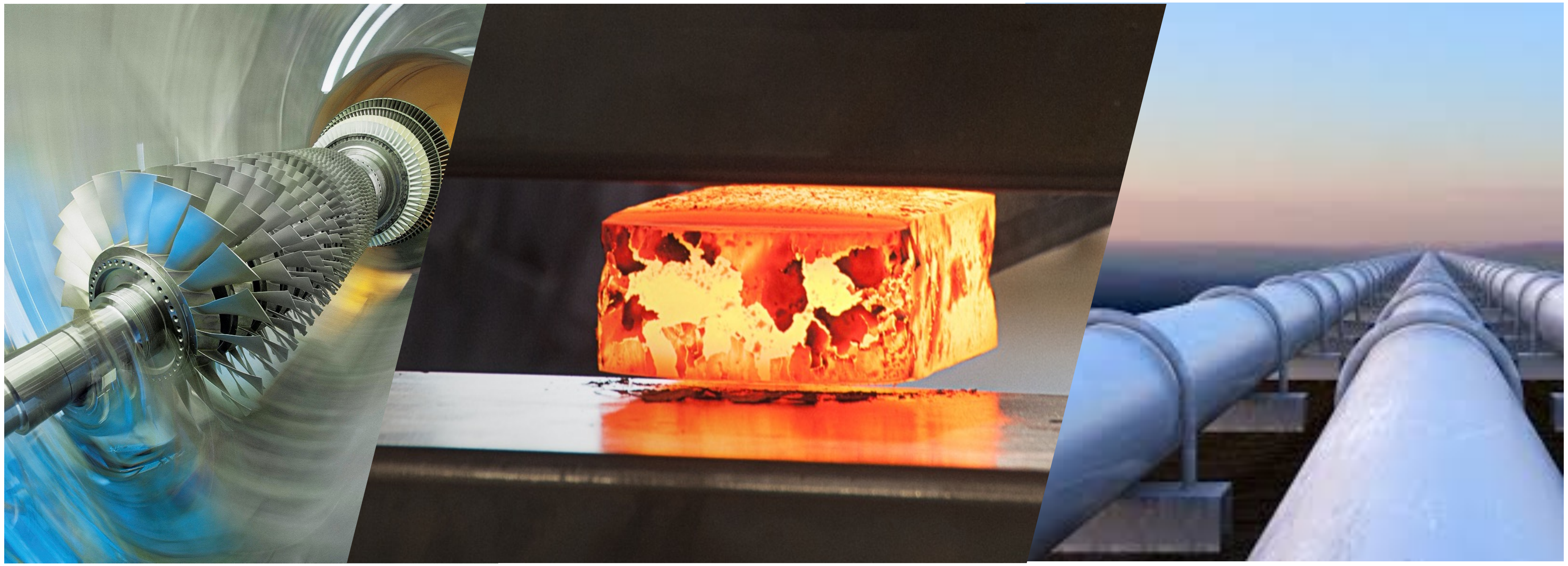
Correlating materials microstructure chemistry and performance in austenitic stainless steels



L.Capolungo

M. Arul Kumar, R.Lebensohn, N. Beets, Q.Q. Ren, Y. Yamamoto, M.P. Brady, J.A. Hawk, Q.Q. Ren, Jon Poplawsky, David Hoelzer, Yuki Yamamoto, Mike Brady, Edgar Lara-Curzio, Misha Glazoff, Jianguo Yu, Feng Zhang , Michael Gao

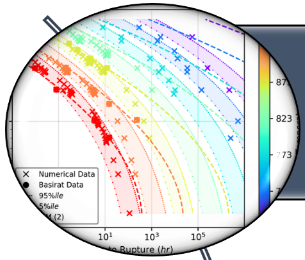
extremeMat: Objectives

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

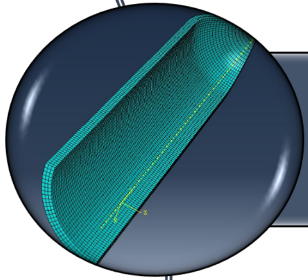
Applications to: conventional austenitic (**347H**, 316H) and ferritic steels (**P91**), **XMAT X351**..

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

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

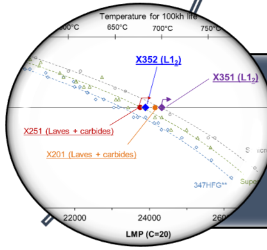


Material lifetime assessment models



Integrated constitutive models

Materials database and analysis tools



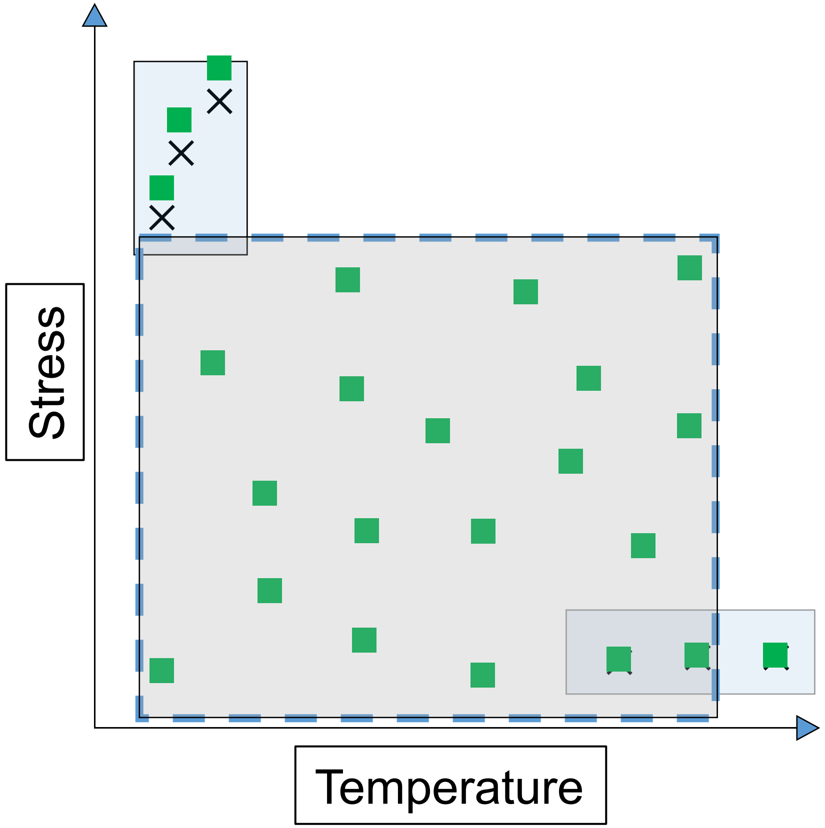
Guidelines for the discovery of new alumina forming alloys

Computational workflow

Microstructure and chemistry informed Polycrystal Model

Mechanical response and materials characterization

→ Database → Surrogate Model → Rupture life predictors / FE materials subroutines



Empirical model support

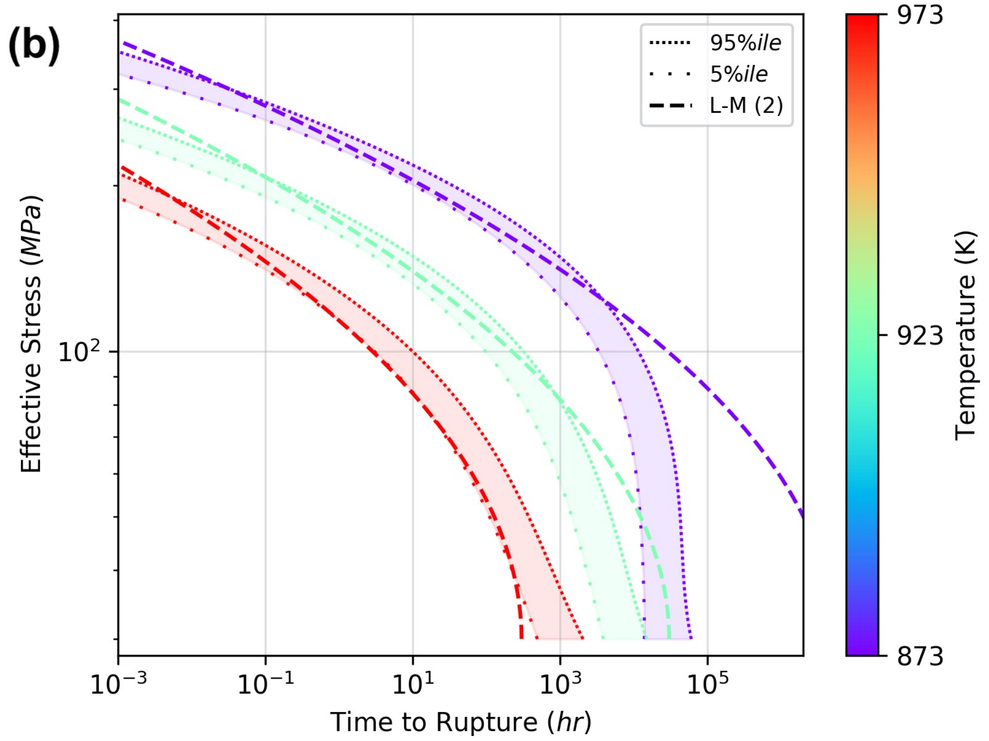
× Experiments

■ High-Fidelity Simulations

ROM Support

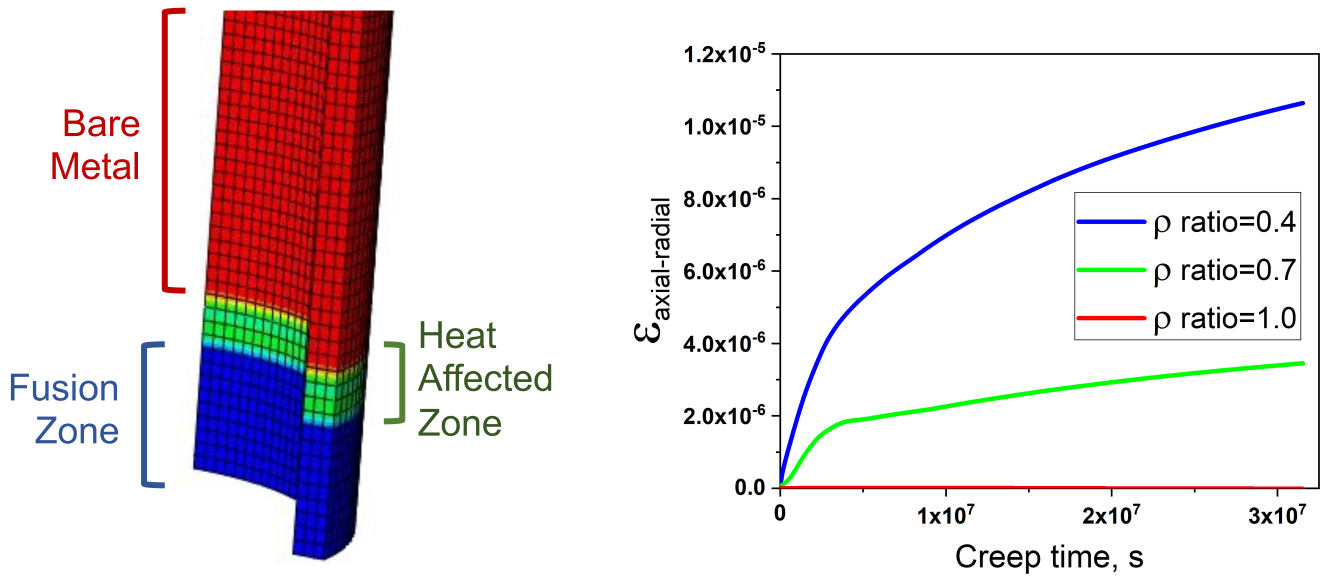
XMAT: accomplishments

LaRupture: Models that predict the failure of steels as a function of microstructure (P91, 347H in progress)



LaRupture: N.Bieberdorf et al. Submitted to IJP
LaRomance: Kumar et al .in preparation

LaRomance© : The suite of constitutive models for plasticity in extreme environments



Both LaRupture and LaRomance predict the impact of microstructure on the mechanical response of steels (Gr91, 347H).

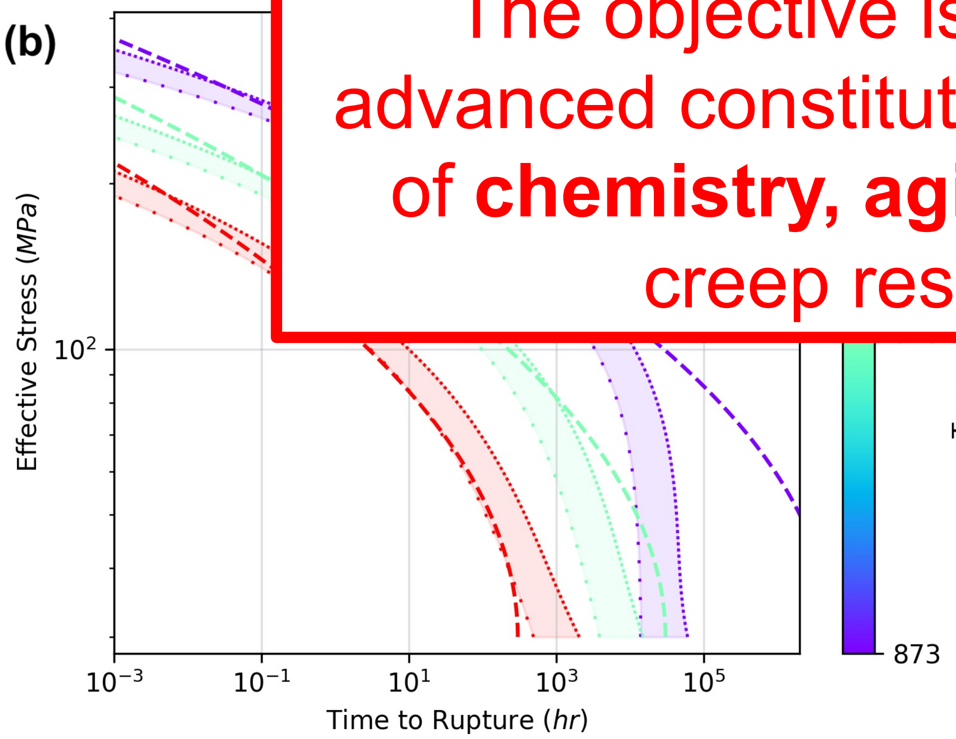
Aging and chemical composition have not been accounted for though. This is the focus of this presentation.

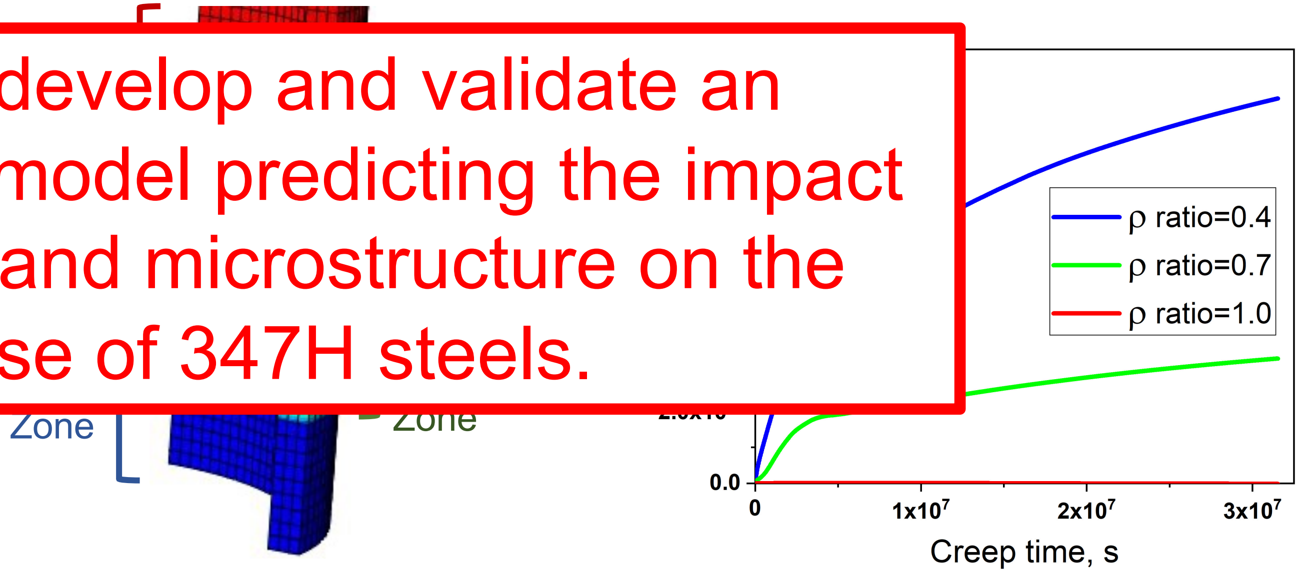
XMAT: accomplishments

LaRupture: Models that predict the failure of steels as a function of microstructure (P91, 347H in progress)

LaRomance© : The suite of constitutive models for plasticity in extreme environments

The objective is to develop and validate an advanced constitutive model predicting the impact of **chemistry, aging** and microstructure on the creep response of 347H steels.





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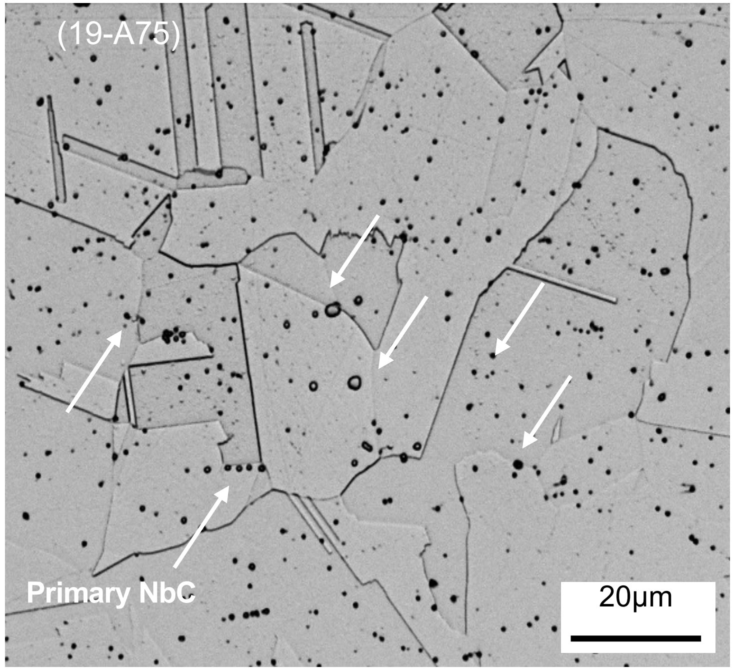
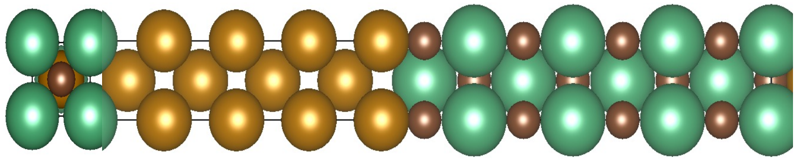
Approach

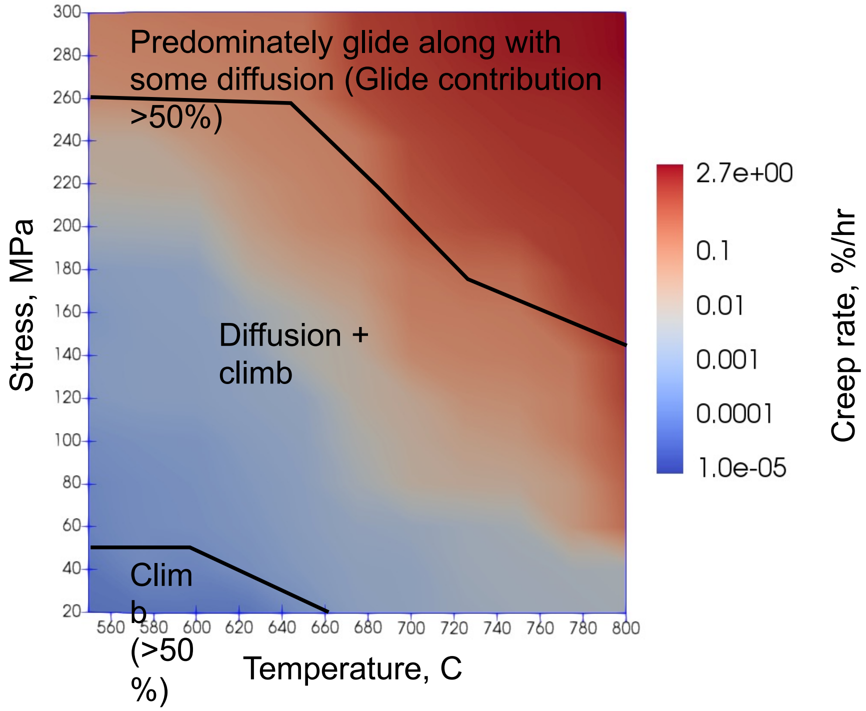
Materials processing and characterization:
The role of aging and chemistry



Understanding materials aging:
DFT and Prisma simulations



Predicting the relationship between microstructure, chemistry and creep response



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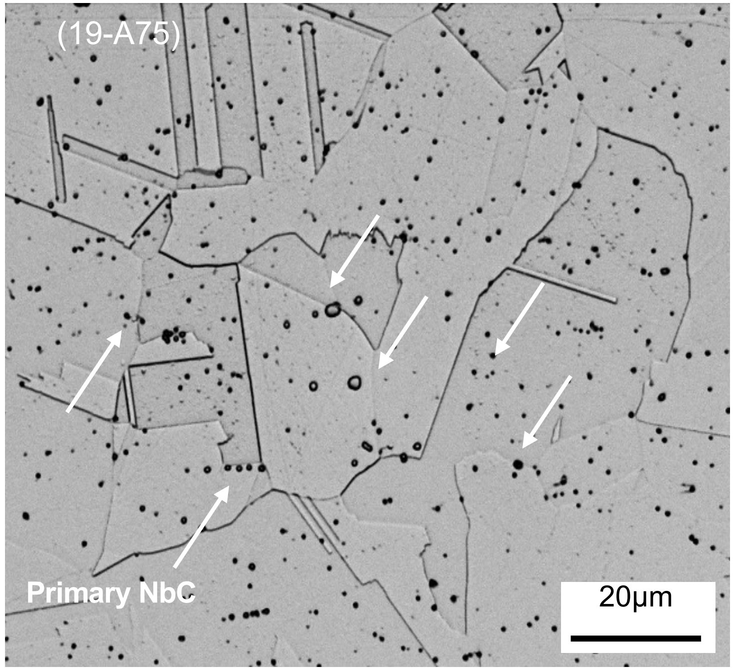

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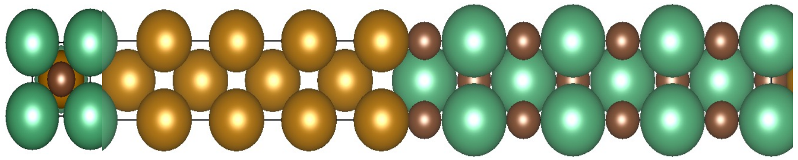

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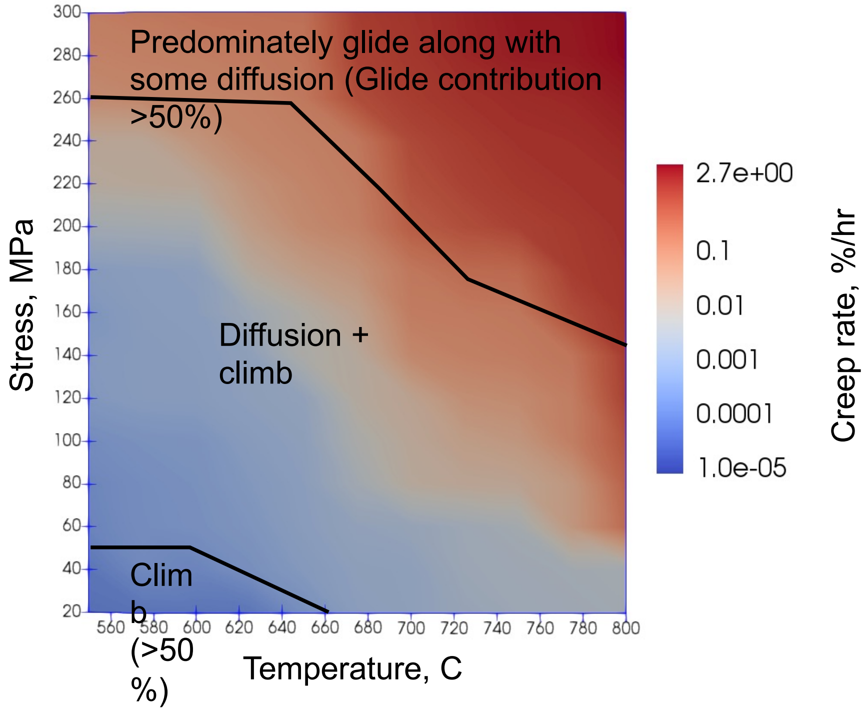

Processing, aging and testing different grades of 347H steels

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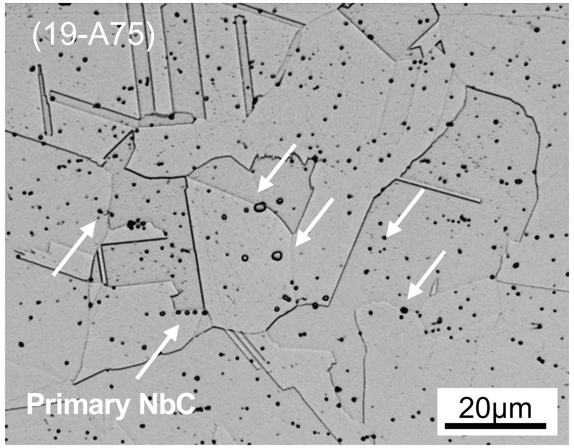
U.S. DEPARTMENT OF ENERGY

- <u>Multiple 347H heats</u>:
  - VIM + TMT + Solution-annealed at 1100°C
    - ➢ *Fully recrystallized austenite grain structure*
    - ➢ *Primary coarse NbC dispersed*
  - Applied additional aging at (at 750°C)
- Predicted <u>phase equilibrium</u> by a thermo-dynamic calculation (ThermoCalc w/TCFE9):
  - At 1100°C: FCC-Fe + NbC
  - At 750°C: FCC-Fe + NbC + Sigma
    - ➢ *Secondary NbC for strengthening*
    - ➢ *Meta-stable $M_{23}C_6$ is also expected*
- Prediction of <u>precipitation kinetics</u>:
  - Nucleation and Growth
  - Compared with experimental results

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**	

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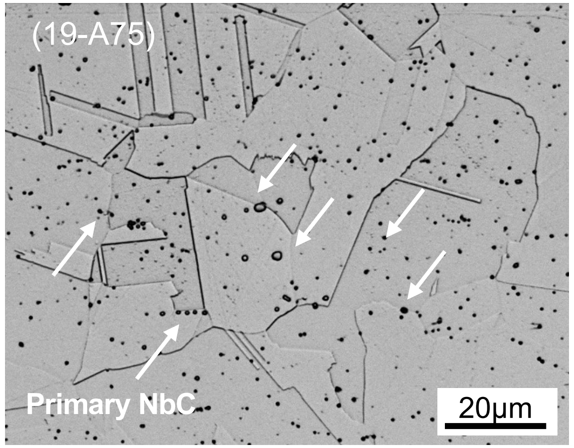

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Tensile and Creep Tests

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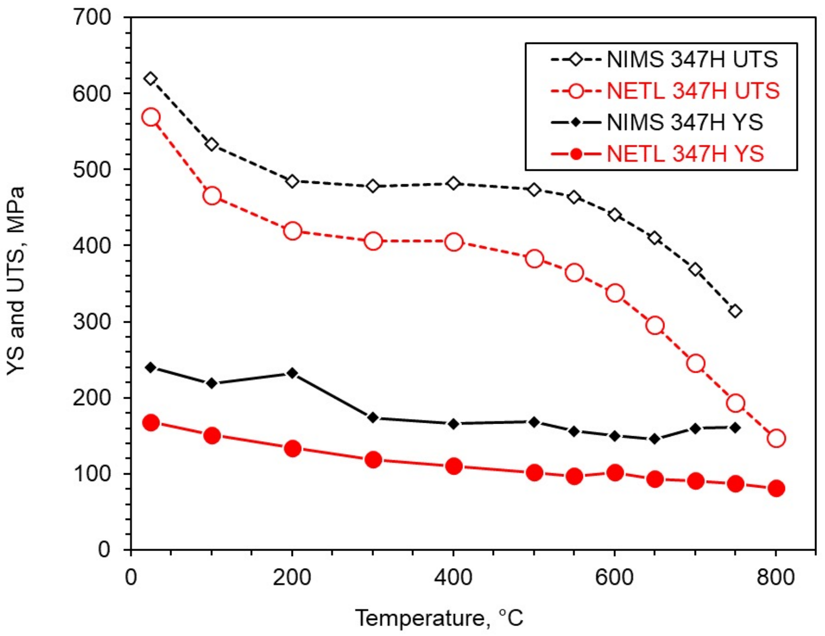
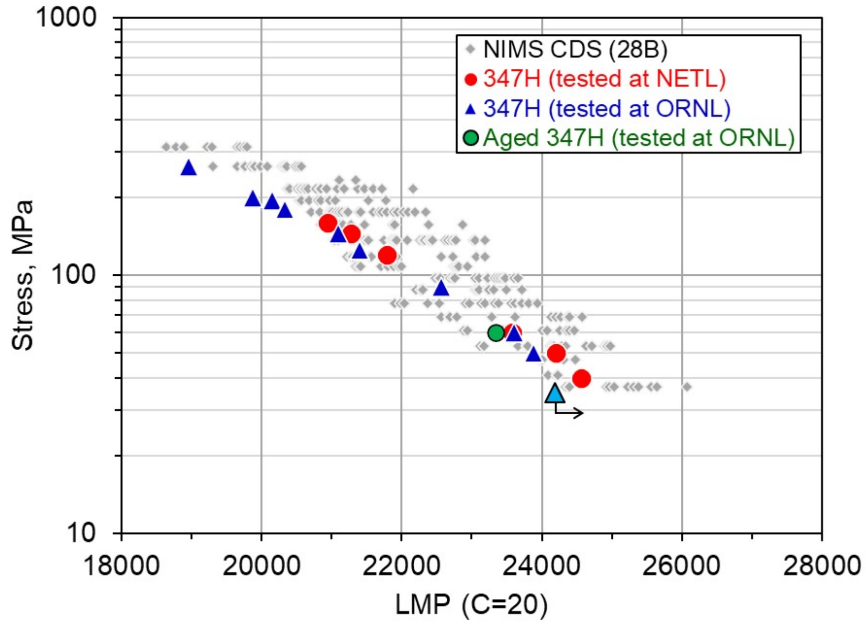
Tensile properties (by NETL)



Creep-rupture properties (ORNL/NETL)



Test Type	Test Conditions	Specimen Condition
Tensile Test	RT to HT (up to 800°C)	Solution-Annealed
	RT and 750°C	Aged at 750°C (for 336 h)
Stress Relaxation Test	300°C	Aged at 750°C (for 336 h)
Creep-Rupture Test (Uni-Axial)	600–800°C, 50–265 MPa	Solution-Annealed
Creep Stress-Jump Test	750°C, 25–45 MPa	Aged at 750°C (for 336 h)
Pressurized Tube Creep Test (Multi-Axial)	700°C, pressure (multi-axial stress), + tension	Solution-Annealed

Tensile and Creep Tests

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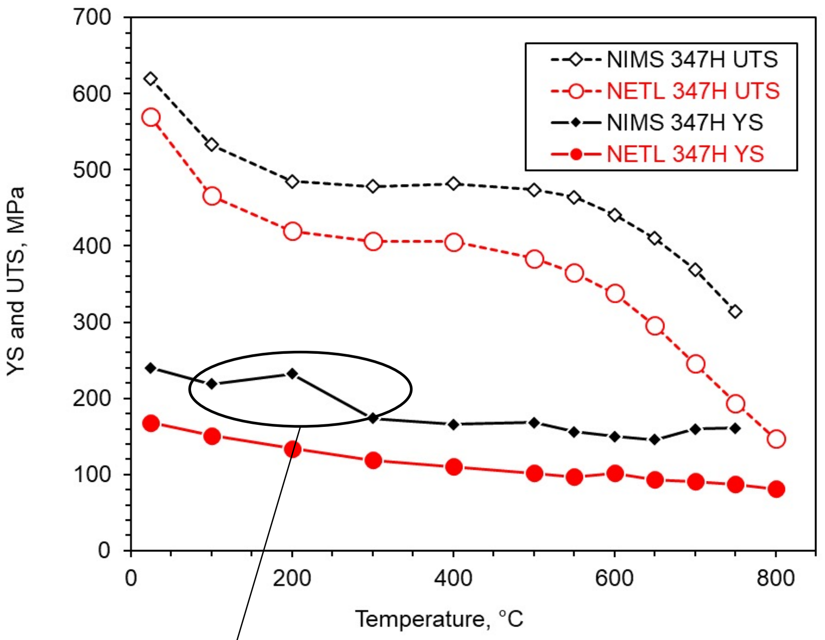
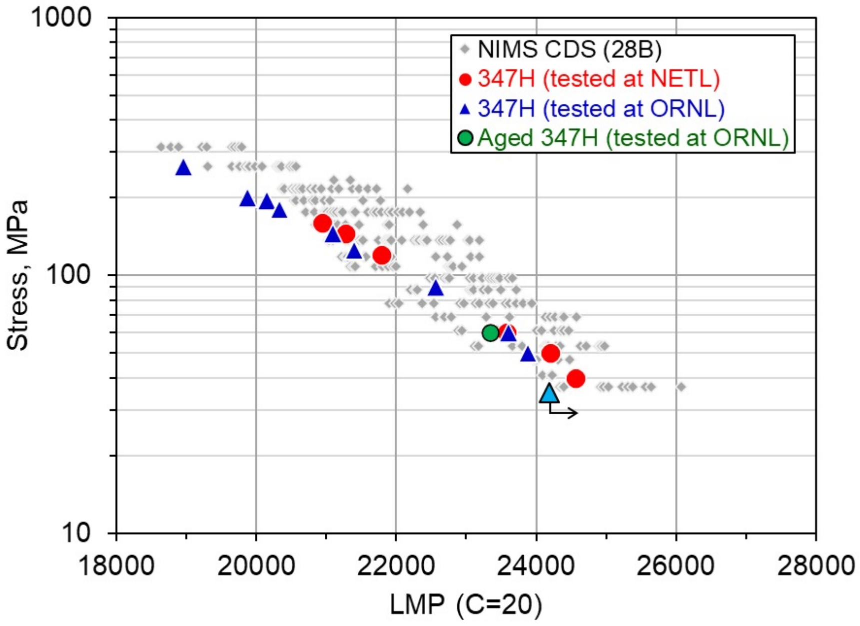


Signature of dynamic strain aging caused by interstitial and substitutional solutes

Creep-rupture properties (ORNL/NETL)



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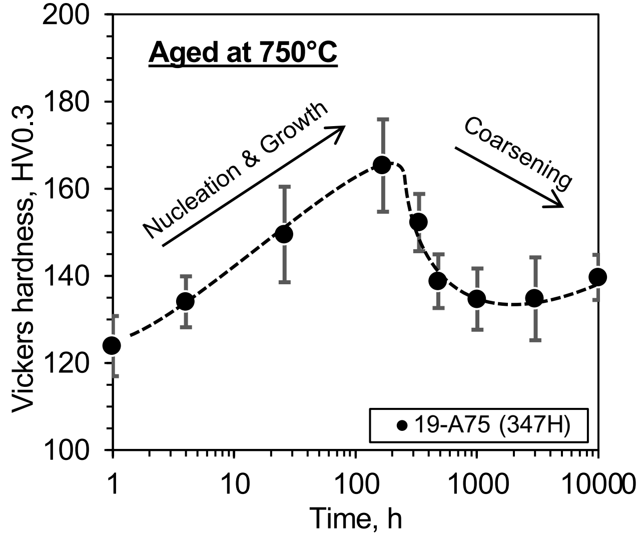
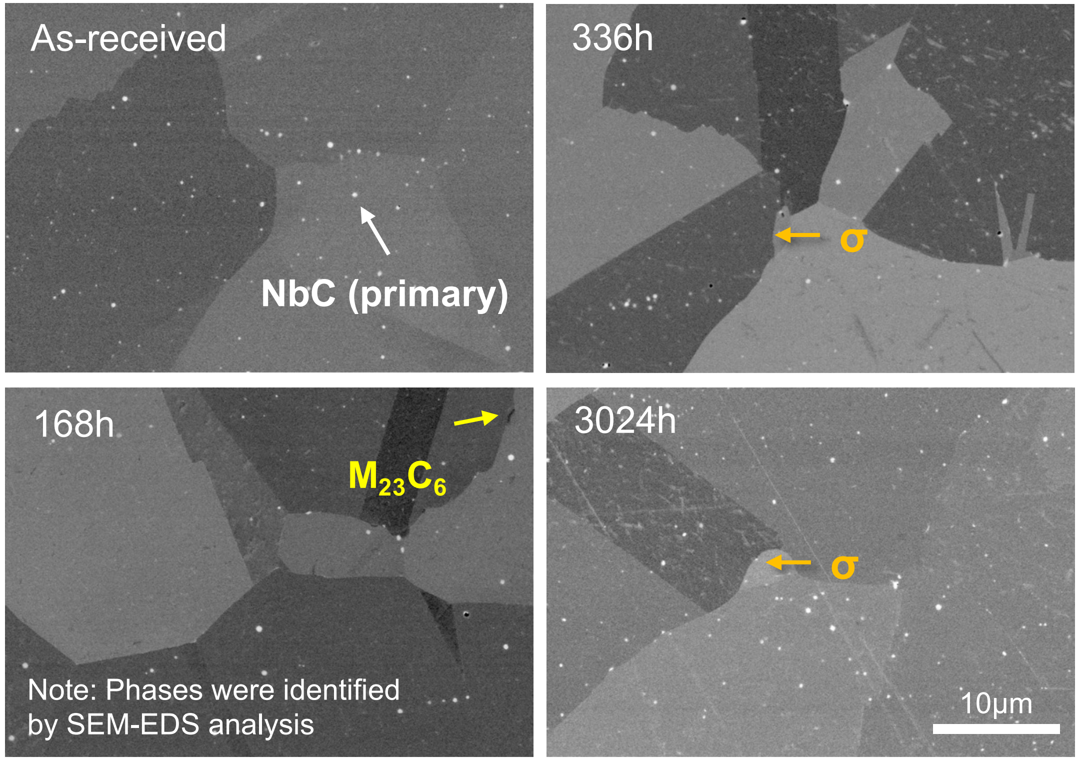
Microstructure Response in 347H During Isothermal Aging at 750°C

- Age hardening was observed
  - Hardness dropped after 168h
  - $M_{23}C_6$ gradually disappeared after the peak, instead sigma started to appear
  - No changes in primary NbC

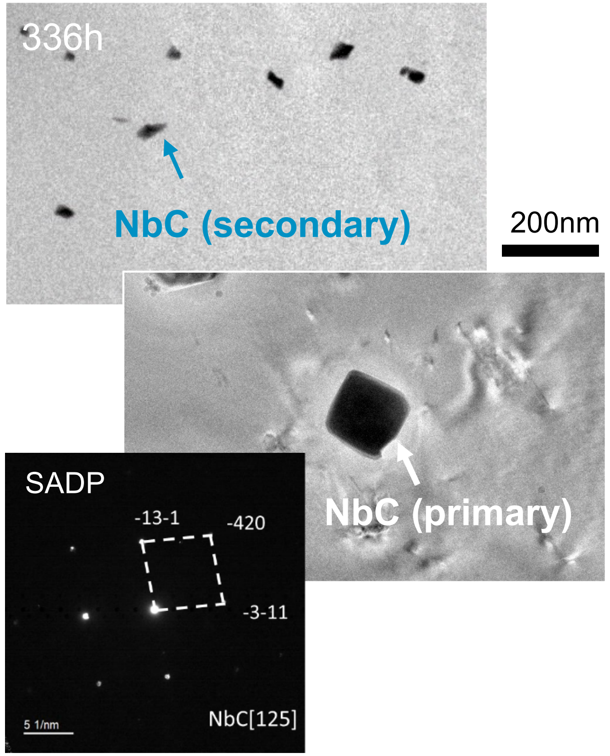
Vickers hardness vs. aging time



SEM BSE images (aged at 750°C)



TEM BF images



Primary NbC → NbC + $M_{23}C_6$ → NbC + $M_{23}C_6$ + σ → NbC + σ

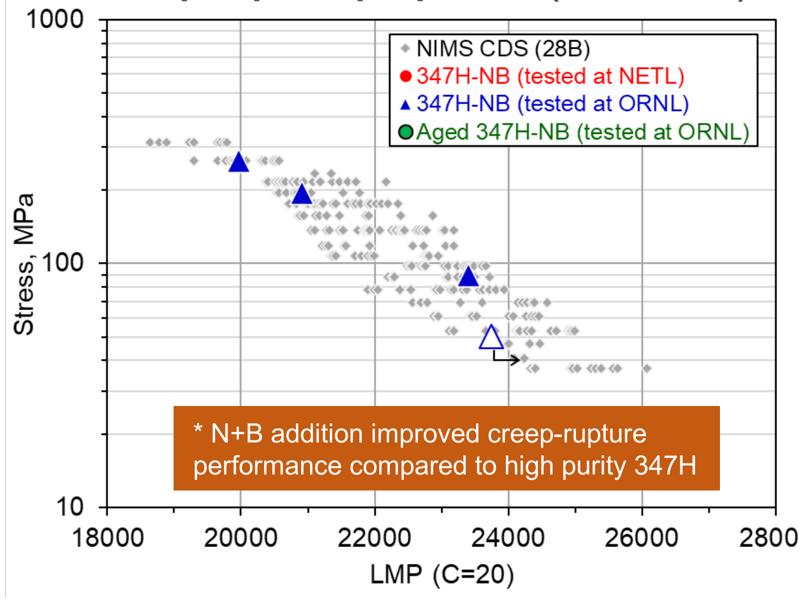
Secondary NbC also observed

AR | 4h 26h 168h | 334/336h | 482h 1008h 3024h

New 347H Heats Reveal Roles of N and B in Precipitation Kinetics

- Uni-axial creep-rupture tests at 600-800°C:
  - At ORNL/NETL
- Isothermal aging of 347H-N and 347H-N+B at 750°C:
  - Hardness measurement
  - Microstructure characterization

Creep-rupture properties (347H-N+B)



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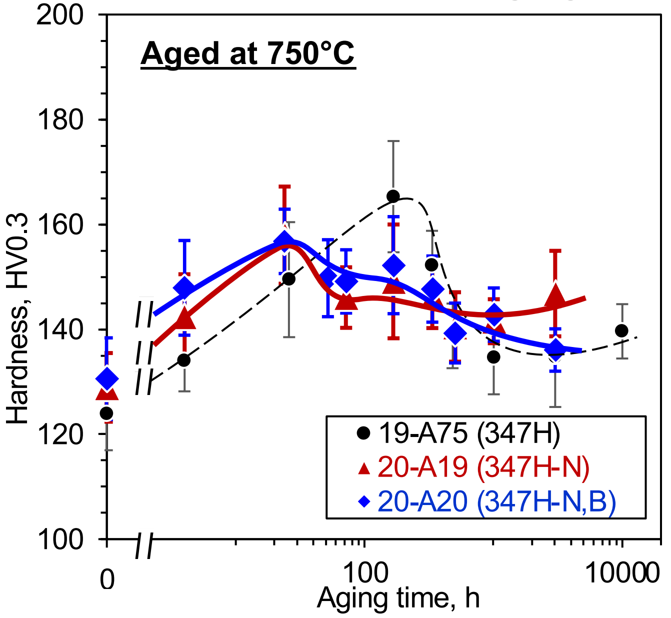
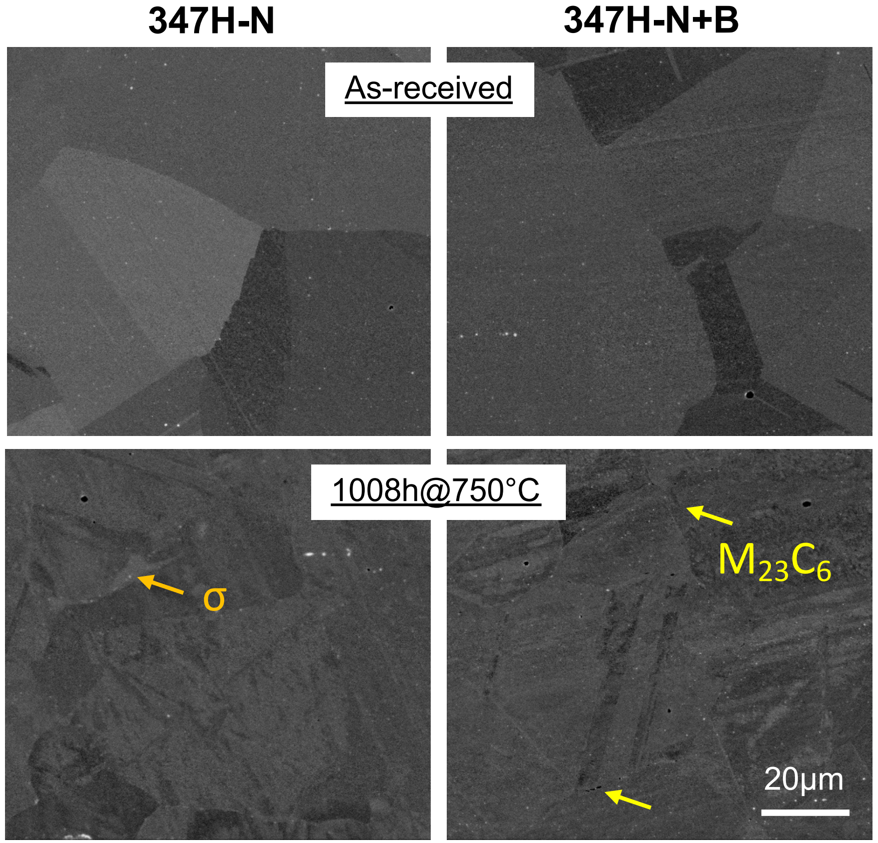


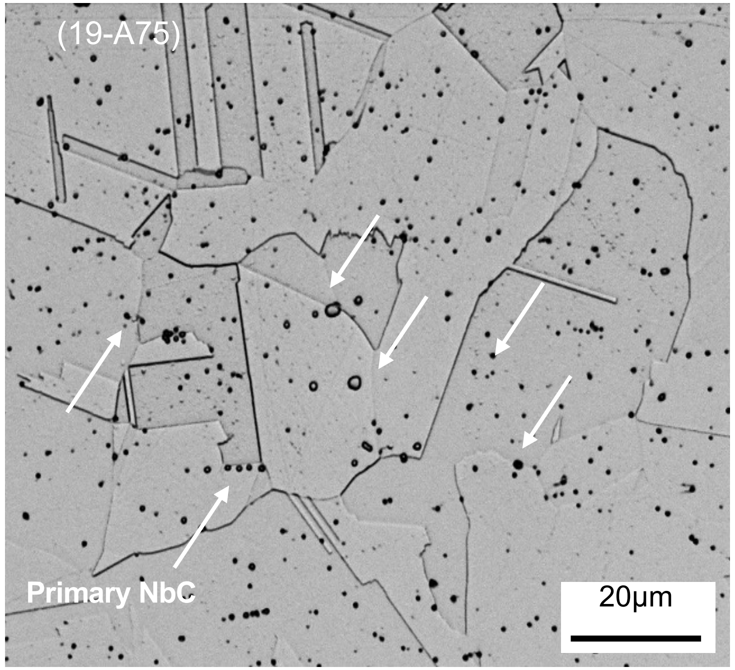
SEM-BSE images of aged heats



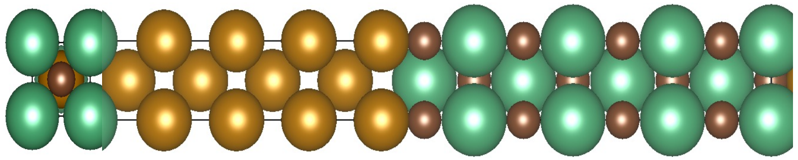
- N addition did not change as-received microstructure
- **B addition increased the stability of $M_{23}C_6$ at 750°C**

Approach

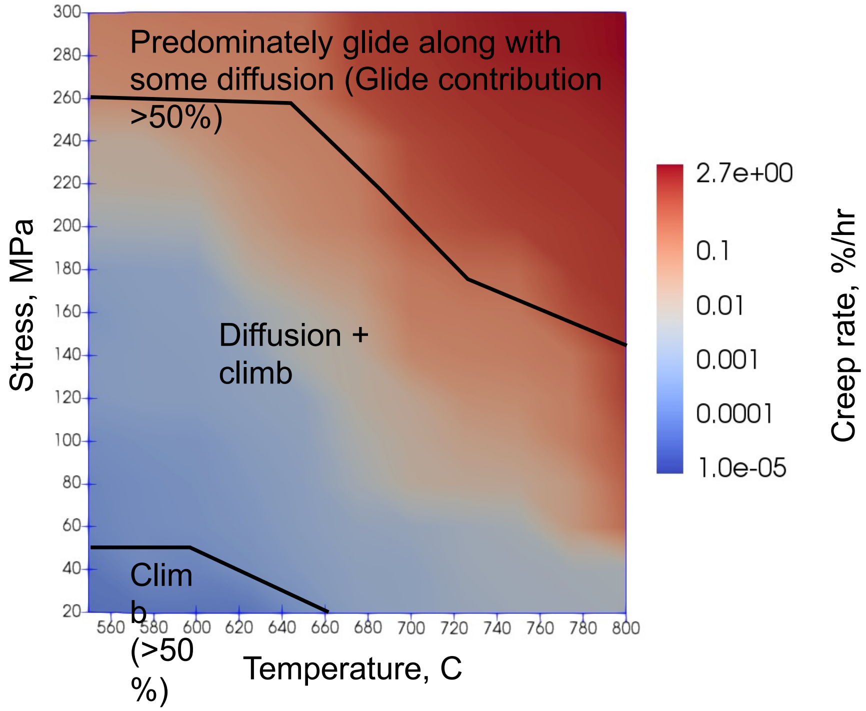
Materials processing and characterization: The role of aging and chemistry



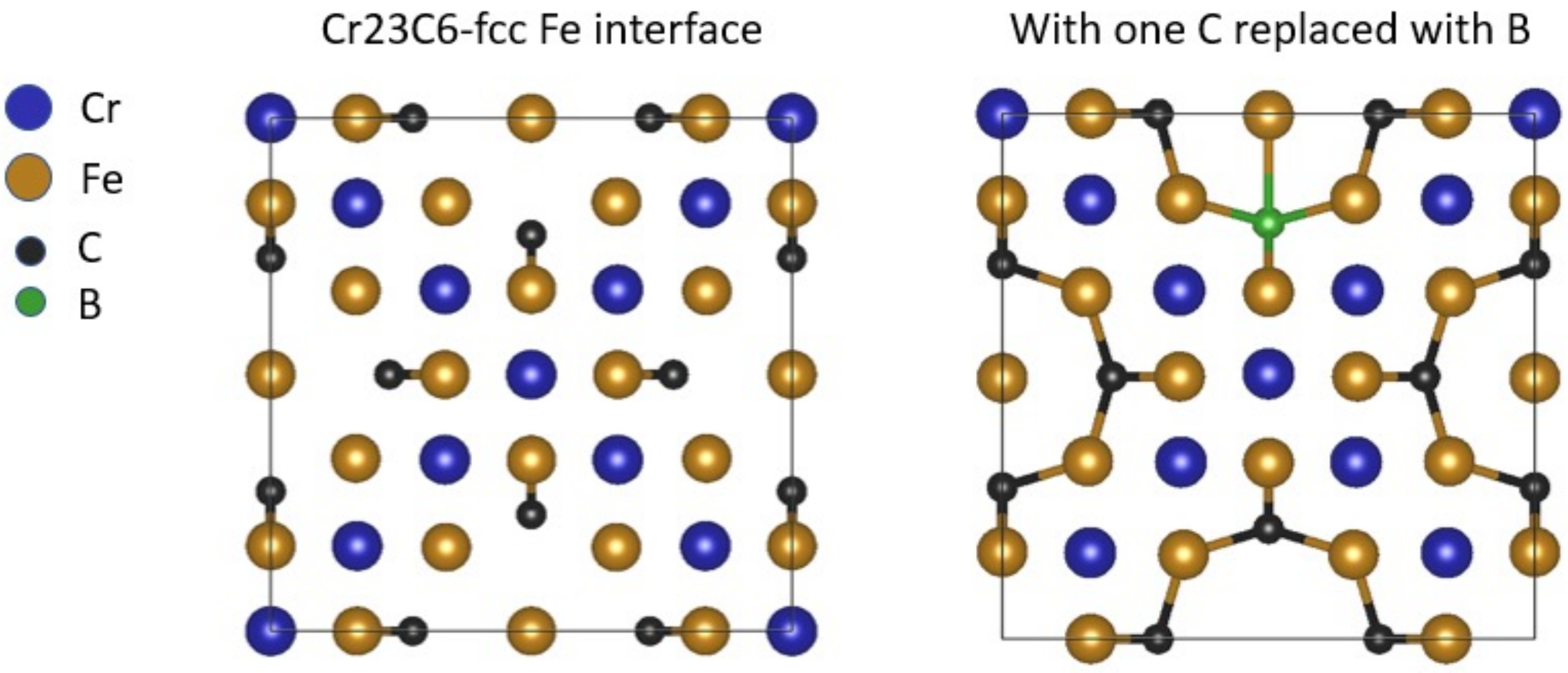
Understanding materials aging: DFT and Prisma simulations



Predicting the relationship between microstructure, chemistry and creep response

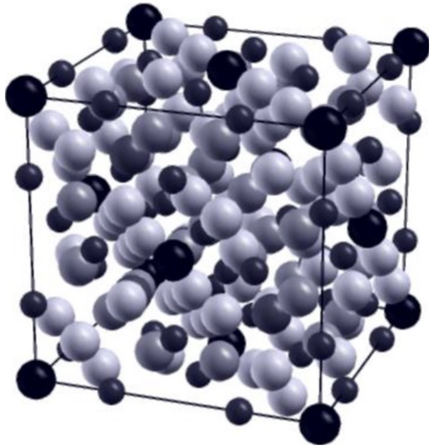


Atom of B at interface reduces fcc-Fe/$M_{23}C_6$ interface energy by 0.1 J/m^2- very significant value



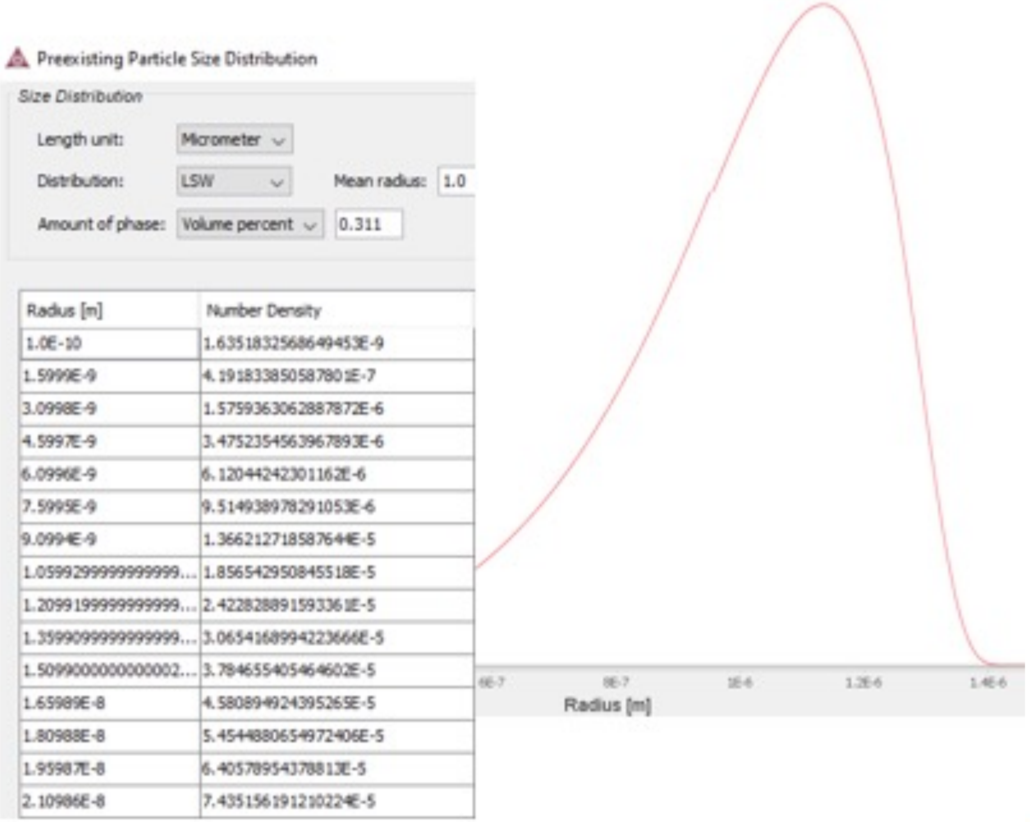
- Fe is projected onto the Cr-C layer.
- Confirmed Fe prefers the "hollow" positions.
- B significantly promotes covalent bonding between Fe-C.

- **Key Conclusion:** several ppm's of B promote ***interface ordering*** and increase stability of precipitates.
- **Interface energy reduction** reflects change in phase stability and in lattice misfit for interface, **enhancing creep retardation**



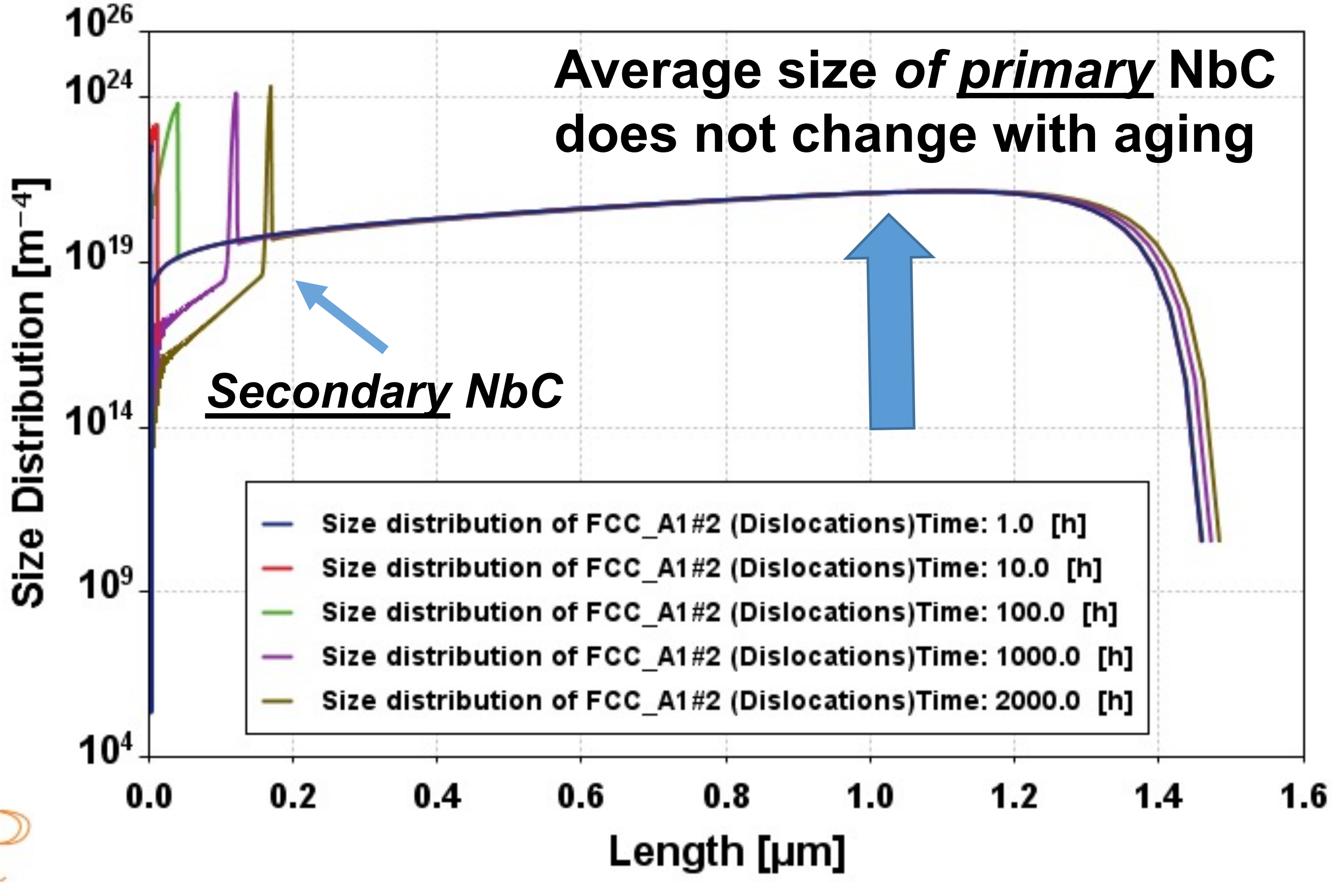
Primary and Secondary Nb(C,N) Particles Bimodal Distributions at 700°C

A *pre-existing* size distribution *<u>of primary NbC is introduced</u>*



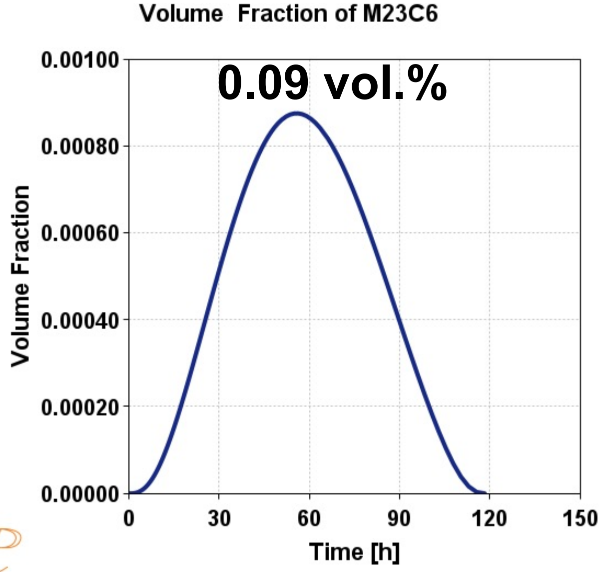
Radius [m]	Number Density
1.0E-10	1.6351832568649453E-9
1.5999E-9	4.191833850587801E-7
3.0998E-9	1.5759363062887872E-6
4.5997E-9	3.4752354563967893E-6
6.0996E-9	6.12044242301162E-6
7.5995E-9	9.514938978291053E-6
9.0994E-9	1.366212718587644E-5
1.0599299999999999...	1.856542950845518E-5
1.2099199999999999...	2.422828891593361E-5
1.3599099999999999...	3.0654168994223666E-5
1.5099000000000002...	3.784655405464602E-5
1.65989E-8	4.580894924395265E-5
1.80988E-8	5.4544880654972406E-5
1.95987E-8	6.40578954378813E-5
2.10986E-8	7.435156191210224E-5

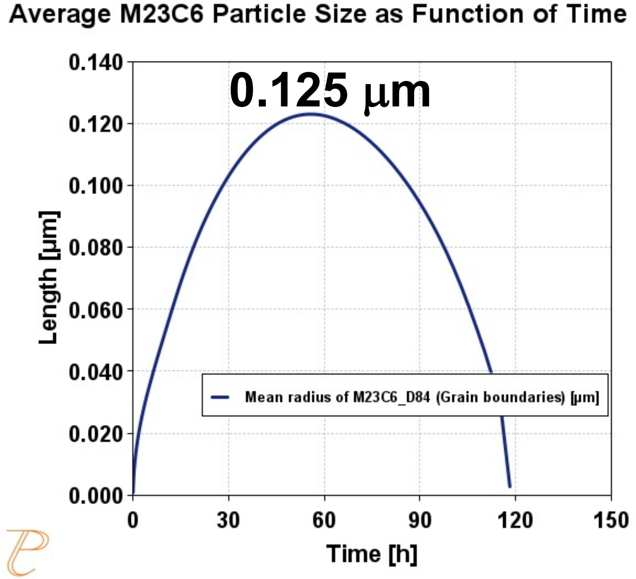
Bimodal Size Distributions of Primary and Secondary Nb(C,N) Particles: time 1h; 10h; 100h;1000h; and 2000h



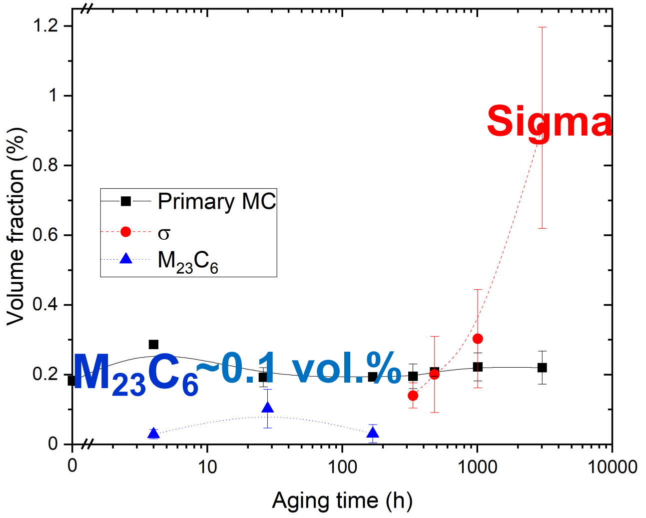
Predictions of aging kinetics and validation against experimental data

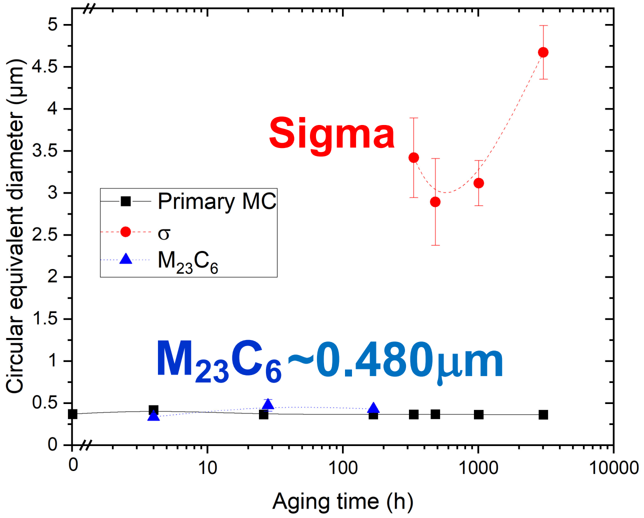
Modeling: $M_{23}C_6$





Experiment





- Prisma simulations are in good agreement with experimental data.
- The evolution volume fraction of M23C6 is consistent with microstructure characterization.
- The model accurately predicts the dissolution of M23C6 to the benefit of the sigma phase.

Approach

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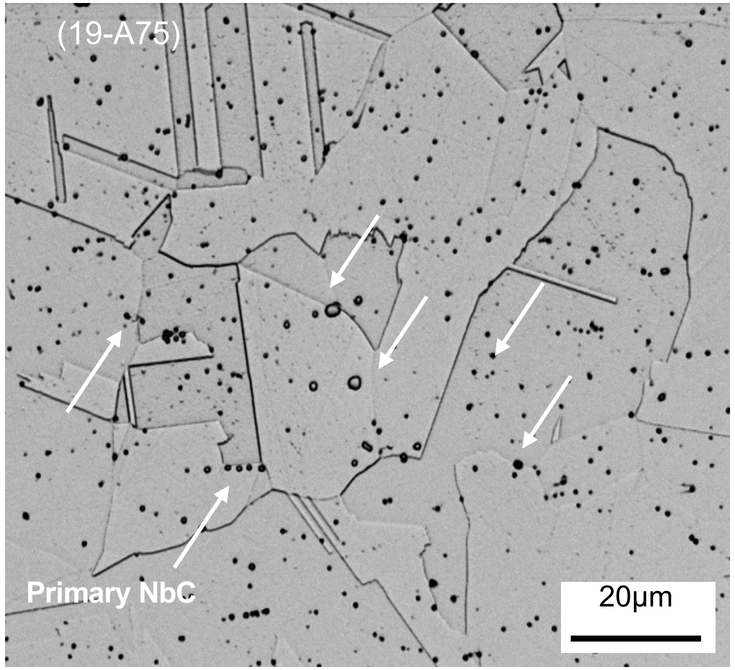

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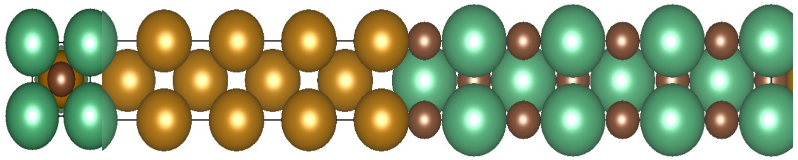
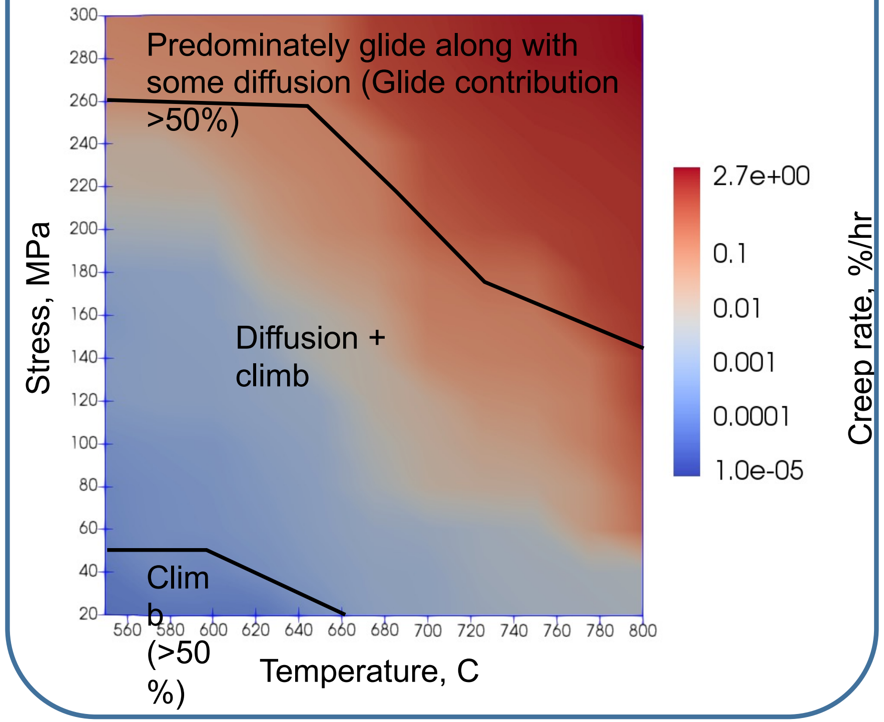


Predicting the relationship between microstructure, chemistry and creep response



A model predicting tensile and creep responses simultaneously

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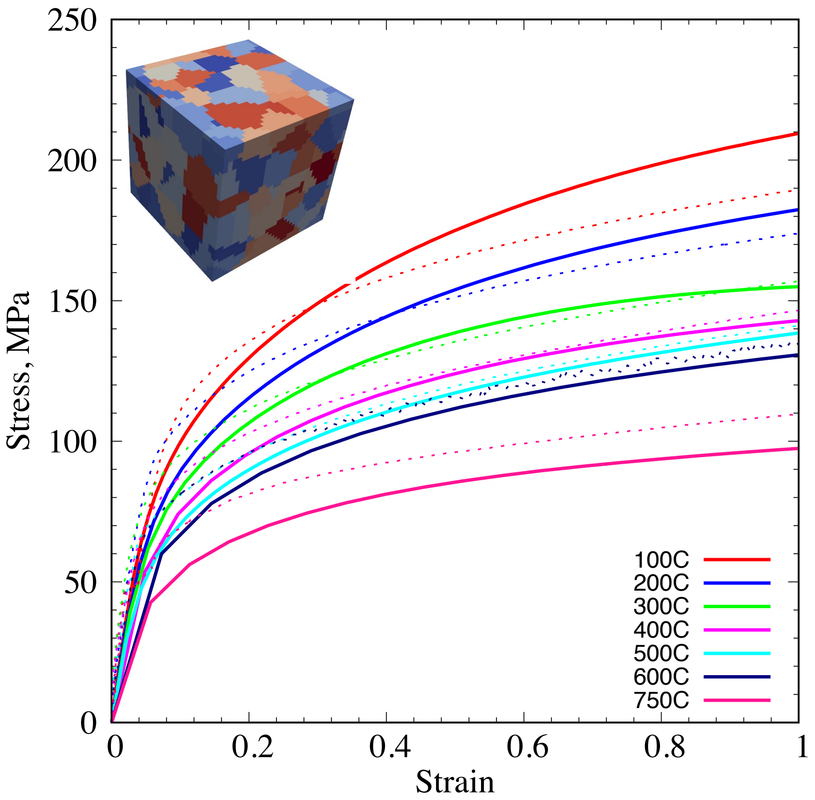
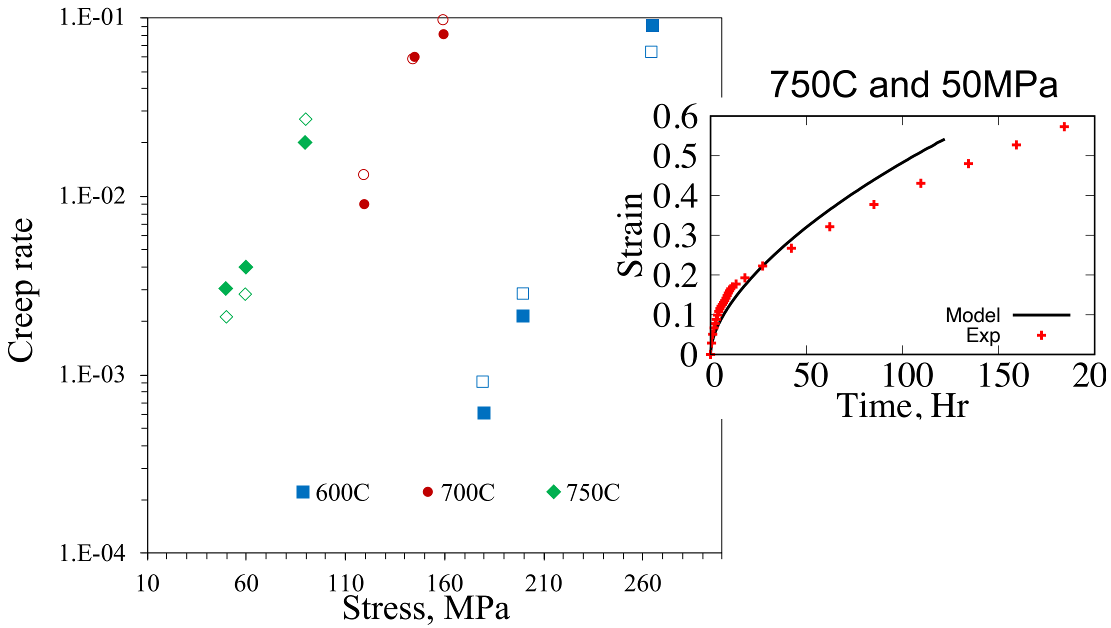
$$\rho_{cell} = 5\times10^{12}m^{-2};\ \rho_{CW} = 1\times10^{11}m^{-2}$$

$$N_{NbC} = 3.5\times10^{17}m^{-3};\ D_{NbC} = 330.0nm$$





- An Advanced polycrystal model was derived to predict the effects of precipitates (M23C6, sigma phase,NbC) and solutes (Cr, Ni) on the mechanical response of 347H like materials.
- All know deformation mechanisms are taken into account
- The model is sensitive to temperature, stress, microstructure and major elements concentration.
- The model can acceptably capture both the creep and uniaxial response of 347H for varying temperatures

A first synthetic deformation map

eXtremeMAT
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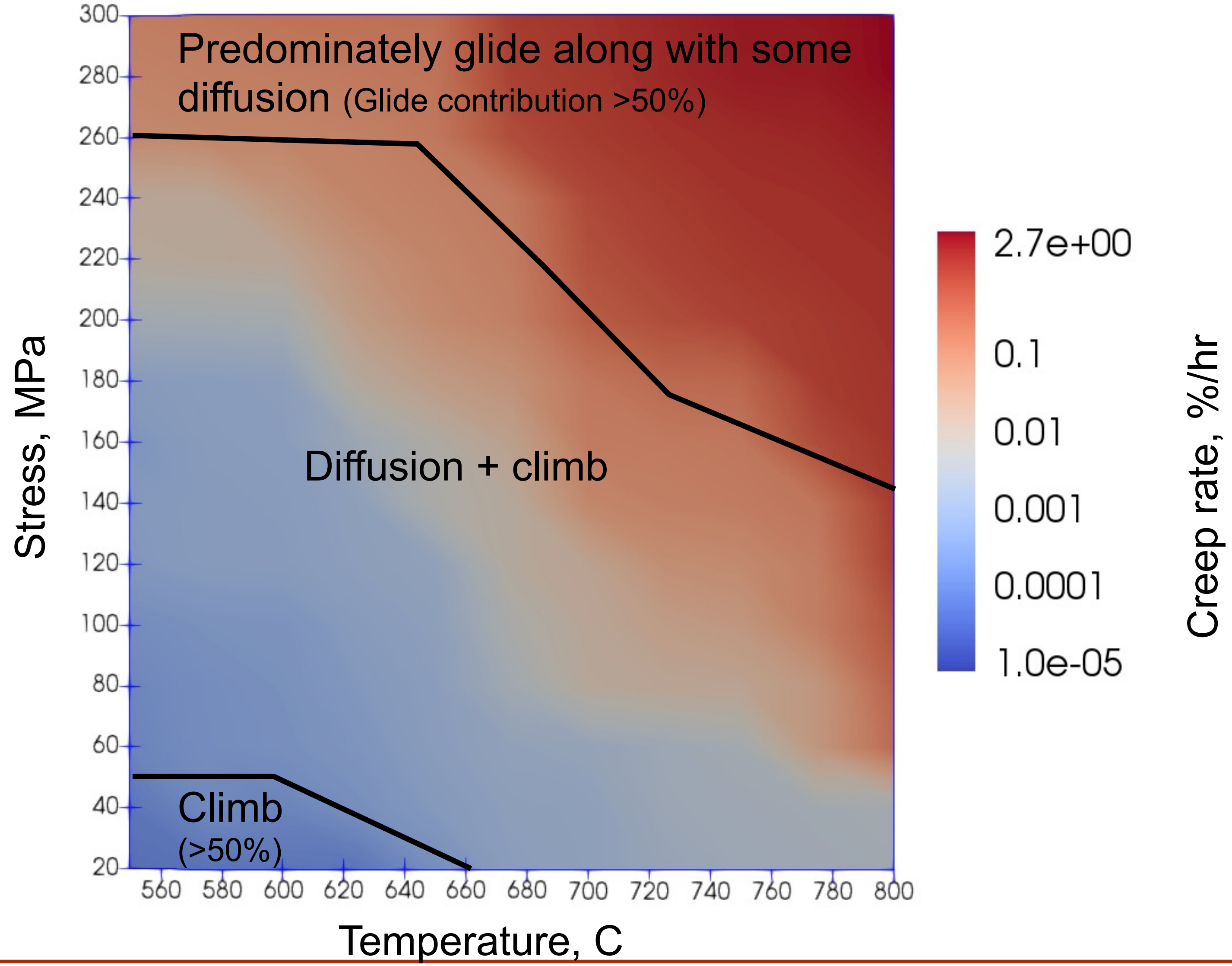
U.S. DEPARTMENT OF ENERGY



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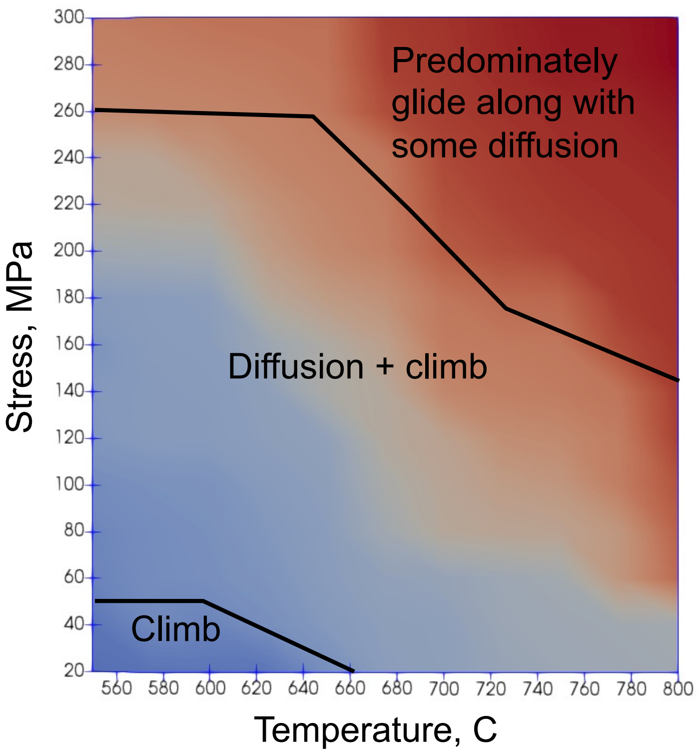
Quantifying the effect of microstructure on the creep response

Case 1: As received 347H steel

$\rho_{cell} = 5\times10^{12}m^{-2}; \rho_{CW} = 1\times10^{11}m^{-2}$

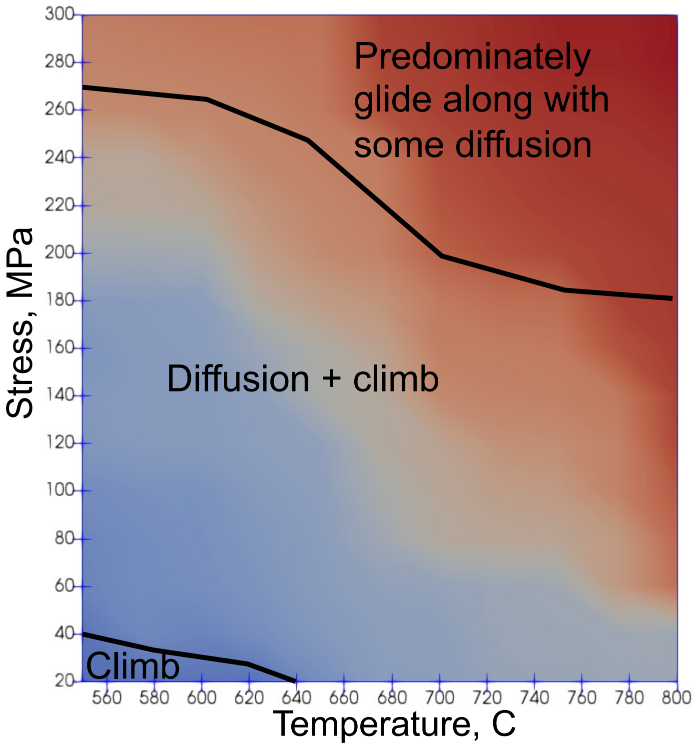
$N_{NbC} = 3.5\times10^{17}m^{-3}; D_{NbC} = 330.0nm$



Case 2: Heat treated but not fully aged

$\rho_{cell} = 2\times10^{12}m^{-2}; \rho_{CW} = 1\times10^{11}m^{-2}$

$N_{NbC} = 3.5\times10^{17}m^{-3}; D_{NbC} = 330.0nm$

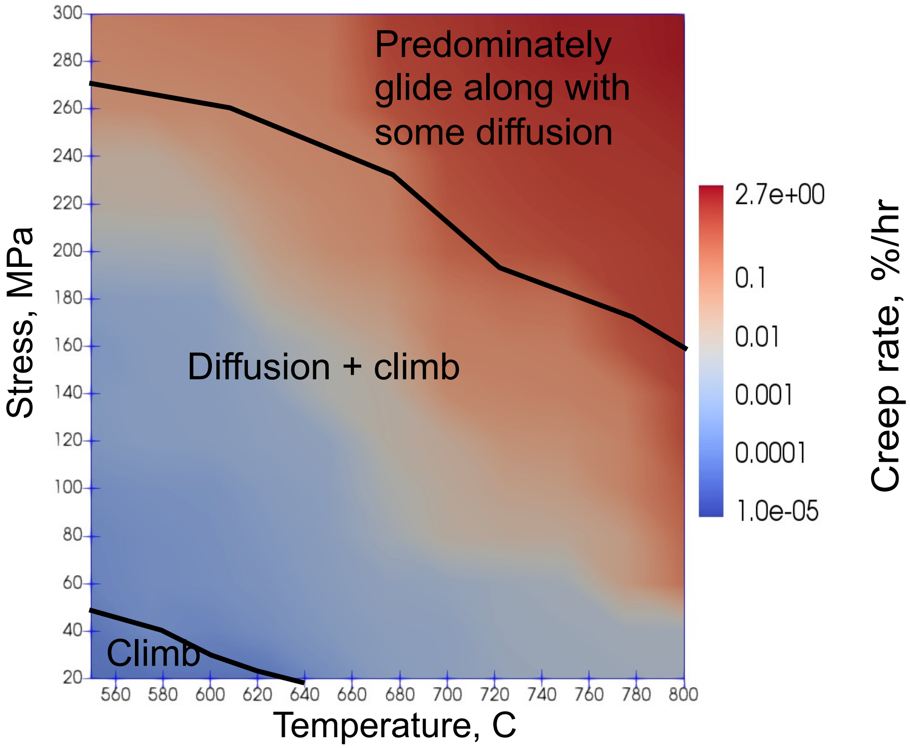


Case 3: Aged at 750C for 336h

$\rho_{cell} = 2\times10^{12}m^{-2}; \rho_{CW} = 1\times10^{11}m^{-2}$

$N_{NbC} = 3.5\times10^{17}m^{-3}; D_{NbC} = 330.0nm$

$N_{NbC}^{s} = 1.0\times10^{17}m^{-3}; D_{NbC}^{s} = 55.0nm$



Quantifying the effect of microstructure on the creep response

Case 1: As received 347H steel

$\rho_{cell} = 5{\times}10^{12} m^{-2}; \rho_{CW} = 1{\times}10^{11} m^{-2}$

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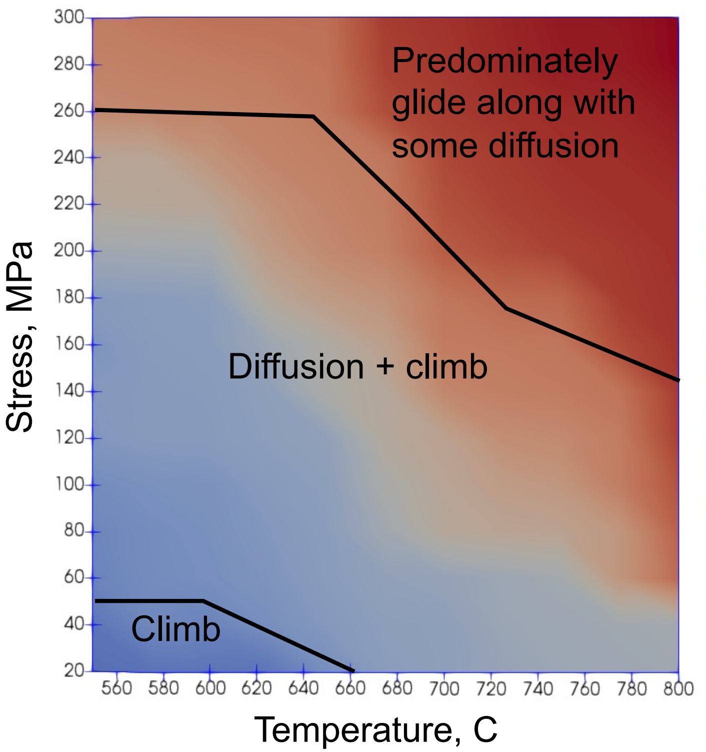
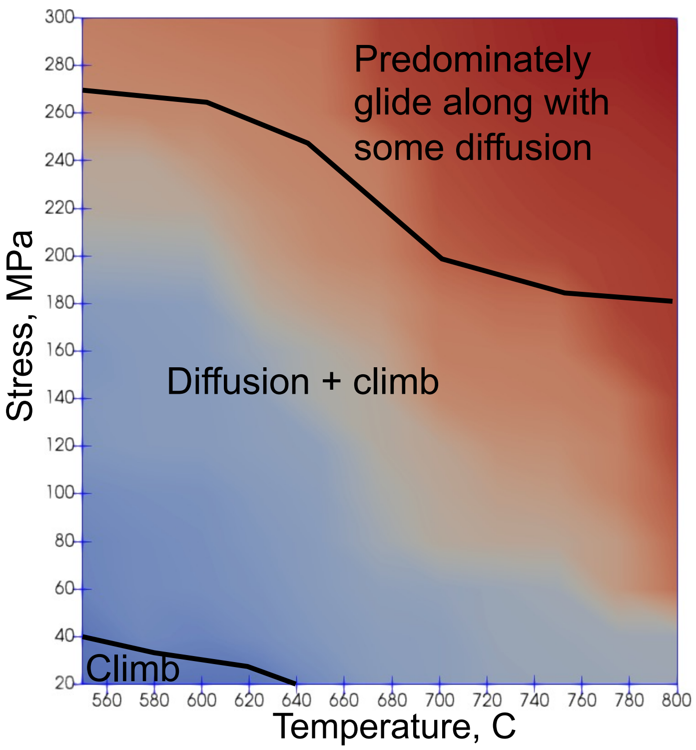


Case 2: Heat treated but not fully aged

$\rho_{cell} = 2{\times}10^{12} m^{-2}; \rho_{CW} = 1{\times}10^{11} m^{-2}$

$N_{NbC} = 3.5{\times}10^{17} m^{-3}; D_{NbC} = 330.0nm$



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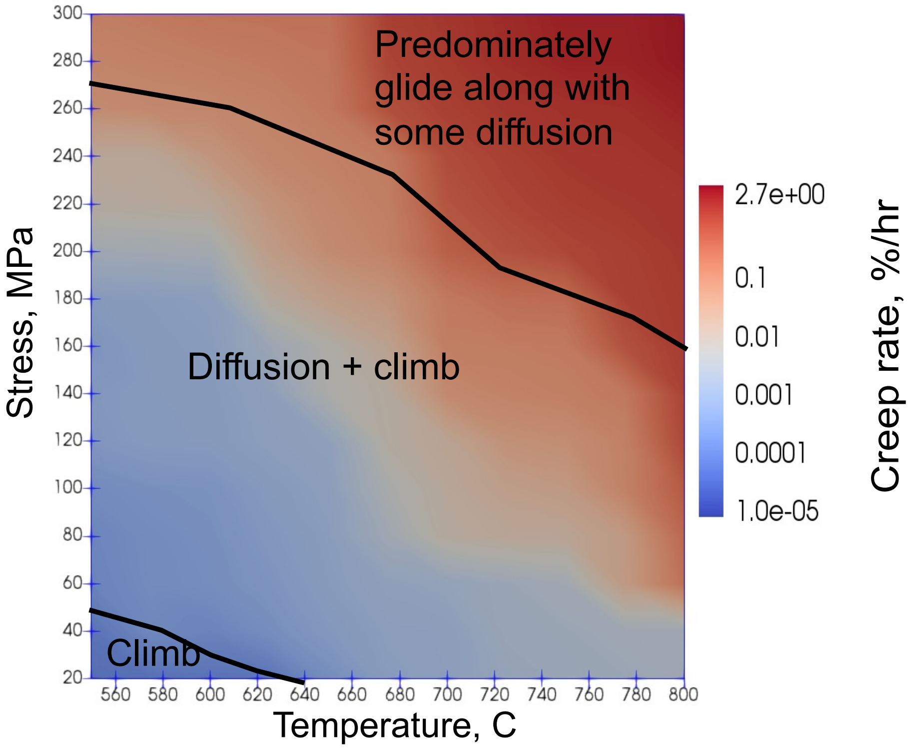
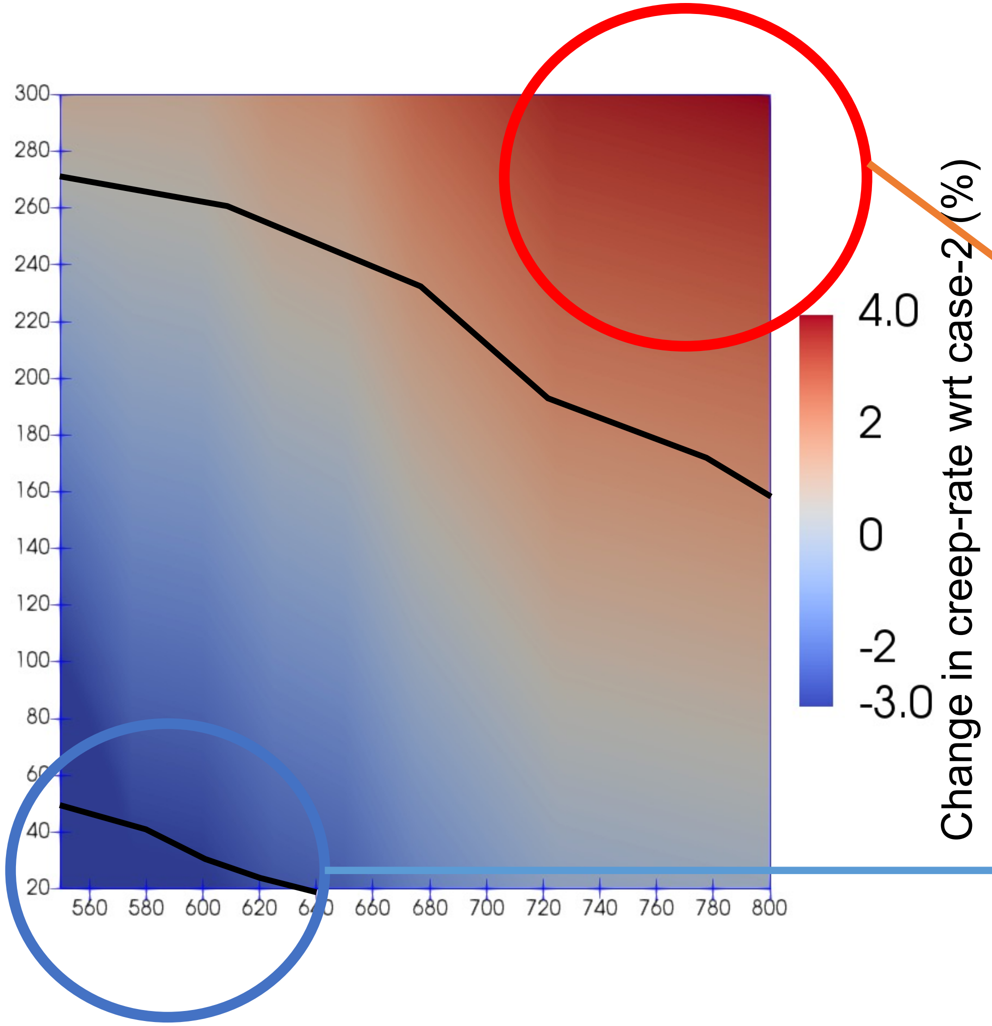
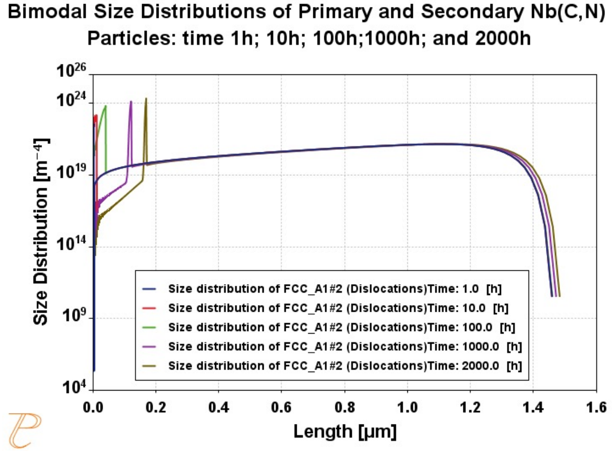


Effect of microstructure on changes in the creep-rate

Case 3: Aged at 750C for 336h

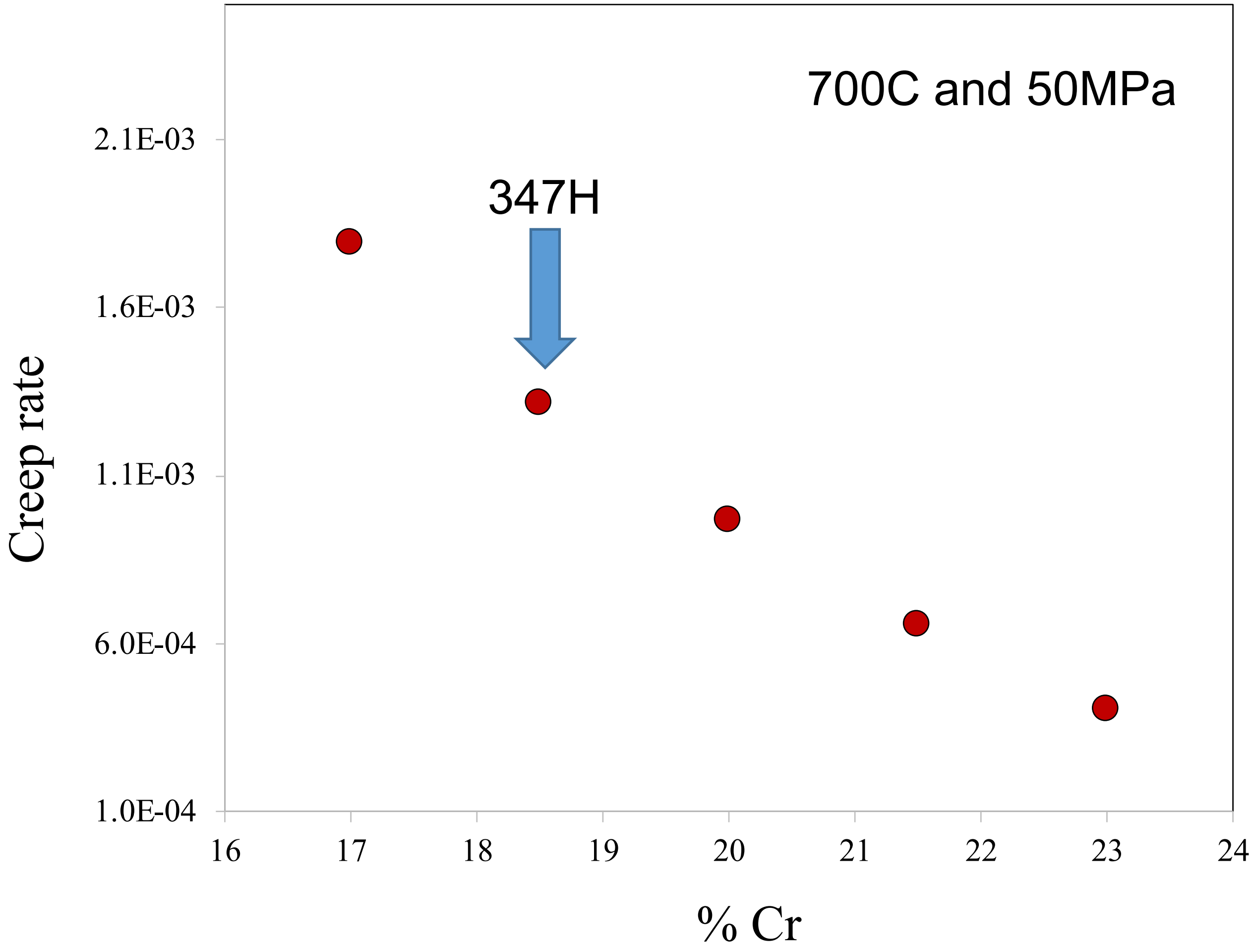


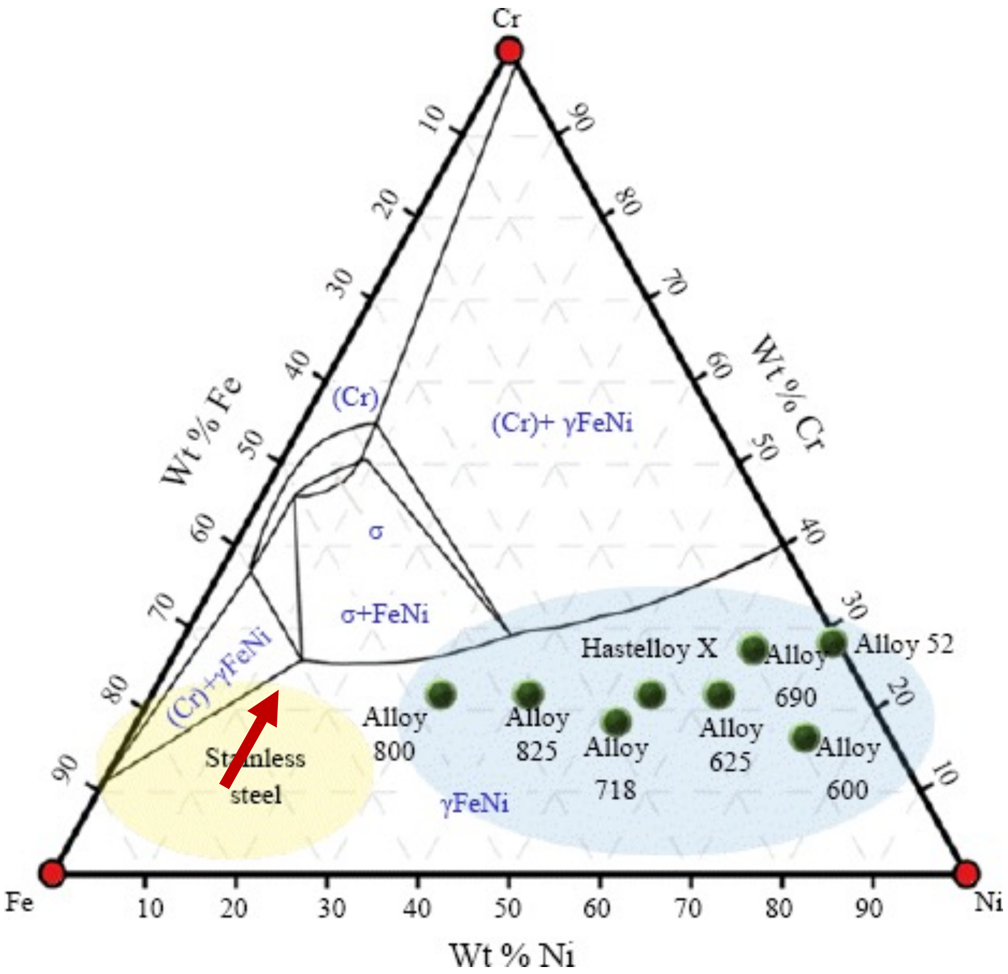


Glide dominated regime: The presence of secondary NbC can accelerate the creep rate (it delays dislocation annihilation→ more dilsocations can migrate)

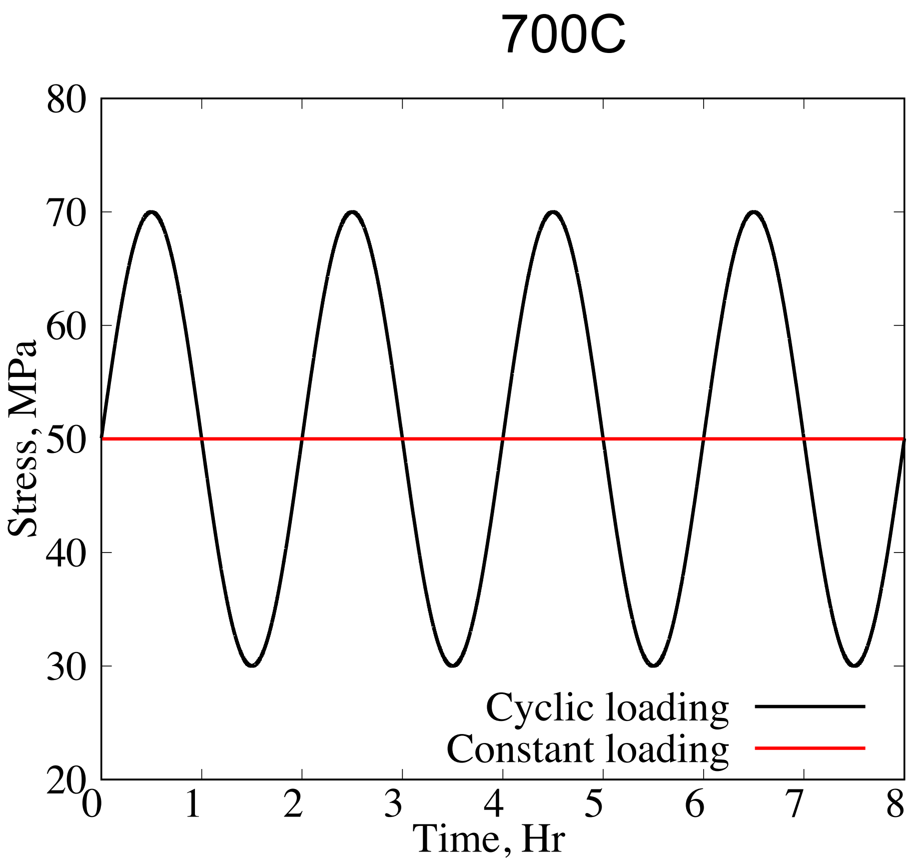
Climb dominated regime: The presence of secondary NbC can decelerate the creep rate (more overall climb events are necessary)

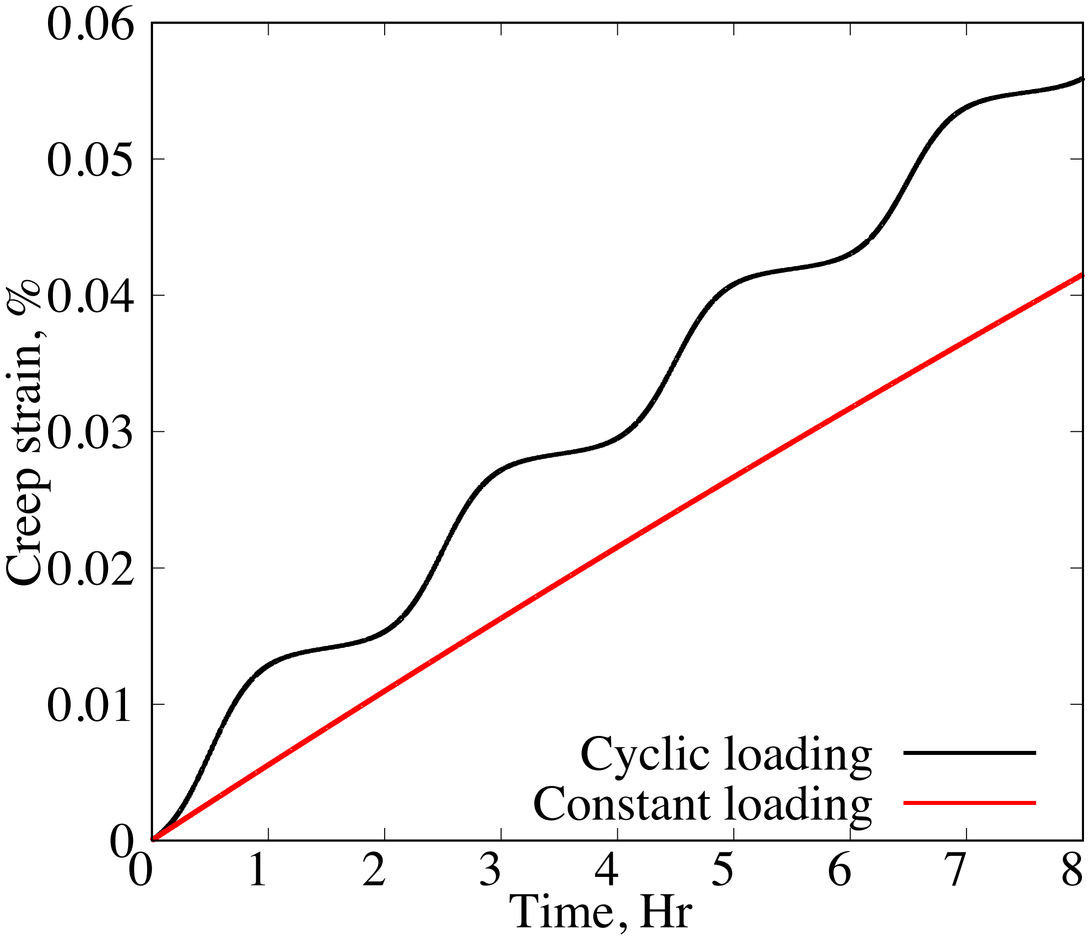
Chemistry effect: % Cr content





Simulation of cyclic loading





Conclusion

LaRupture: Models that predict the failure of steels as a function of microstructure (P91, 347H in progress)

LaRomance© : The suite of constitutive models for plasticity in extreme environments

LaMap: An experimentally validated (partially) predictor of the effects of microstructure and chemistry on the creep response of 347H steels