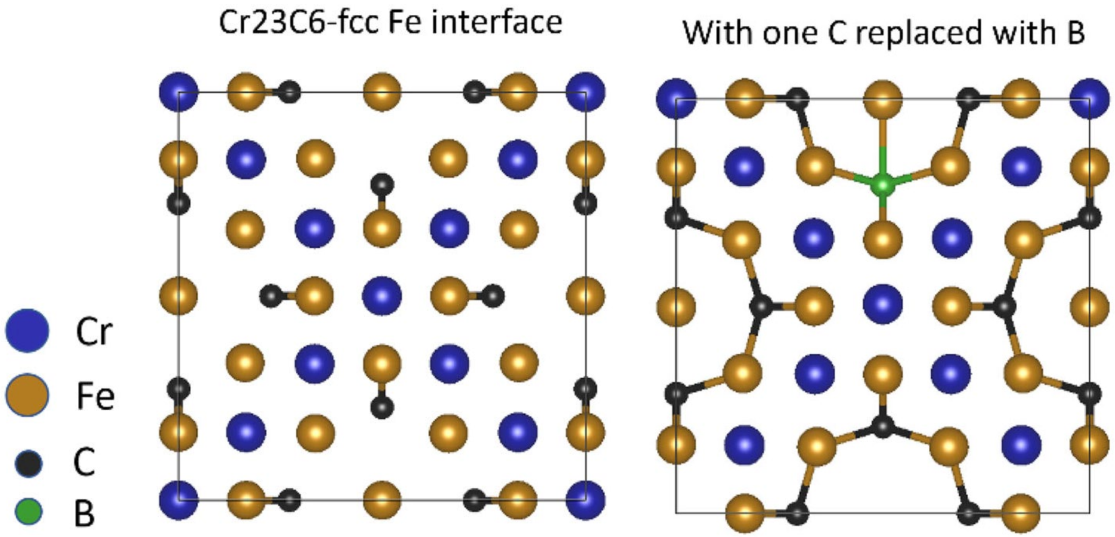


Glazoff et al. JOM 2022

No B

With B





Sigma (001) // FCC Fe (111) Interfacial Energy

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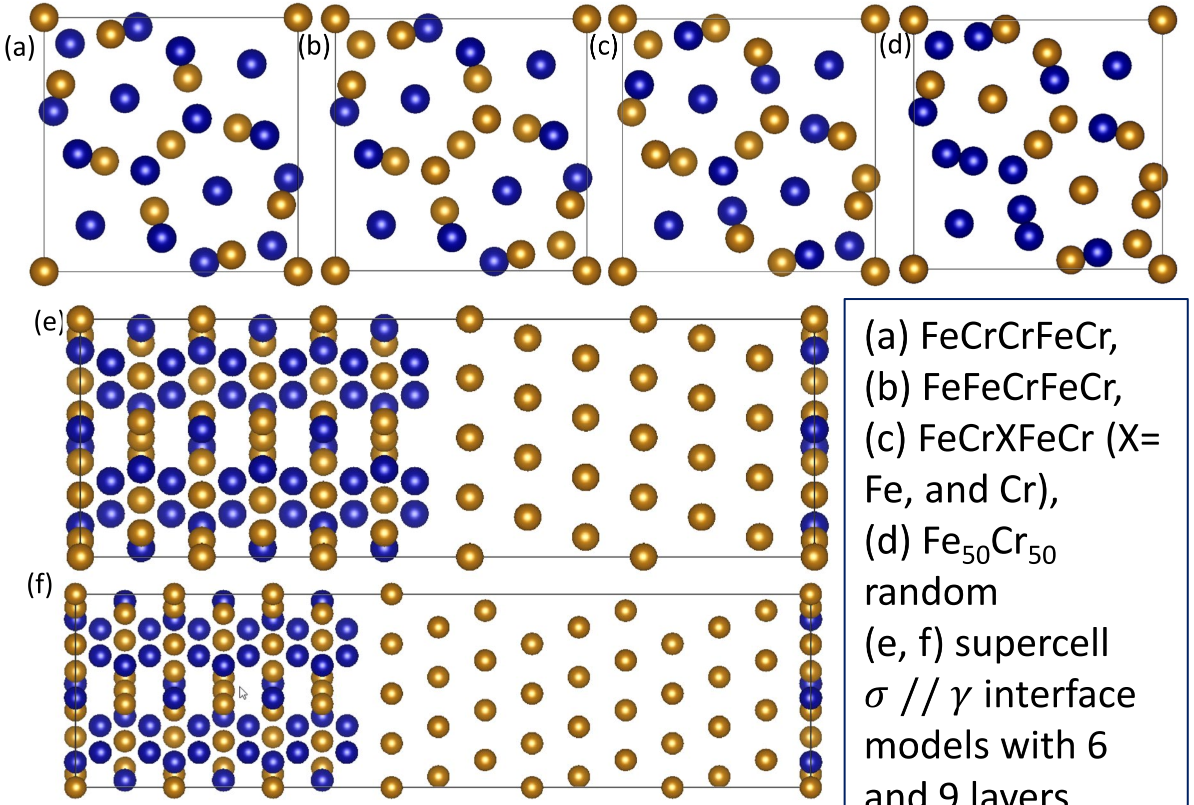

(a) FeCrCrFeCr, (b) FeFeCrFeCr, (c) FeCrXFeCr (X= Fe, and Cr), (d) $Fe_{50}Cr_{50}$ random (e, f) supercell σ // γ interface models with 6 and 9 layers

Table 1. The bulk and interface energy of FCC Fe and different configuration of sigma phase, and their lattice parameters.

	$A_2B_4C_8D_8E_8$	Number of atoms	Energy/ atom	a(Å)	b(Å)	c(Å)	α	β	γ	γ_{int} J/m^2
	Fe	4	-8.085	7.70	8.90	12.58	90.00	90.00	90.00	--
Sigma	FeFeCrFeCr	30	-8.854	8.64	8.64	4.42	90.00	90.00	90.00	--
Sigma	FeCrCrFeCr	30	-9.055	8.67	8.67	4.44	90.00	90.00	90.00	--
Sigma	FeCrXFeCr	30	-8.821	8.67	8.66	4.49	90.00	90.00	89.97	--
Sigma	$Fe_{50}Cr_{50}$	90	-8.775	8.66	8.63	13.52	89.91	90.03	89.86	--
Interface	FeFeCrFeCr//Fe	162	-8.465	8.64	8.64	26.71	90.00	90.00	90.00	0.080
Interface	FeCrCrFeCr//Fe	162	-8.562	8.67	8.67	26.75	90.00	90.00	90.00	0.131
Interface	$Fe_{50}Cr_{50}$//Fe$^{(i)}$	162	-8.243	8.66	8.63	30.00	89.91	90.03	89.86	--
Interface	$Fe_{50}Cr_{50}$//Fe$^{(ii)}$	198	-8.205	8.66	8.63	35.81	89.91	90.03	89.86	--

(i) Six layers of FCC Fe
(ii) Nine layers of FCC Fe

The corrected thermodynamic database allows to predict concurrent precipitation with TC Prisma

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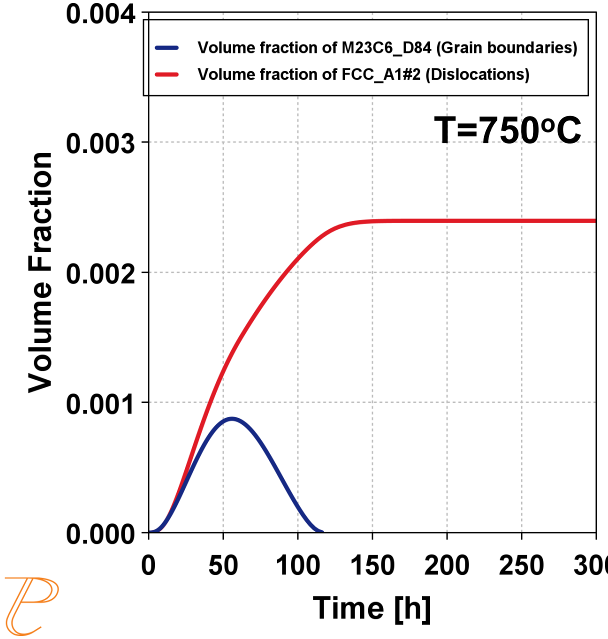
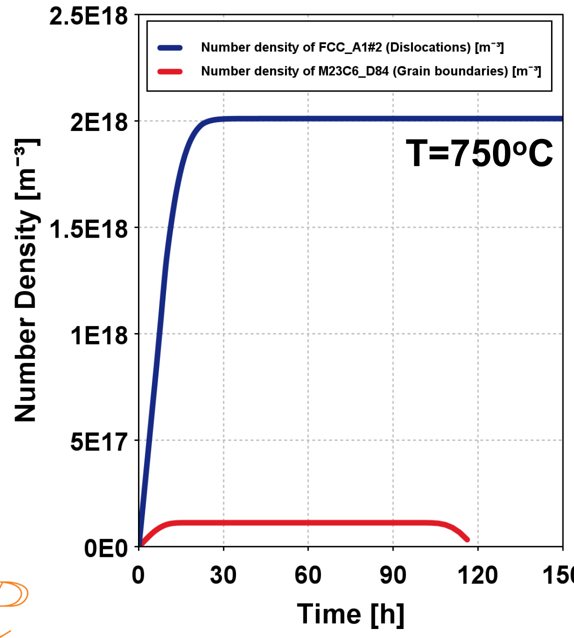
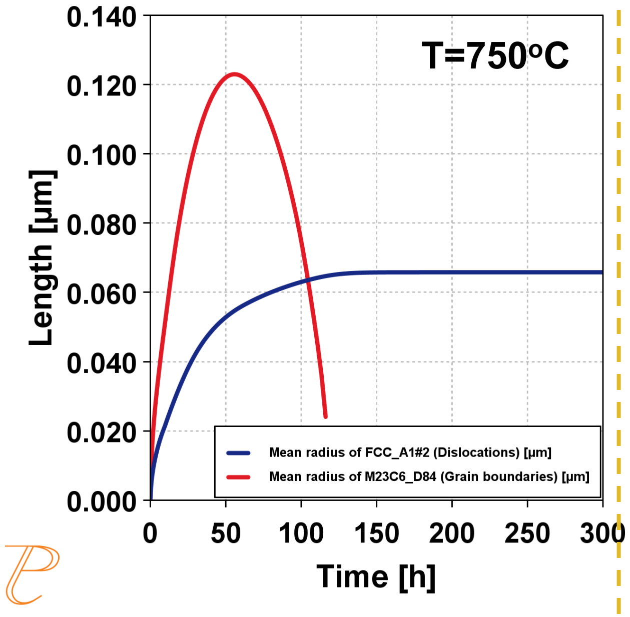
Volume Fractions of M23C6 and NbC



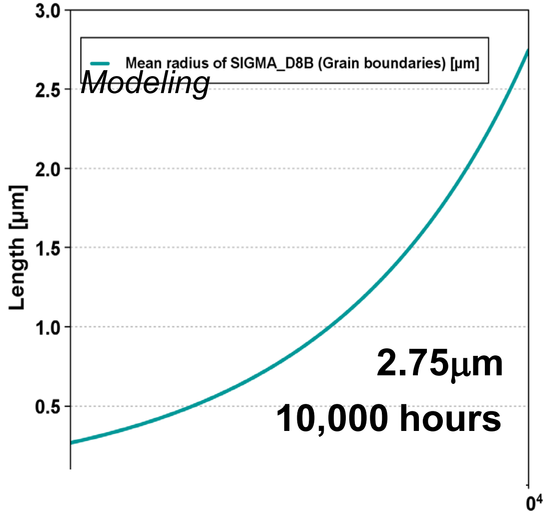
M23C6 & NbC Particle Number Density, m^(-3)



M23C6 and NbC Particle Size(s) as Function of Time



Sigma Phase Precipitation - up to 10,000 hours



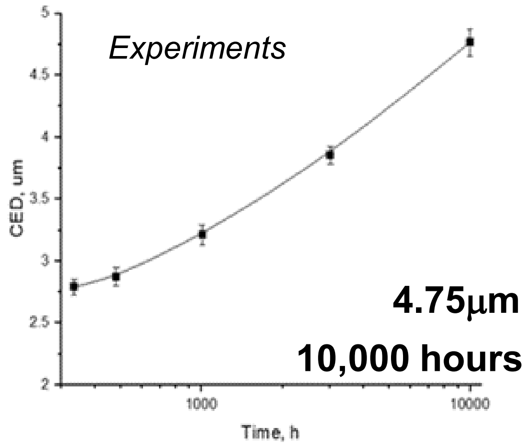


Table	Modeling and experimental $M_{23}C_6$ precipitation data of 347H stainless steels at 750°C			
	Aging time of $M_{23}C_6$ formation	Volume fraction, %	Number density[a]	Size, µm
Simulation	0 through 120 h	0.09	1.1×10^{17} m^{-3}	0.125
Experimental[37]	4 h, 24 h, and 168 h	0.10	4.7×10^{14} m^{-3}	0.480

[a]The original experimental result, 6.0×10^9 m^{-2}, was presented in {m^{-2}}. If recalculated into {m^{-3}}, we will obtain the value given in Table III, i.e., 4.7×10^{14} m^{-3}.

The kinetics of concurrent precipitation are captured.

The volume fractions of precipitates are captured.

Number densities and size are off

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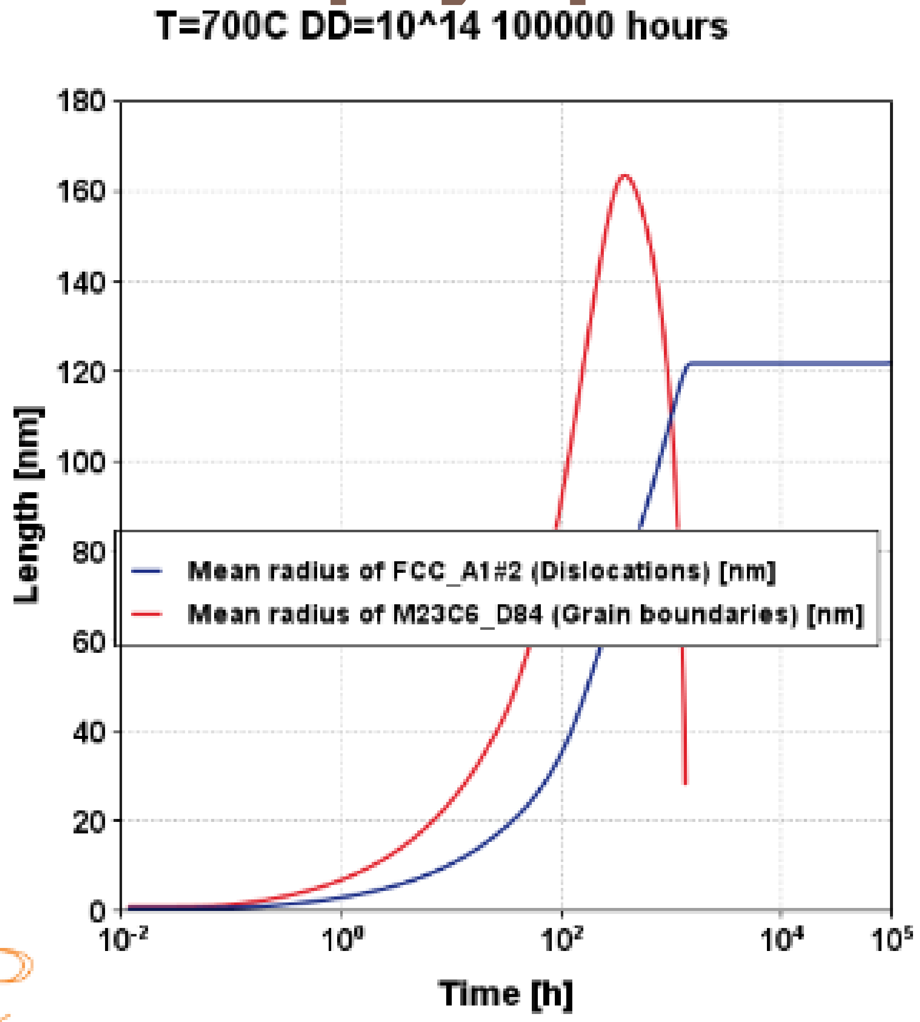
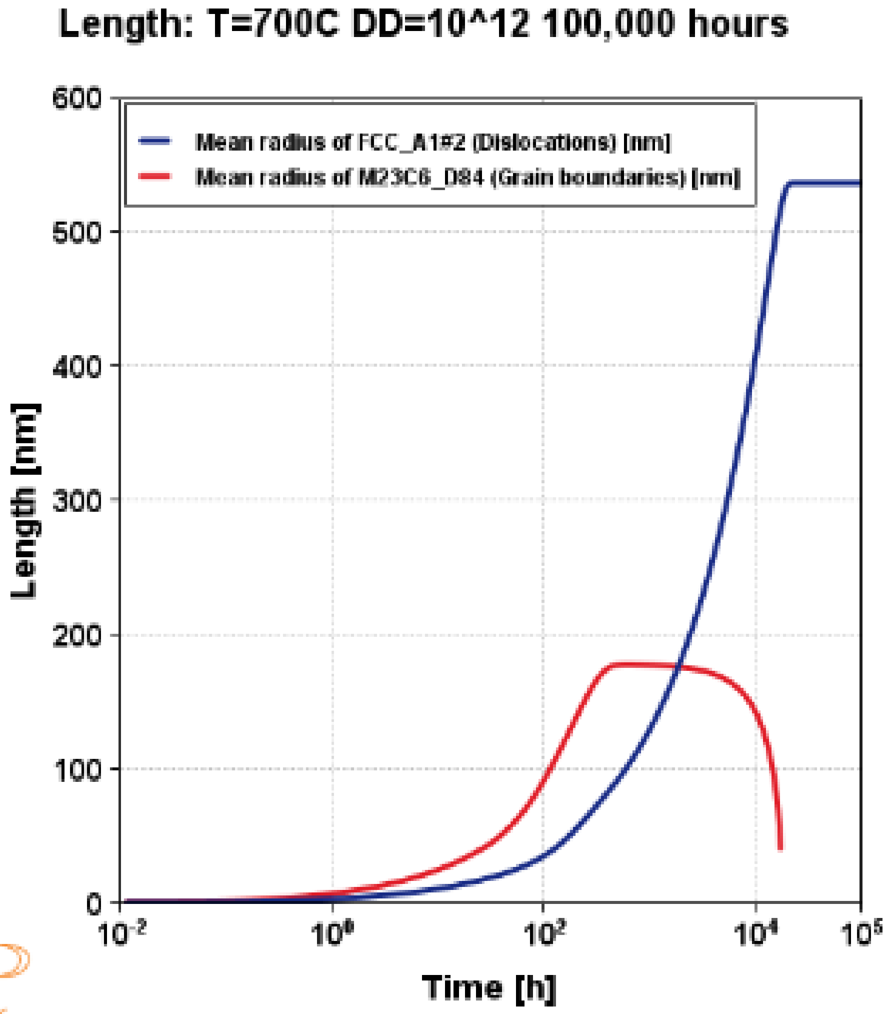
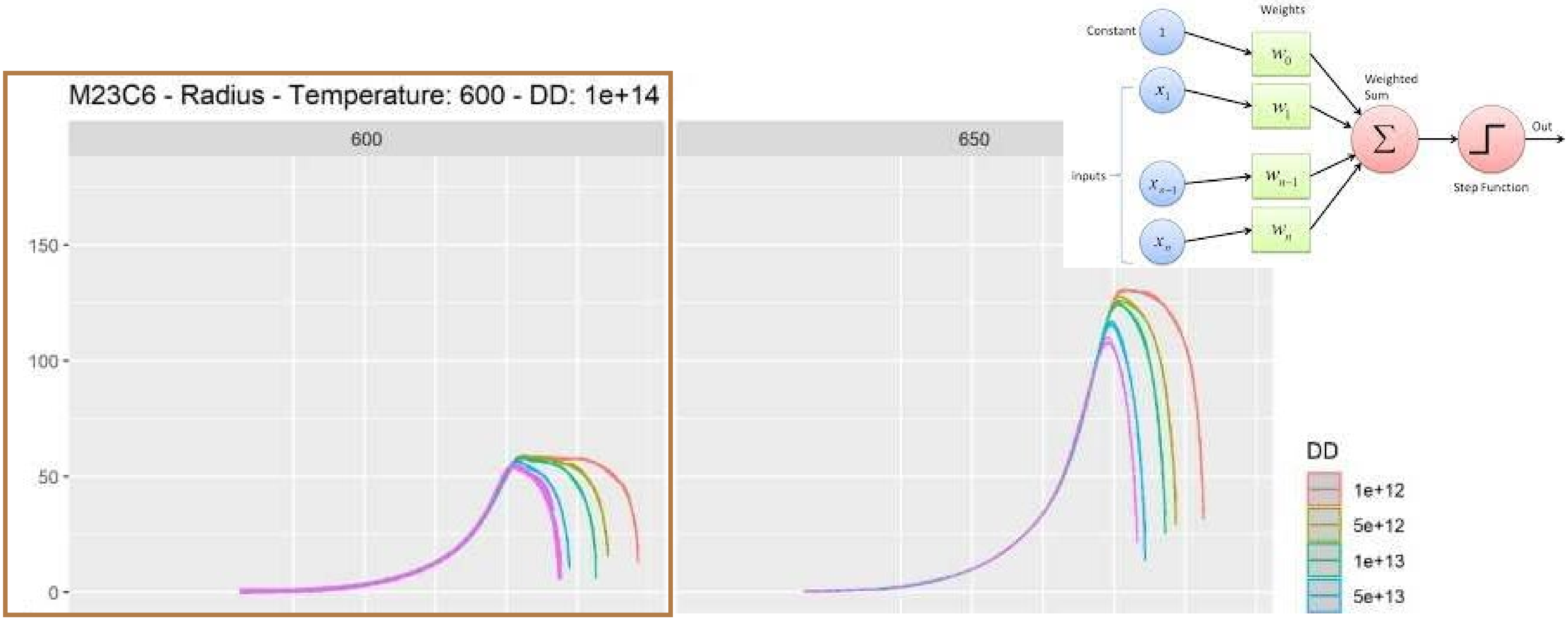
The new model is utilized to predict the Microstructure on precipitate content: dislocations play a prominent role





ML algorithms are being utilized to predict precipitate evolution

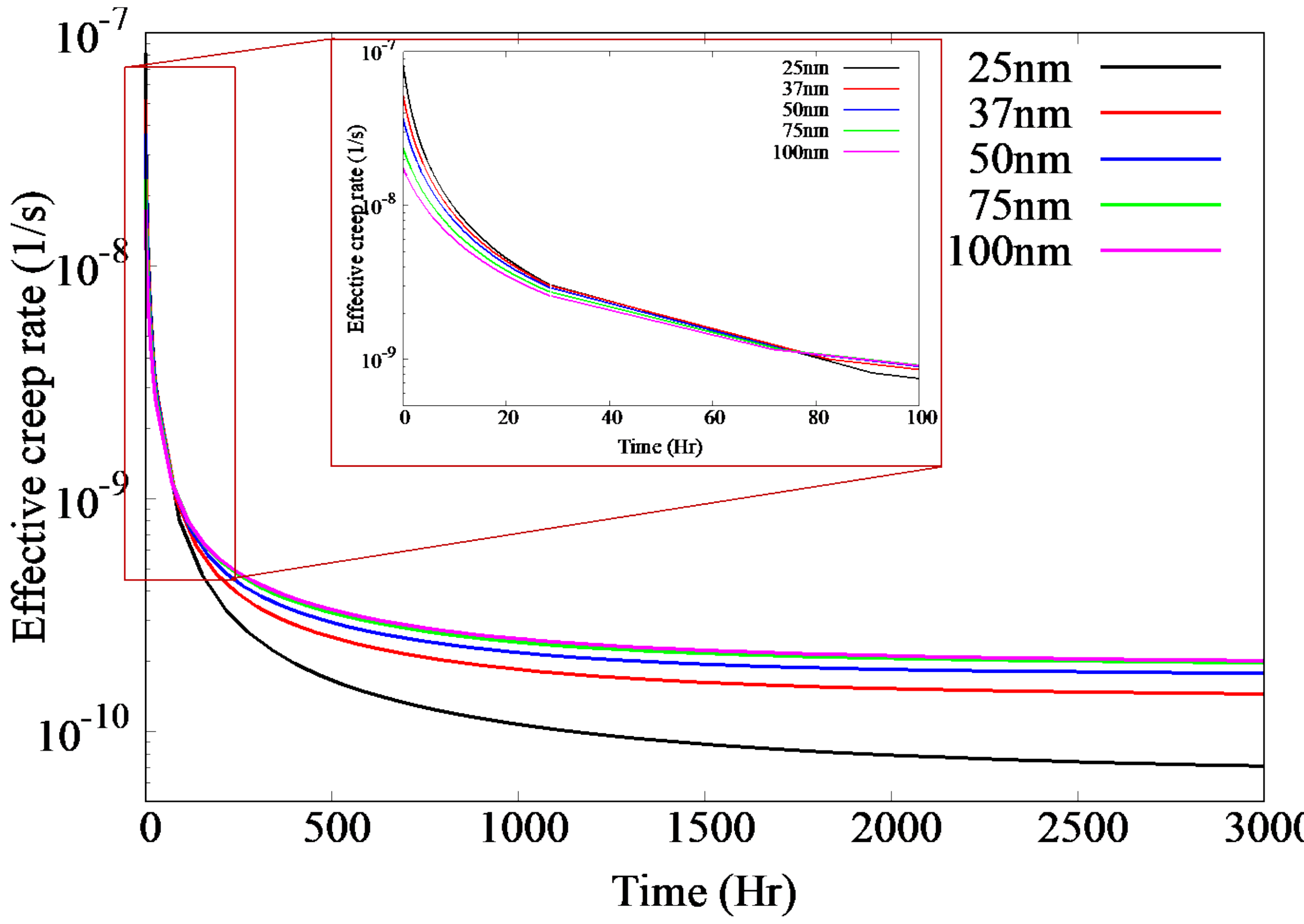


Courtesy of Cedric Neumann (battelle)

Precipitate "strengthening"

Gr91 subjected to creep at 600C under 100MPa stress

Increasing the size of precipitates which reduces the solute content in the matrix can lead to an increase in the creep rate



Precipitate "strengthening"

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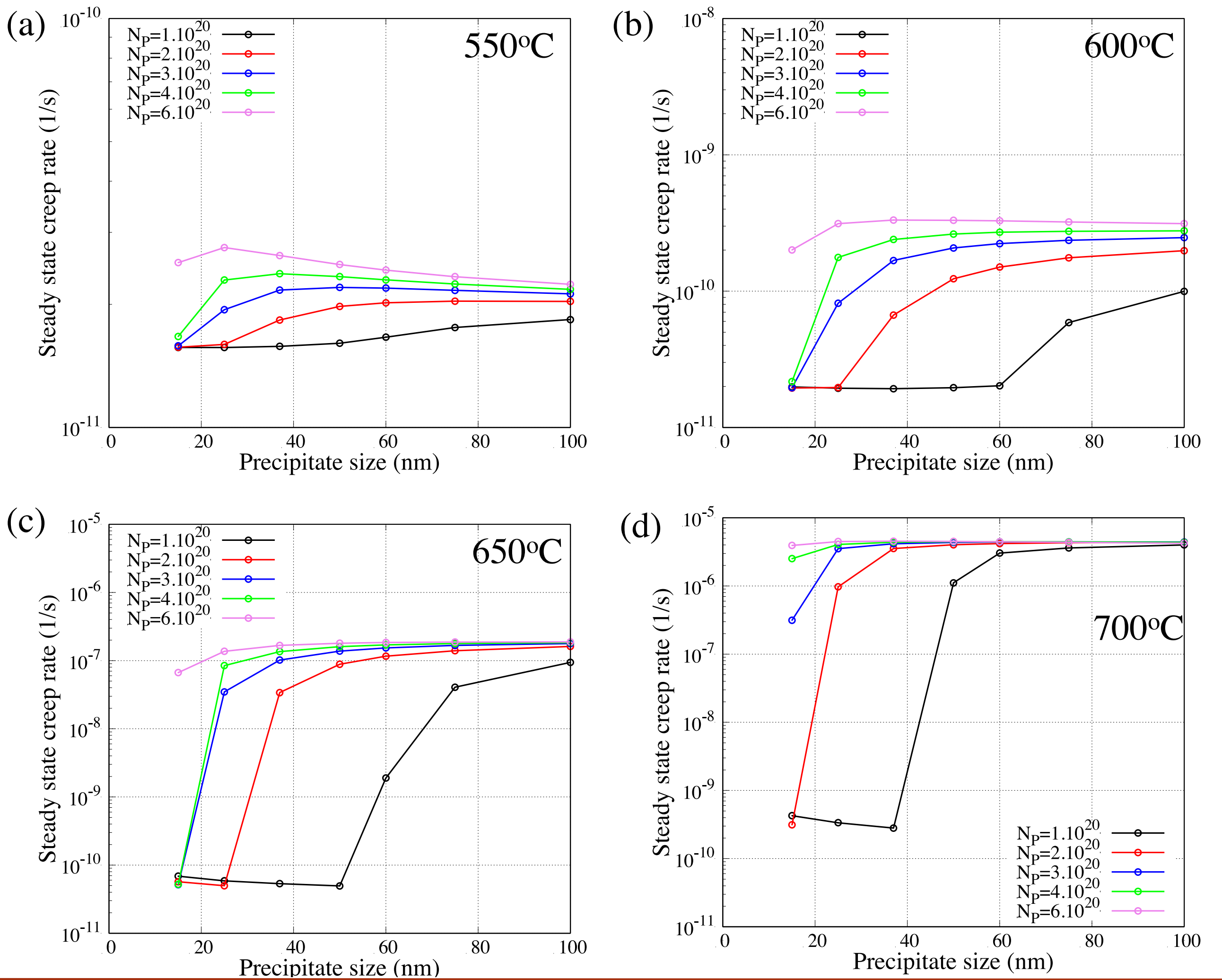
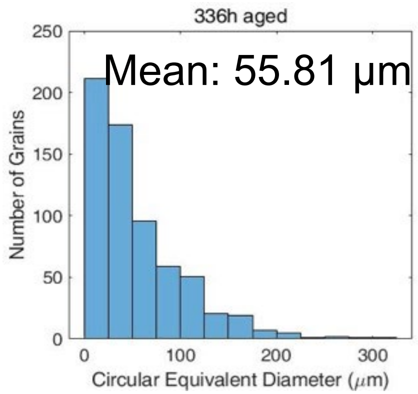
Increasing the size of precipitates which reduces the solute content in the matrix can lead to an increase in the creep rate.

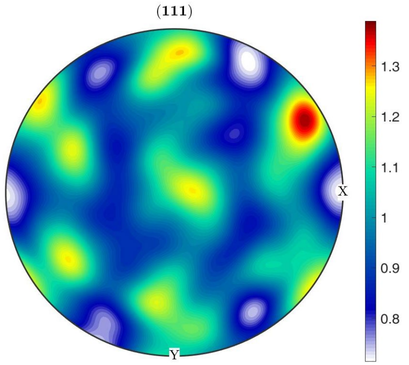
Increasing the size of promotes dislocation recovery thus benefiting the activation of diffusive processes (e.g. Nabarro Herring).

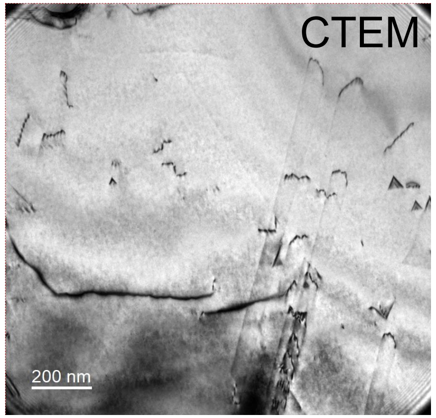
Overall the density and size of precipitates can either increase of decrease the steady state creep rate.

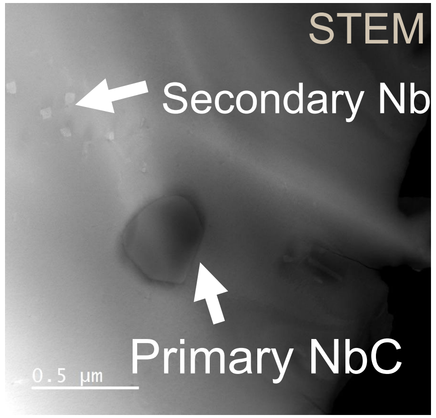


Effect of thermal aging on creep behavior: model vs experiments

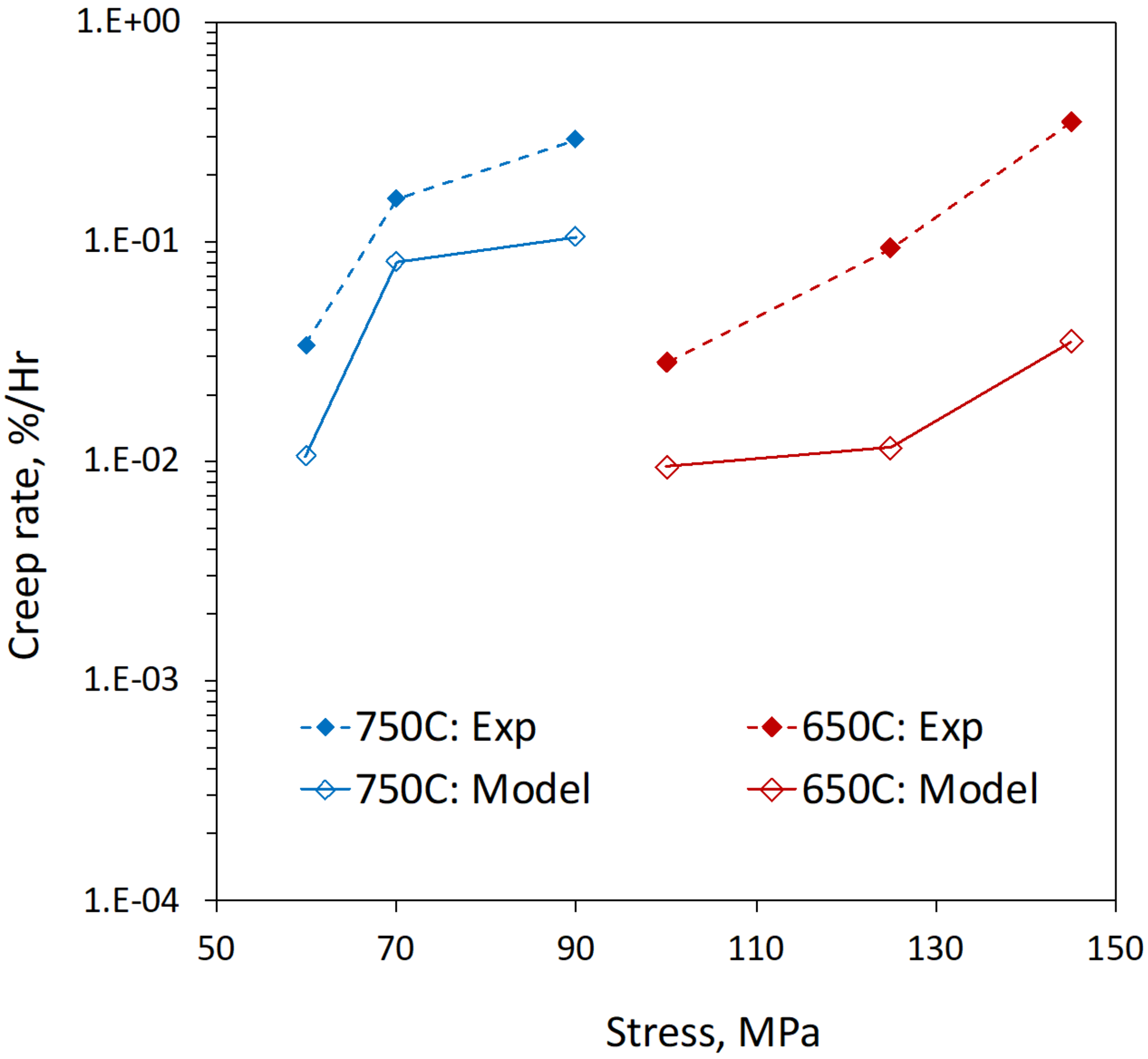








Dislocation density: $\rho = 3.5 \pm 1.5 \times 10^{12} \mathrm{m}^{-2}$
Primary NbC: N= 3.5 × 10^{17} /m^3, and D= 330 nm
Secondary NbC: N = 2.5 × 10^{19} /m^3, and D = 31.5 nm



Scientific advances allowing to relate microstructure, composition and performance

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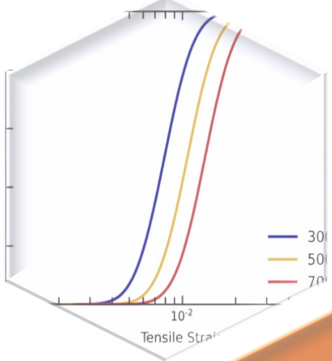
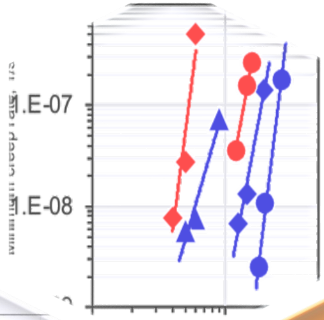


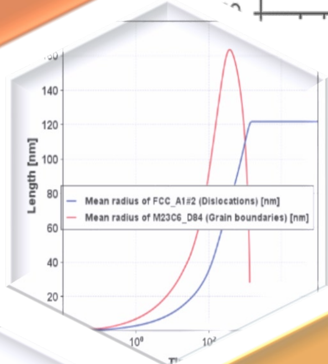
Cavity nucleation model: mechanism and microstructure sensitivity



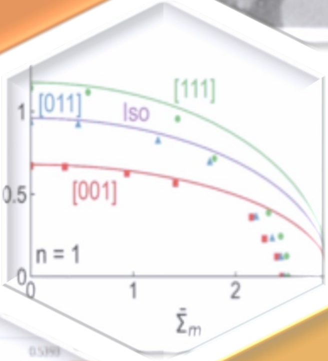
Processed and characterized 12 alloys

Characterized precipitate formation during anneal as a function of composition

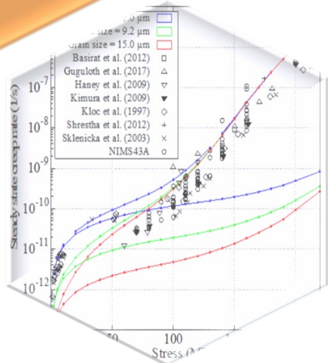
Predicted the kinetics of concurrent precipitation and dissolution from DFT and TC-Prisma

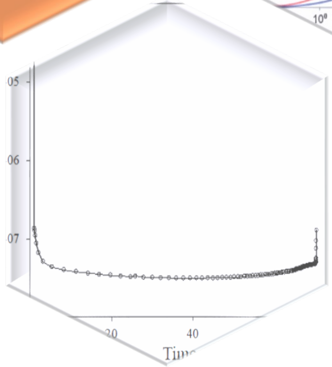


Cavity growth: growth rate under viscoplastic flow

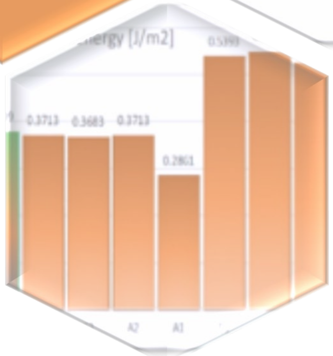


Quantified the role of microstructure onm the steady primary and secondary creep response of Gr91





3D model predicting the primary secondary and tertiary creep response of BCC and FCC steels



Quantified on the basis of DFT the role of trace elements

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eXtremeMAT-H2

eXtremeMAT https://edx.netl.doe.gov/extrememat

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APPROACH

BENEFIT

Reduce the time & cost for alloy qualification & certification

High–Fidelity Constitutive Model Capturing effects of **alloy microstructure** and deformation & damage processes

Database of responses with experimental data and ***synthetic data*** generated over wide range of conditions

Surrogate (reduced order) models.

Data Driven Alloy Life Predictors

Engineering Models for embedding in FEM packages

Improved physics-based mechanistic models to inform alloy design. Reduce time & cost for alloy development

Improved component design, eliminate over design, enable predictive maintenance

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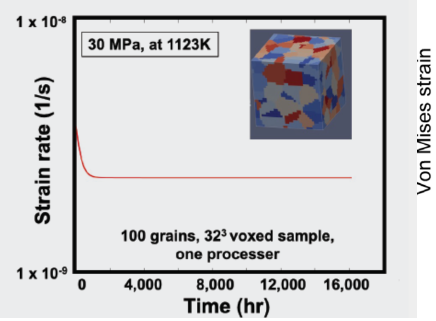
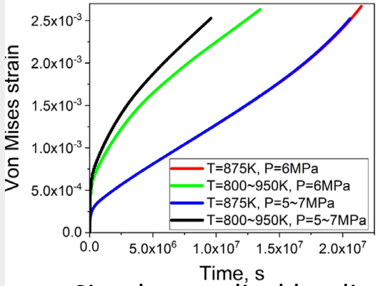
Accomplishments & Advancements

- ★ Mechanistic model can simulate 10 years of creep behavior in ~5 hours
- ★ Incorporation of complex stress states representative of real service conditions
- ★ Incorporation of *microstructural evolution (coarsening)* during service in predictive models

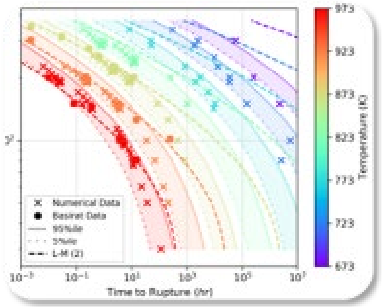
Alloy performance in hydrogen at elevated temperatures and long service duration

Mechanistic model can simulate 10 years of creep behavior in ~5 hours

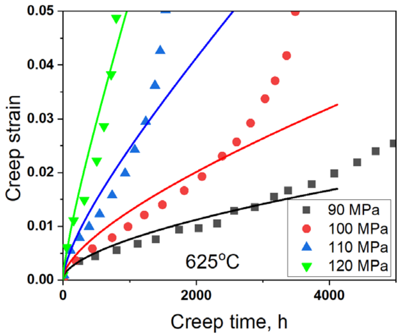


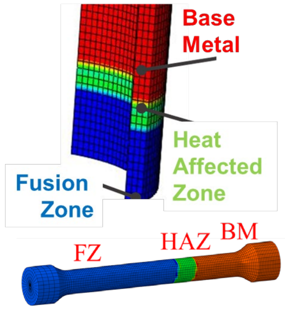


Simulate cyclical loading



Accurately predict creep life from a limited number of short-term





Framework for predicting the performance of welds

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H-MAT: Hydrogen Materials Consortium

NATIONAL ENERGY TECHNOLOGY LABORATORY

https://h-mat.org/

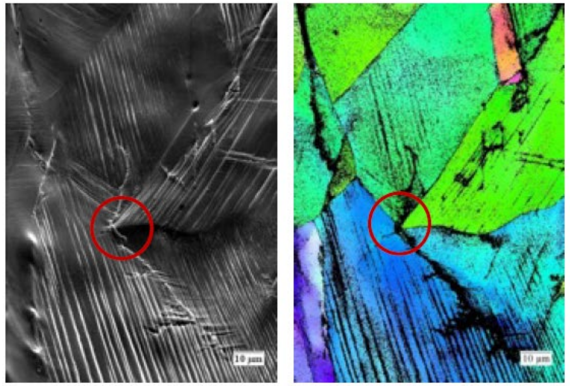
Effects of hydrogen on performance of polymers and metals – transportation & storage

Atomic level simulations

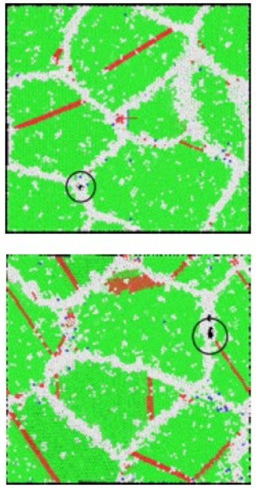
Science question:

- **Can we generalize inelastic field evolution at stress concentrations to predict of crack nucleation?**
- **How do hydrogen-defect interactions lead to fatigue crack nucleation?**

Experimental observation of fatigue crack nucleation



Both experimental and computational investigations show triple points and twin boundary intersections as active damage sites



MD simulations of damage evolution w/o and w/ H

From: Kevin Simmons, PNNL & Christopher San Marchi Sandia, XMAT Workshop, March 30, 2022

HyMARC: Hydrogen Materials Advanced Research Consortium

NATIONAL ENERGY TECHNOLOGY LABORATORY

https://www.hymarc.org/

g/models.html

HyMARC Hydrogen Materials Advanced Research Consortium

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Hydrogen Storage Systems Modeling

The U.S. Department of Energy (DOE) develops and maintains systems models for screening the performance of hydrogen storage materials. These models are available for download and use by the broad research community.

Detailed model descriptions and references detailing the models' validation are available in the supporting information. These models are open for use by material developers and storage system designers, but caution should be used when applying these models to materials and operating conditions that have not been validated.

Models Available for Download

Hydrogen Vehicle Simulation Framework

The Hydrogen Vehicle Simulation Framework is a MATLAB/Simulink tool for simulating a light-duty vehicle powered by a PEM fuel cell, which in turn is fueled by a hydrogen storage system. The framework is designed so the performance of different storage systems may be compared on a single vehicle, maintaining the vehicle and fuel cell system assumptions. This model requires MATLAB and Simulink.

Hydrogen Vehicle Simulation Framework User Manual

Download Systems Models

1. Read the terms of use.
2. Register to download the models.

Get Started

Metal Hydride Acceptability Envelope

The Metal Hydride Acceptability Envelope allows the user to evaluate the distance (in rectangular or cylindrical coordinates) between two surfaces or walls inside the bed containing the metal hydride material, needed to attain determined targets with selected material properties. This model requires Microsoft Excel.

Metal Hydride Finite Element Model

The Metal Hydride Finite Element model is a 3D model, developed under COMSOL 4.2a, that allows the user to see the thermochemical behavior of a storage system composed of sodium aluminum hydride material. The storage bed is based on a shell-and-tube, finned heat transfer system, with the structure and geometry of the United Technologies Research Center prototype.

Tankinator: Hydrogen Tank Mass and Cost Estimator

The Hydrogen Tank Mass and Cost Estimator, or "Tankinator", is used to cross-compare various pressure vessel types to estimate gravimetric, volumetric, and cost performance of hypothetical tanks in the conceptual phases of design. The Tankinator tool provides an estimate of basic tank geometry and composition from a limited number of geometric and temperature inputs. This model requires Microsoft Excel.

- ★ **Sandia National Laboratories,**
- ★ **National Renewable Energy Laboratory,**
- ★ **Pacific Northwest National Laboratory**
- ★ **Lawrence Livermore National Laboratory**
- ★ **Lawrence Berkeley National Laboratory.**

Accelerate discovery of solid-state materials for on-board vehicular hydrogen storage.

XMAT: new scope to address H effects on crep and embrittlement of metals as a function of microstructure

General scope: XMAT will develop, verify and validate research tools that predict how the mechanical performance of 347H and NI-based superalloys is affected by H, mechanical loads and thermal loads.

Materials studied: conventional and additively manufactured austenitic (**347H**, 316H) and ferritic steels (**P91**), **Ni-based superalloys**

Applications to:
Gasifiers, H gas turbines

BENEFITS of XMAT : Efficiently using materials under extreme environments and enabling rapid qualification of new materials.

Synergy between modeling and experiments leads **to quantification of the uncertainty in materials performance.**

Guidance to experimental programs

Improved component design ***eliminates over-design and enables predictive maintenance to avoid failure***

Reduce the time and cost for alloy qualification and certification

eXtremeMAT Towards a digital twin of microstructure evolution and performance of metals

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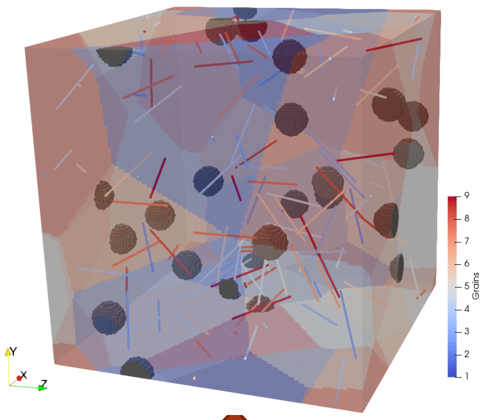
Microstructure

H partial pressure

Stress

Temperature



Mechanical tests

- H effects on creep is poorly studied
- H effects on tensile response is well known (decrease in toughness, embrittlement)
- Creep/ creep fatigue is less studied (increase in creep rate, increase in power law exponent).. Although new studies are poring in

Digital Twin

- Local H content at traps as a function of experimental conditions and microstructure?
- Does H increase the likelihood of crack nucleation, does it simply weakens preexisting cracks, does H affect precipitation kinetics?

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Scientific gaps in relating microstructure composition and performance

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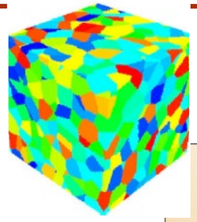
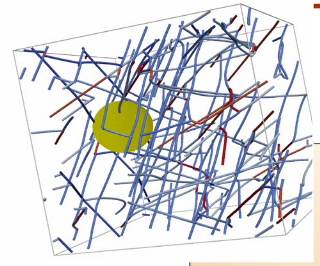
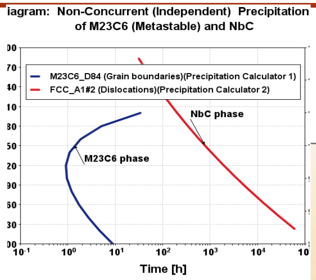






Plasticity

- Dislocation glide
- *Solute vs precipitate strengthening*
- Dislocation climb
- *Vacancy mediated*
- ***H assisted plasticity***

Damage

- *Cavity nucleation*
- Cavity growth
- Cavity coalescence
- Crack formation

Aging

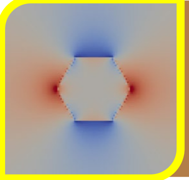
- *Second phase evolution*
- *Effect on plastic response and damage*
- ***H concentration?***

Oxidation

- Scale growth
- Cracking
- volatilization

Effects of **microstructure** (grain size, texture, precipitates, dislocation content,solutes), **stress** (3D, time evolution), **temperature** (time evolution) on material performance

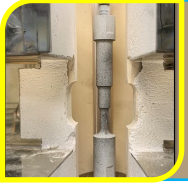
eXtremeMAT Thrusts and main tools to be delivered



1.0 Computational Modeling & Simulation Team

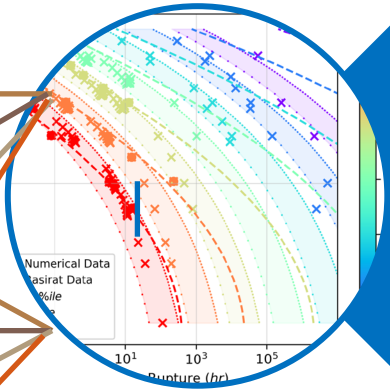
Energy Data eXchange

2.0 Uncertainty Quantification team

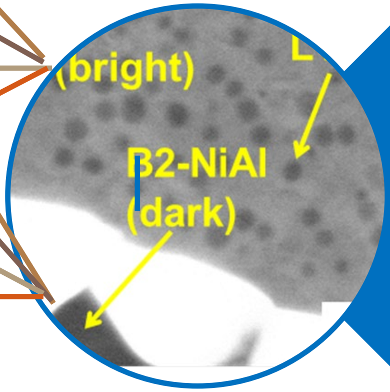


3.0 Experimental Validation Team

4.0 Manufacturing Team



Thrust 1: Material Lifetime & Performance Predictors



Thrust 2: Microstructure evolution predictor

FWP: cliff notes

1. Dislocation/H interactions (SFE, Mobility)

2. H segregation at interfaces & toughness

3. EVPFFT + chemo-mechanical module to show H distribution in the microstructure

4. Modeling H effects on plasticity and on damage nucleation .

5. Uncertainty Quantification

6. Characterization of the mechanical response under hydrogen environment

7. Atom Probe Tomography to study H redistribution

8. Microstructure and internal stress characterization

NETL

LANL

ORNL

Development of new capabilities

extremeMat-H2:

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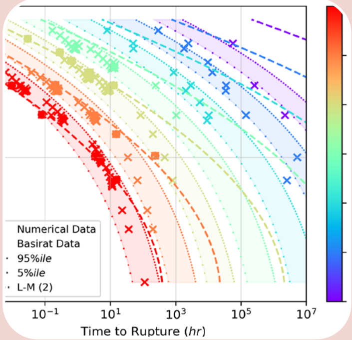

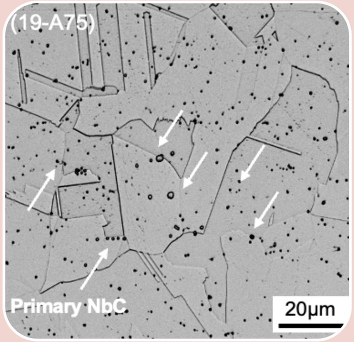

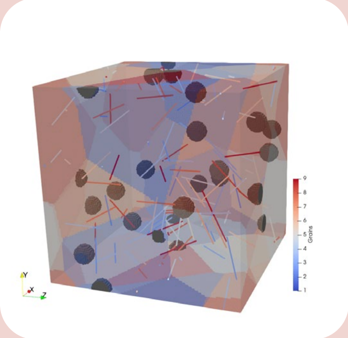

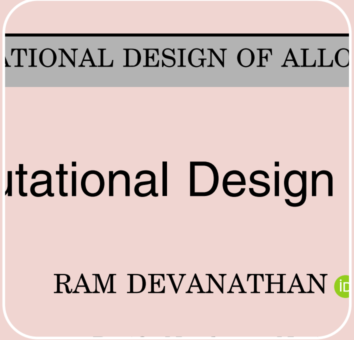

LaRupture:

Demonstration of predictiveness

Precipitation modeling:

Integration of precipitation effects into EVPFFT

Software releases and licensing:

EVPFFT

LaRupture

Discrete defects dynamics

Scientific manuscripts:

Nucleation models

Damage models

Precipitation

Creep and characterization data

Large overview paper

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