Improved Models of Long Term Creep Behavior of High Performance Structural Alloys for Existing and Advanced Technologies Fossil Energy Power Plants

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Abhinav Saboo[1], Qiaofu Zhang[1], Jiadong Gong[1], Greg Olson[1,2], David Dunand[2]

[1]QuesTek Innovations LLC

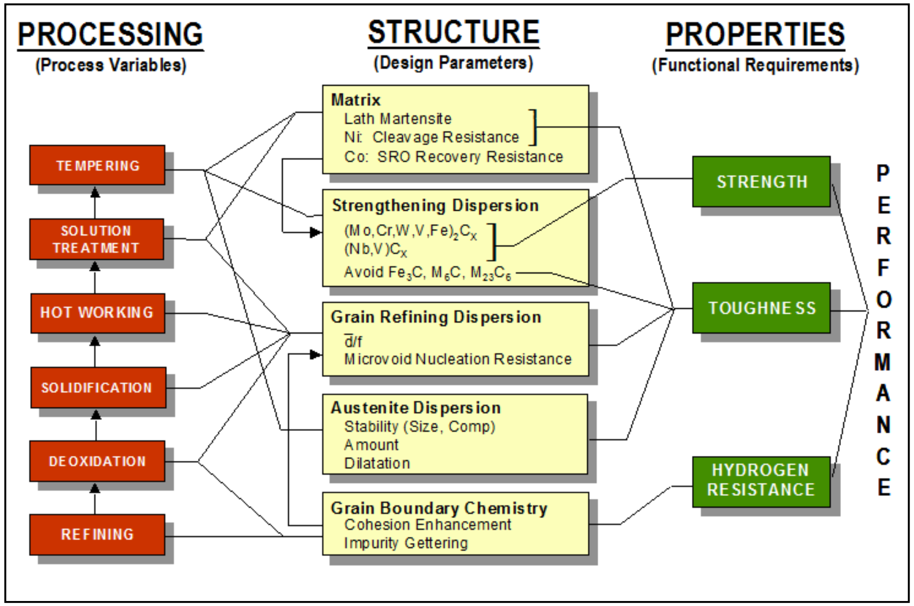
[2]Northwestern University

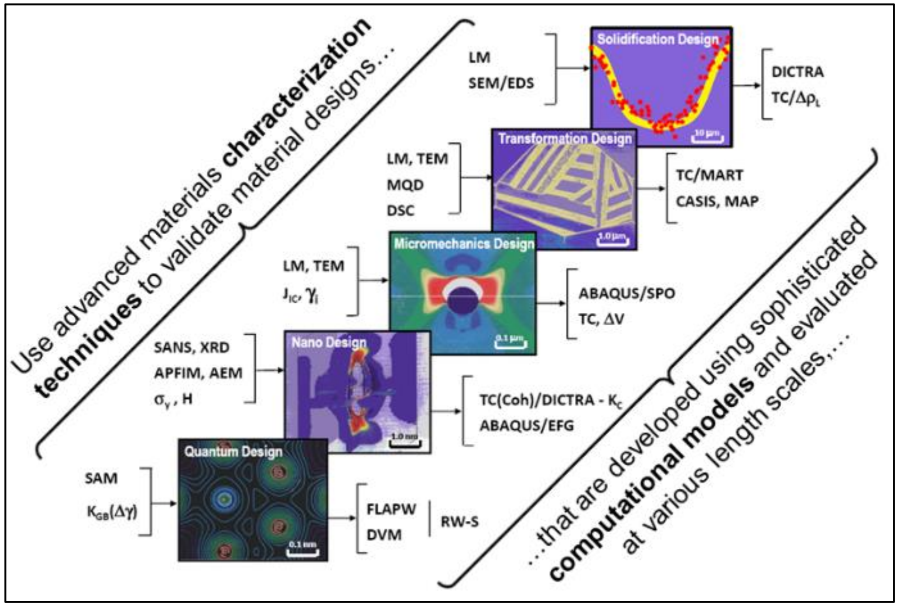
Introduction – QuesTek Innovations LLC

- Global leader in Integrated Computational Materials Engineering (ICME)
- Business model: design, develop and patent new materials and processes; license to Producers/OEMs/End-users
- In-house software, databases and models work across a range of alloy systems
- 12 US patents awarded; 18 US patents pending (>50 Foreign Patents filed)

QuesTek's Materials Design Process

- Systems-based design approach utilizing computational tools to model key process-structure and structure-property linkages
- Replacing the legacy trial-and-error approaches with parametric materials design
  → *Faster, cheaper, targeted material performance*





Multi-scale modeling of process-structure-property relationship for material design

U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

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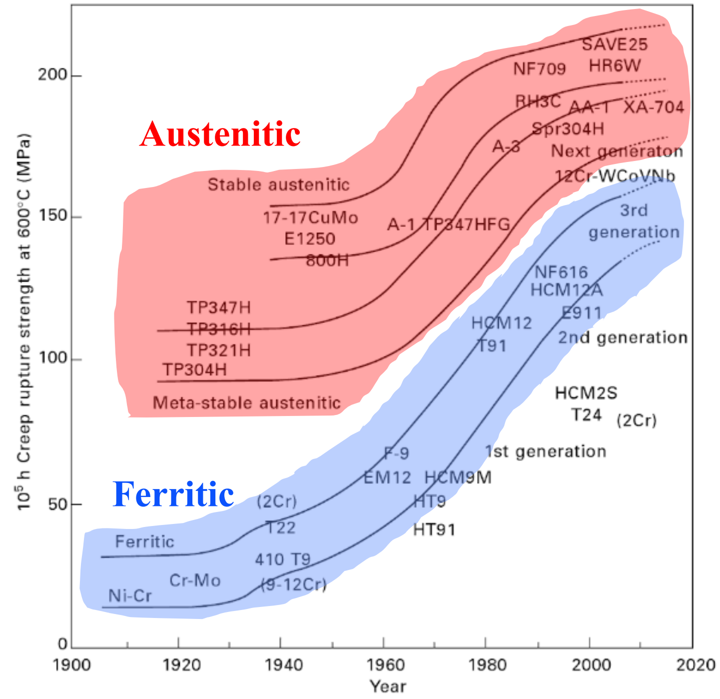
High performance structural alloys - Steels

- The hottest part of the boiler can have hoop stress as high as **100 MPa** and temperatures of around **550 ˚C or higher**
- Performance determined by 100,000 hours creep rupture strength at 600 ˚C
- Austenitic steels have better performance but more expensive than ferritic
- High performance **CSEF** (Creep Strength Enhanced Ferritic) **steels** developed
  - 9-12 %Cr steels like **Gr. 91**, Gr. 122 steels
  - Additions of Mo,V,Nb,W,B for formation of stable microstructure resistant to creep

Historical improvement of creep rupture strength of boiler steels [1]



Composition of Grade 91 steels (wt%)

	C	Si	Nb	V	N	Ni	Cr	Mo	Cu
Grade 91	0.09	0.29	0.072	0.22	0.044	0.28	8.7	0.90	0.032

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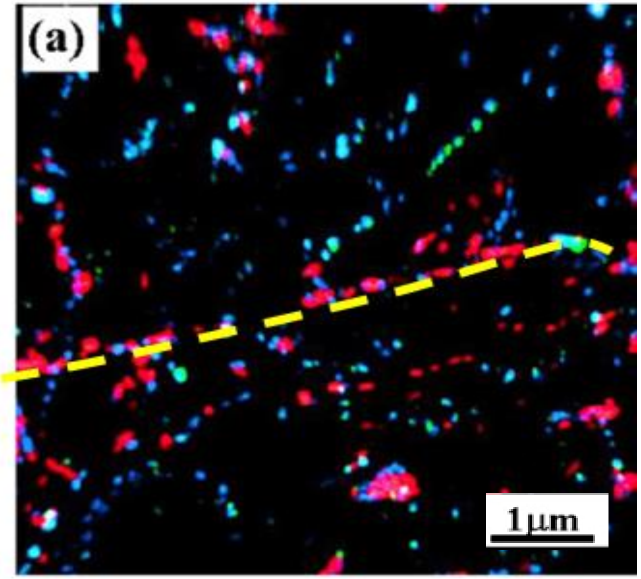
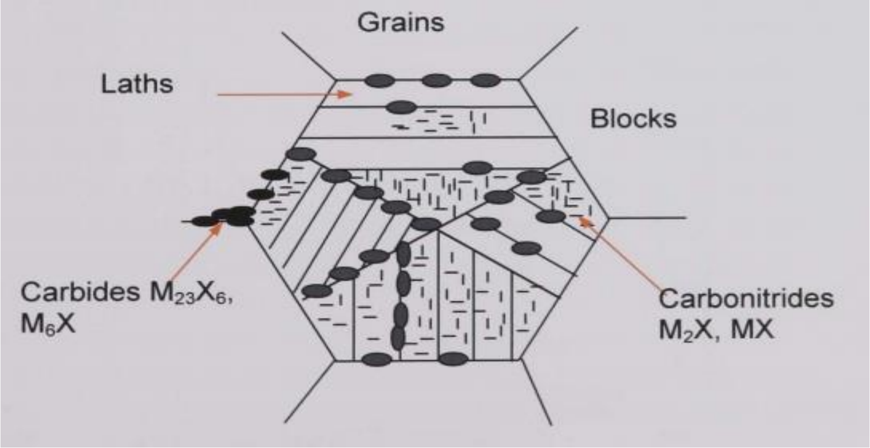
[1] Abe, Fujio, Torsten-Ulf Kern, and Ramaswamy Viswanathan, eds. Creep-resistant steels. Elsevier, 2008.

About Grade 91 steels - Microstructure

- Tempered martensitic hierarchical microstructure – PAGB, block and packets, laths
- $M_{23}C_6$ precipitates on PAGB and lath boundaries
- Nano-sized MX precipitates homogeneously distributed in the grains

TEM micrographs of carbon replica from as heat treated Grade 91 steels[1]





$(Fe, Cr, Mo)_{23}C_6$

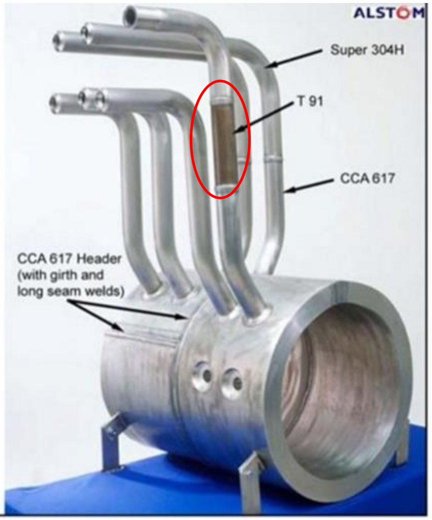
VX

NbX

[1] Sawada, K., et al. "Microstructural degradation of Gr. 91 steel during creep under low stress." Materials Science and Engineering: A 528.16 (2011): 5511-5518.

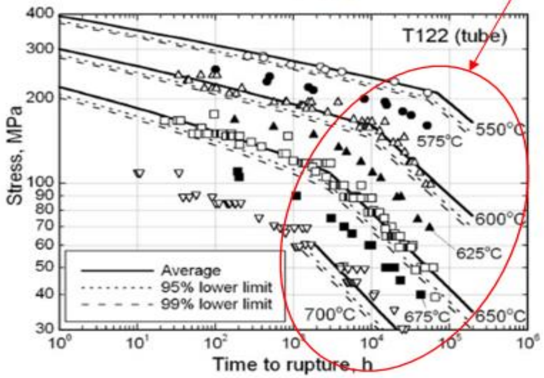
Problem statement

- The problem:
  - Loss of creep strength in long term creep in ferritic steels
  - Overestimation of allowable stress by extrapolation of short term data.
- The goal:
  - To develop a physics-based mechanistic long term creep model for existing ferritic alloys
  - Use the model in efficient design of power plant

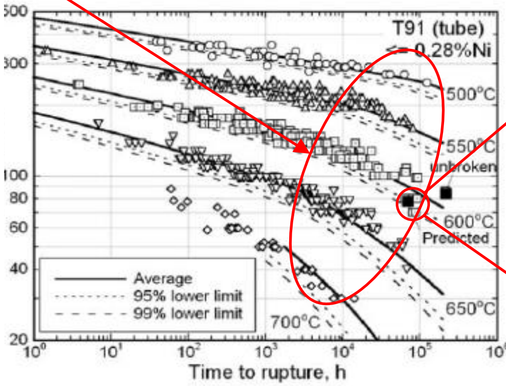


Steeper creep strength drop

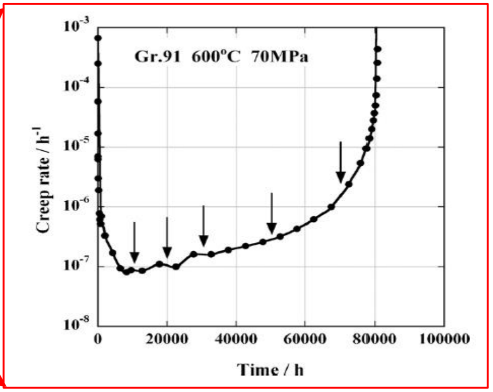
T122[1]



T91



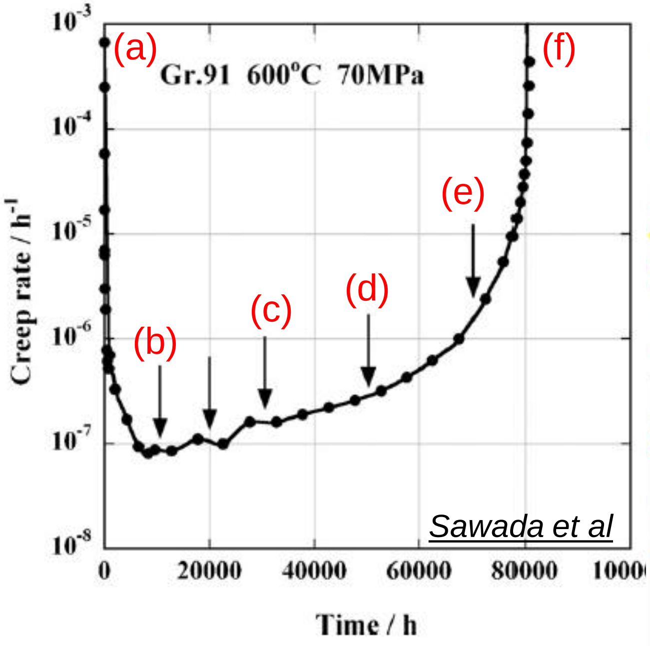
[2]



[1] Kimura, K et al (2008). STRESS DEPENDENCE OF DEGRADATION AND CREEP RUPTURE LIFE OF CREEP STRENGTH ENHANCED FERRITIC STEELS. 601-615. 10.1361/cp2007epri0601.

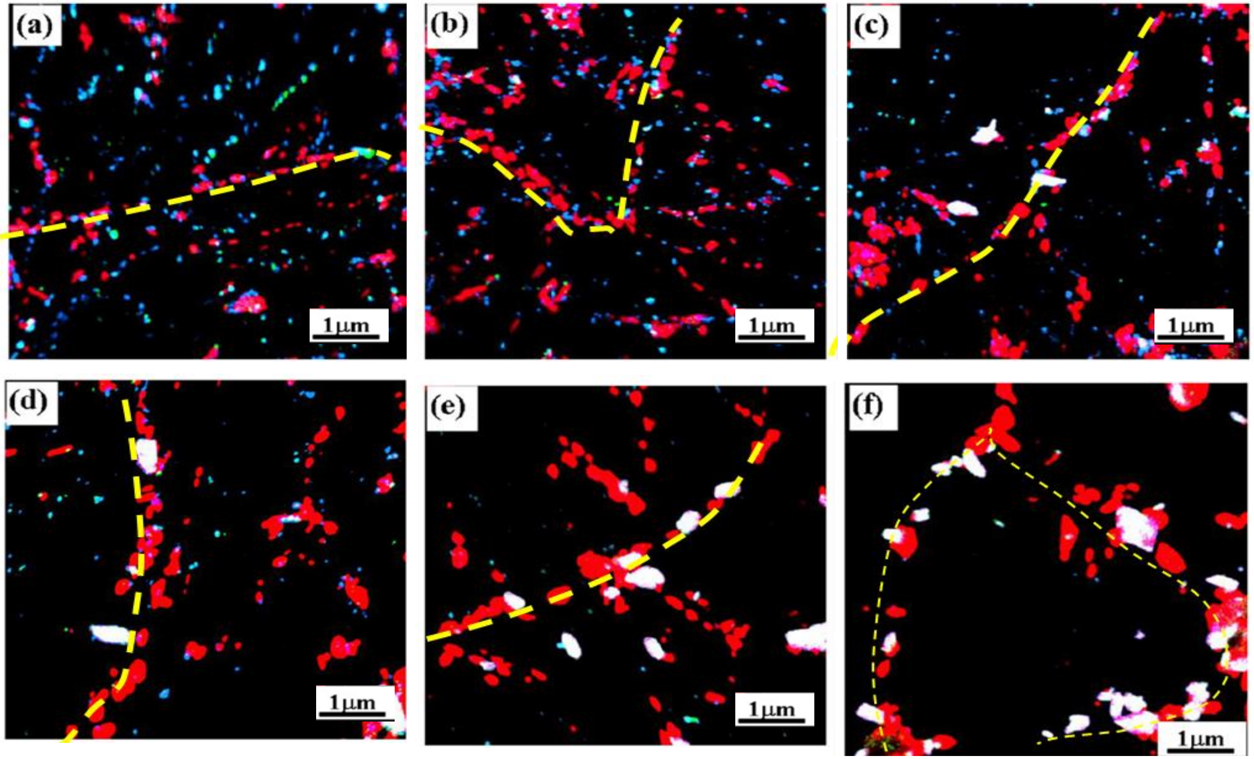
[2] Sawada, K., et al. "Microstructural degradation of Gr. 91 steel during creep under low stress." Materials Science and Engineering: A 528.16 (2011): 5511-5518.

Microstructural evolution during creep



Sawada et al

Microstructures from Sawada et al



$(Fe, Cr, Mo)_{23}C_6$

VX, NbX

Z-Phase

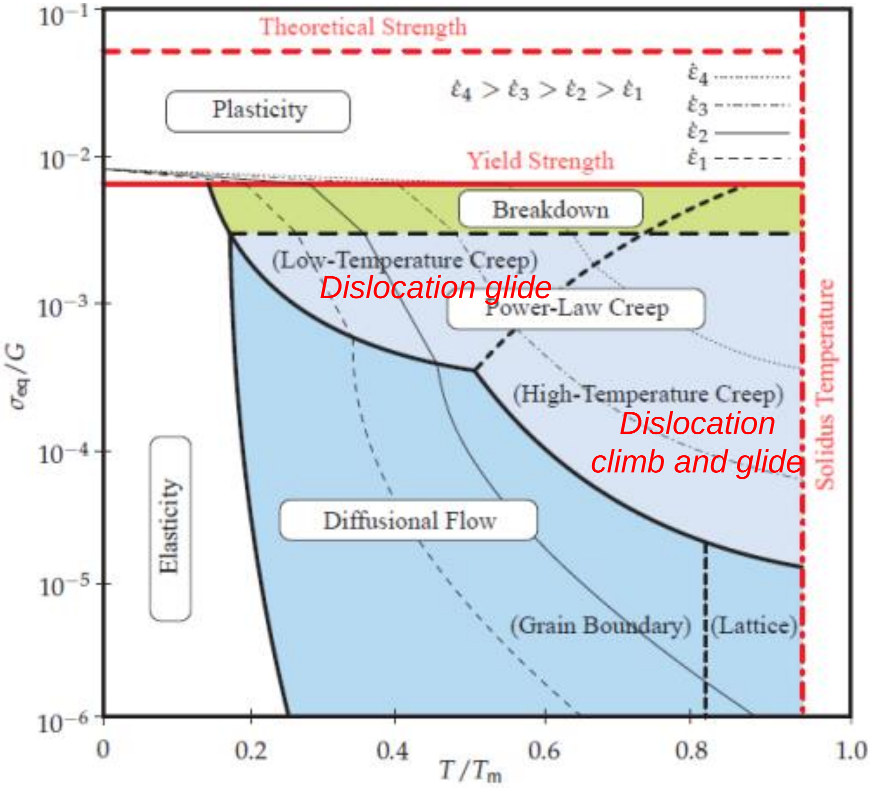
Dissolution of MX strengthening phase due to precipitation of Z-Phase responsible for accelerated creep deformation

Need for a microstructural sensitive creep model

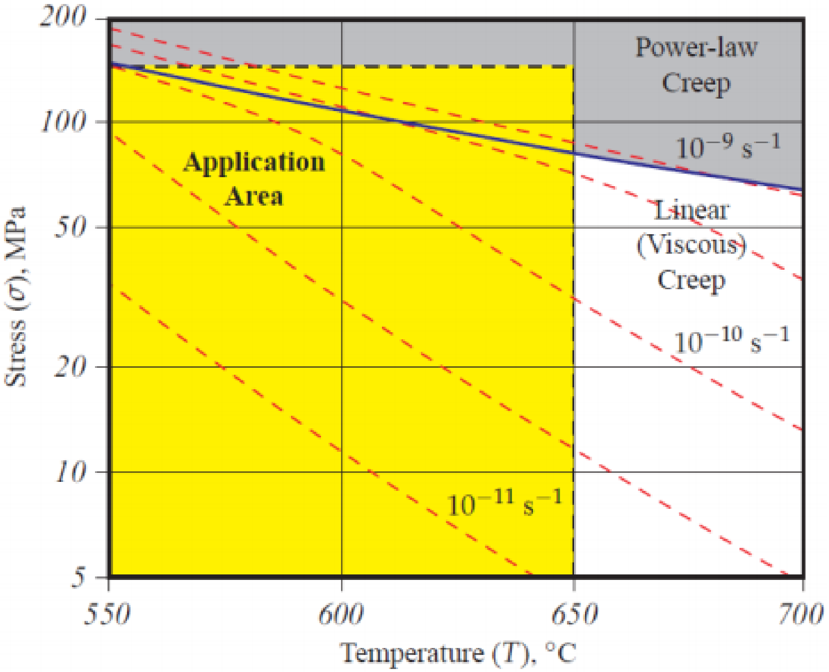
Sawada, K., et al. "Microstructural degradation of Gr. 91 steel during creep under low stress." Materials Science and Engineering: A 528.16 (2011): 5511-5518.

Creep model – deformation-mechanism maps

General deformation-mechanism map



Deformation-mechanism map for Grade 91 steels



Application area includes combination of power-law creep (dislocation glide and climb) and diffusional creep

Kalyanasundaram, Valliappa. *Creep, fatigue and creep-fatigue interactions in modified 9% Chromium-1% Molybdenum (P91) steels*. University of Arkansas, 2013.

Creep model

- According to the Orowan's equation, steady state creep rate for the dislocation type creep is given by (assuming that the glide time is negligible compared to the climb time):

$$\dot{\epsilon} = \rho_m b v \;= \rho_m b \,\frac{\lambda}{t} = \rho_m \; b \;\frac{\lambda}{t_c + t_g}$$

$$\approx \; \rho_m \; b \;\frac{\lambda}{t_c}$$

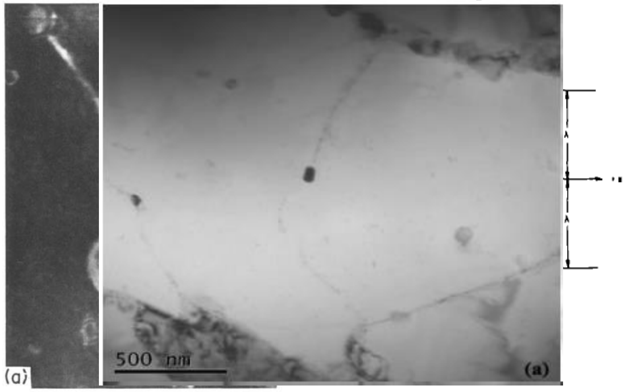
- What controls the climb time?

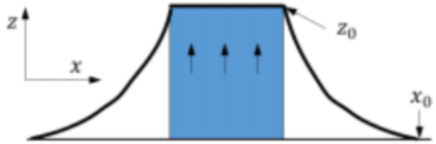
$$t_c = t_{general\ climb} + t_{local\ climb} + \; t_{detachment}$$

- λ is the inter-particle spacing (**Microstructural Input**)

Dislocation pinning – detachment mechanism in oxide strengthened Ni[*]

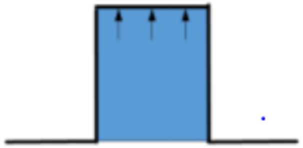
Pinning of dislocation by the MX particles in Gr.91 steels





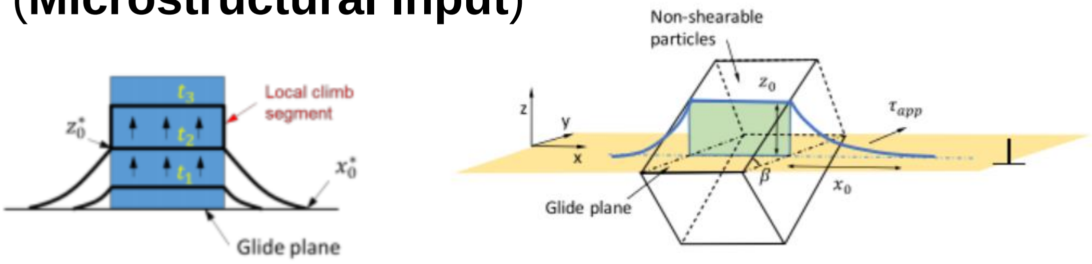
General Climb

Dominant at low Stresses



Local Climb

Dominant at high Stresses



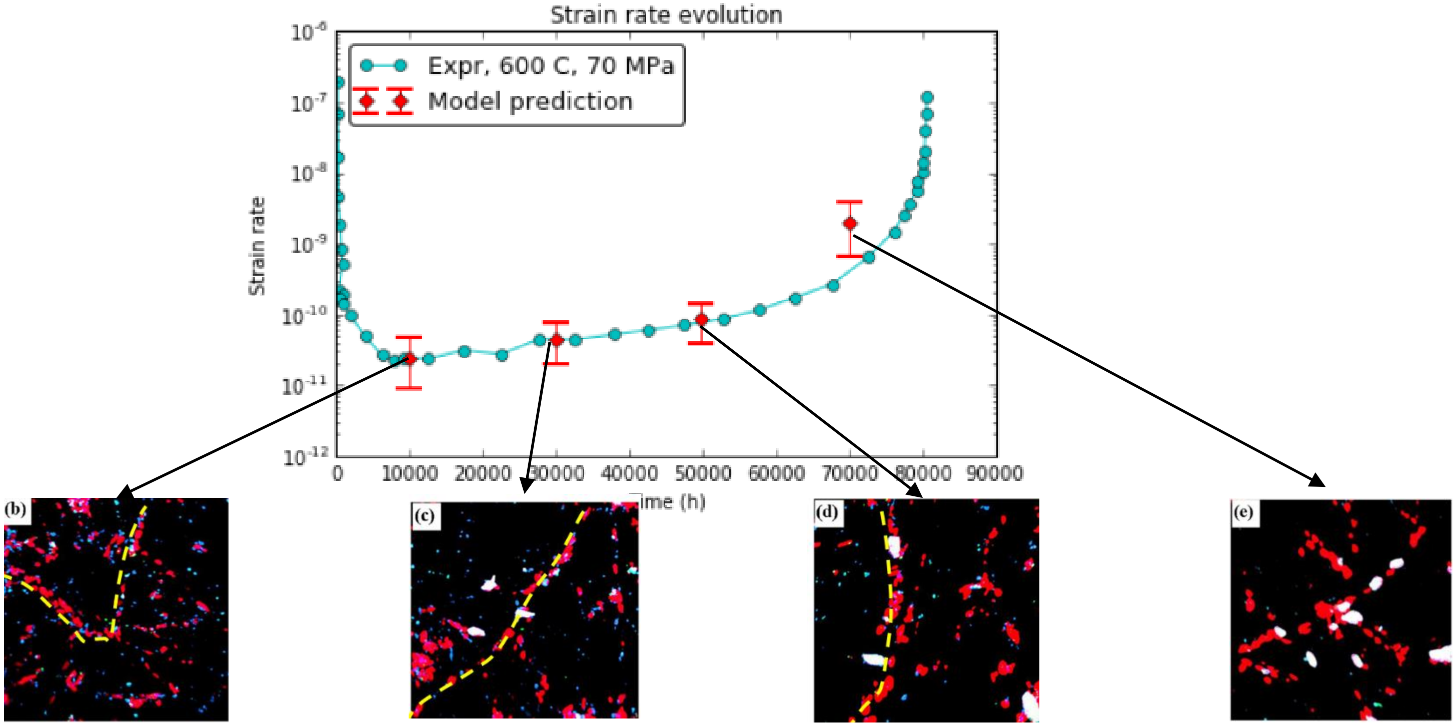
General + Local climb

In reality, this mode is observed

[1] E. Arzt and J. Rosler, "The Kinetics of Dislocation Climb over Hard Particles .2. Effects of an Attractive Particle Dislocation Interaction," *Acta Metall.*, vol. 36, no. 4, pp. 1053–1060, 1988.

Results – Strain Rate vs Time

Microstructural inputs and service conditions → Creep Model → $\dot{\epsilon}_{creep} = f(time)$



Microstructures from Sawada et al

Experimental data[1]:	MX area density = 8.28e12 MX radius = 21 nm	MX area density = 8.58e12 MX radius = 16.3 nm	MX area density = 8.755 e12 MX radius = 17.7 nm	MX area density = 5.3e12 MX radius = 17.7 nm

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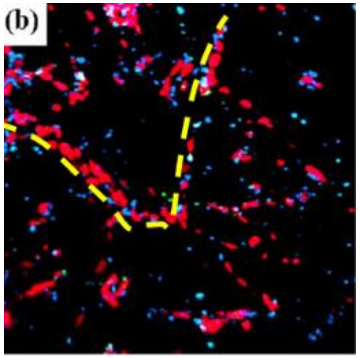
[1] Sawada, K., et al. "Microstructural degradation of Gr. 91 steel during creep under low stress." Materials Science and Engineering: A 528.16 (2011): 5511-5518.

Results – Minimum Strain Rate vs Stress

Microstructural inputs and service conditions → Creep Model → $\min(\dot{\epsilon}_{creep})$

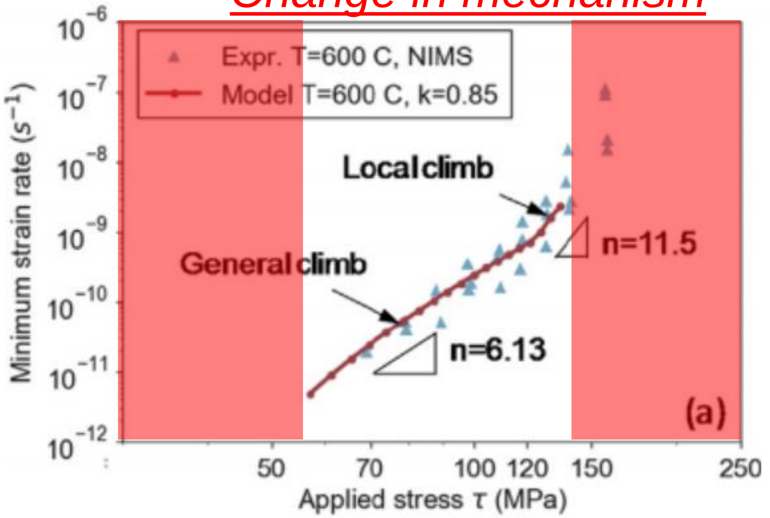
Microstructures from Sawada et al [2]



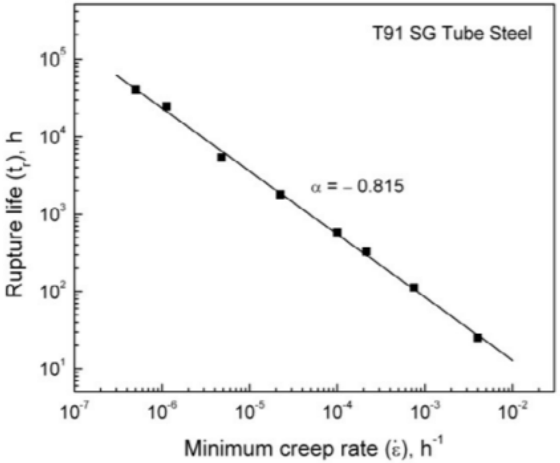
MX area density = 8.28e12

MX radius = 21 nm

Change in mechanism



Monkman-Grant Relation for Gr.91 steels [1]



- Assuming identical microstructure at different stress level
  - Difficult to model creep at different temperatures
- Use minimum creep rate with Monkman-Grant relationship to get creep lifetimes
  - Requires phenomenological relations → not desirable

[1] Palaparti, DP et al. "Creep properties of Grade 91 steel steam generator tube at 923K." *Procedia Engineering* 55 (2013): 70-77.

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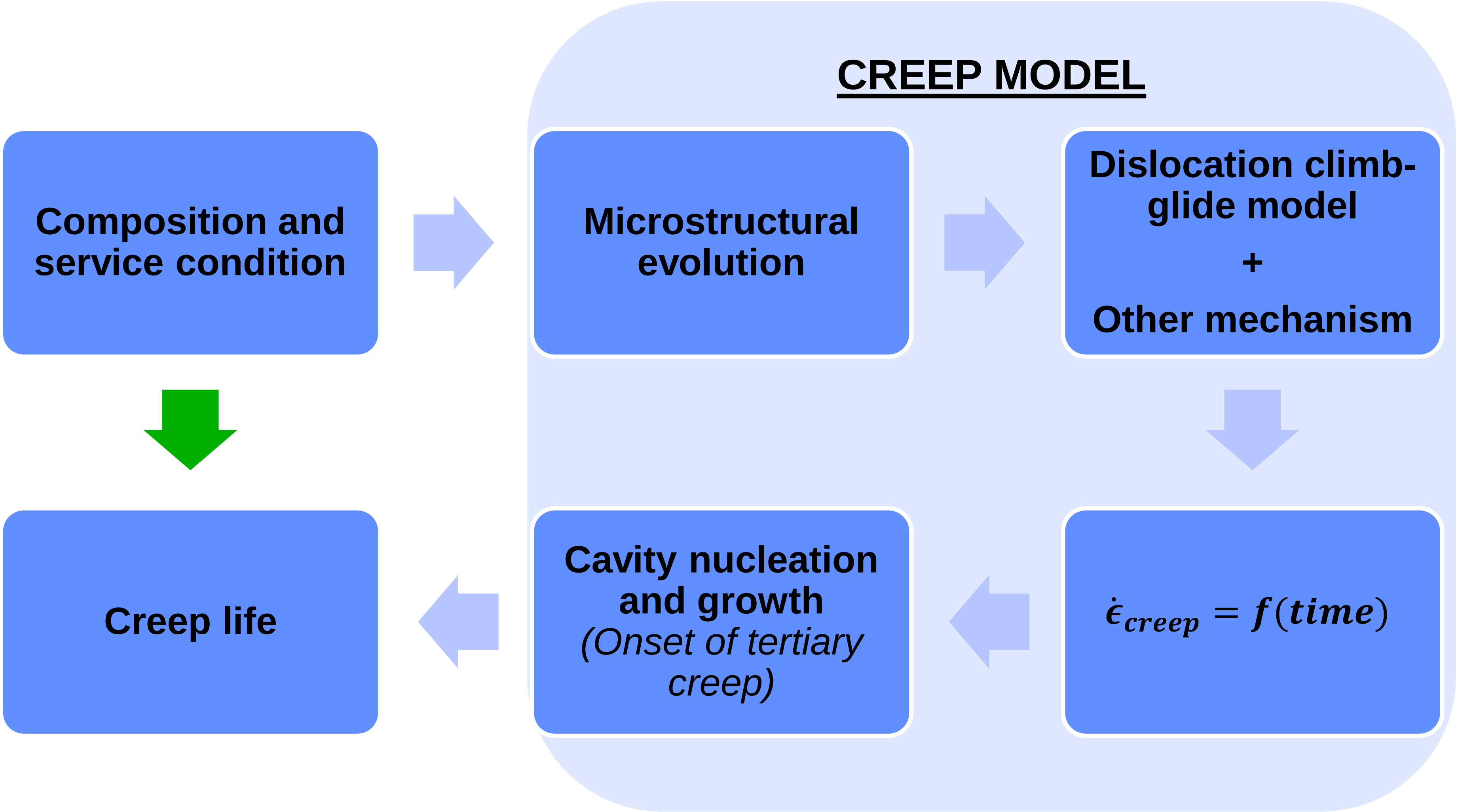
[2] Sawada, K., et al. "Microstructural degradation of Gr. 91 steel during creep under low stress." Materials Science and Engineering: A 528.16 (2011): 5511-5518.

Complete creep model



CREEP MODEL

Composition and service condition

Microstructural evolution

Dislocation climb-glide model

+

Other mechanism

$\dot{\epsilon}_{creep} = f(time)$

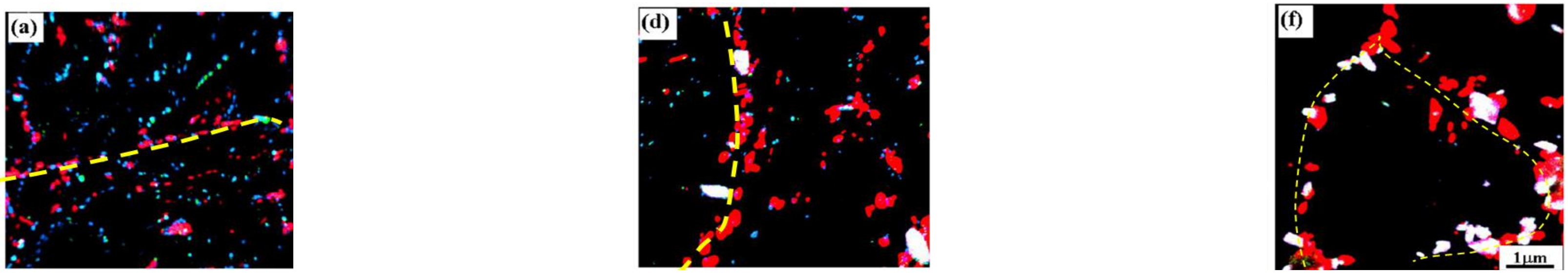
Cavity nucleation and growth *(Onset of tertiary creep)*

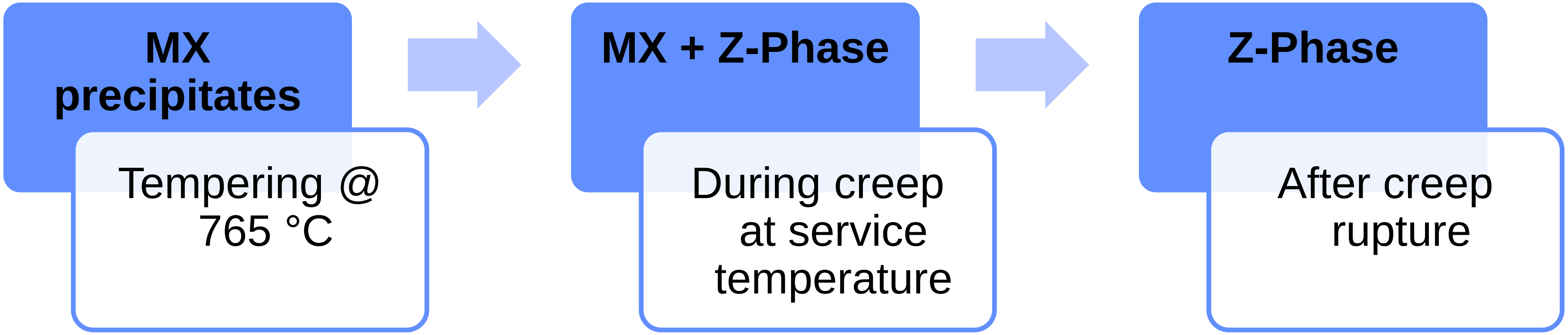
Creep life

Modeling microstructure evolution

- Modeling evolution of precipitates as function of time, temperature and composition using CALPHAD-based approaches
- Utilize *PrecipiCalc*® simulation tool for modeling dissolution of MX particles by Z-Phase precipitates

Microstructures from Sawada et al





MX precipitates

Tempering @ 765 °C

MX + Z-Phase

During creep at service temperature

Z-Phase

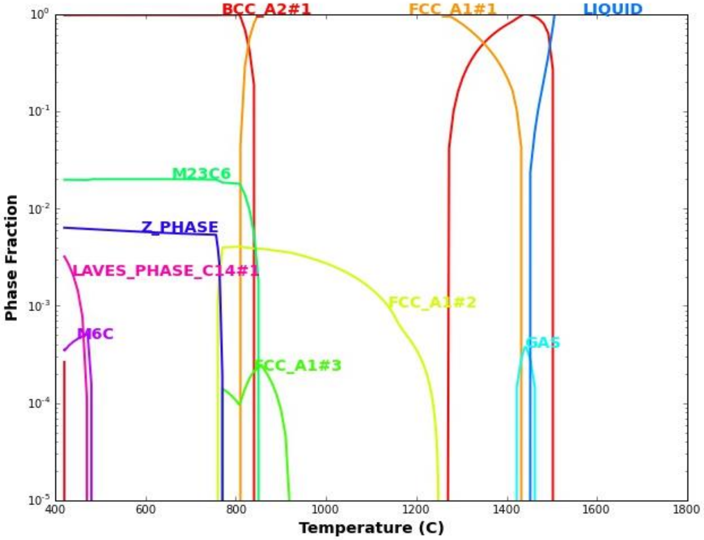
After creep rupture

Sawada, K., et al. "Microstructural degradation of Gr. 91 steel during creep under low stress." Materials Science and Engineering: A 528.16 (2011): 5511-5518.

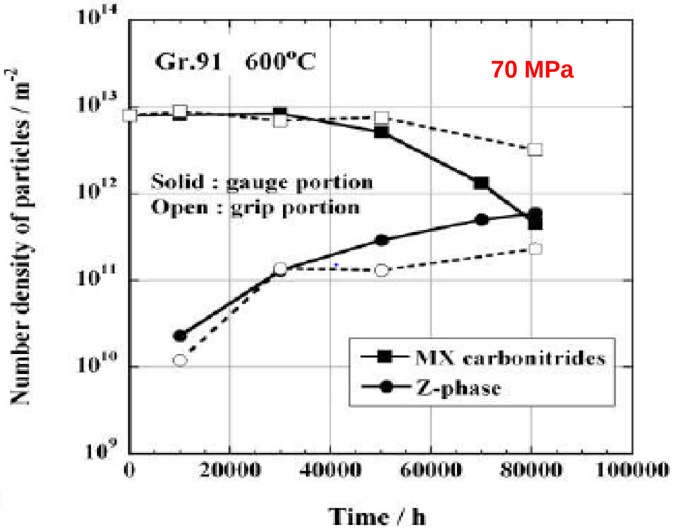
About Z-Phase (Cr(V,Nb)N)

- Thermodynamically most stable nitride at service temperature
- **High interfacial energy** coupled with already depleted matrix due to (V,Nb)N precipitates cause **slow nucleation**
- Consumes beneficial MX precipitates
- Evidence of heterogeneous nucleation on MX precipitates
  - Need to incorporate this mechanism in precipitation modeling

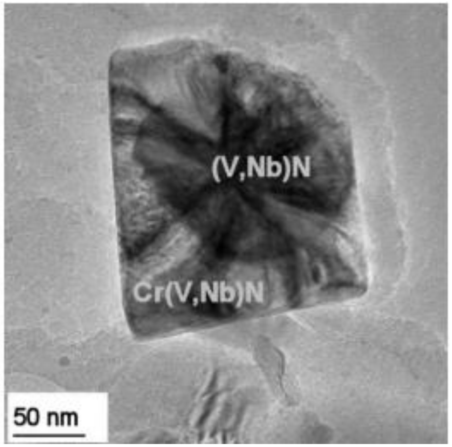
Step diagram for Gr.91 steels



Number Density of Z and MX[1]



Heterogeneous Nucleation[2]

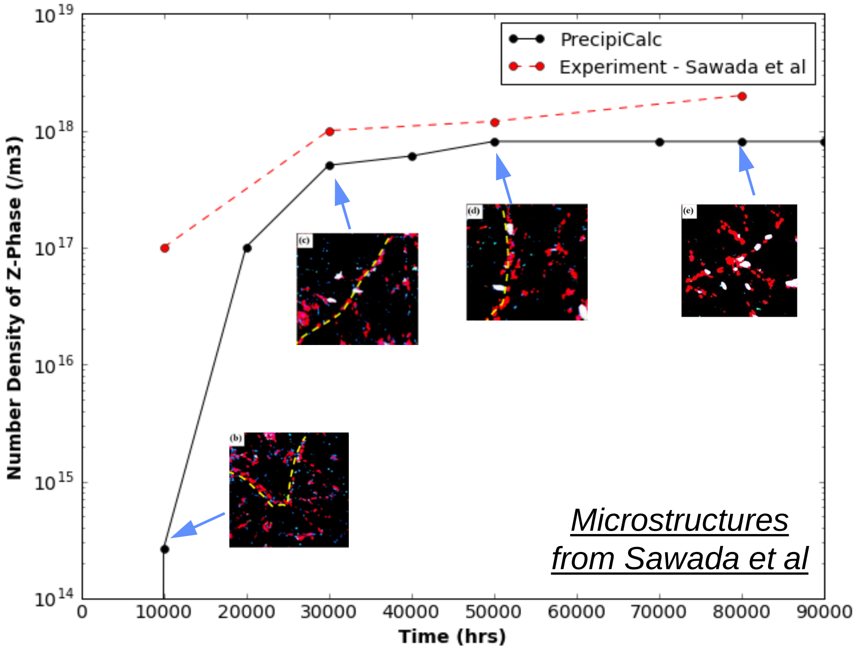


[1] Sawada, K., Kushima, H., Hara, T., Tabuchi, M. and Kimura, K., 2014. Heat-to-heat variation of creep strength and long-term stability of microstructure in Grade 91 steels. Materials Science and Engineering: A, 597, pp.164-170.

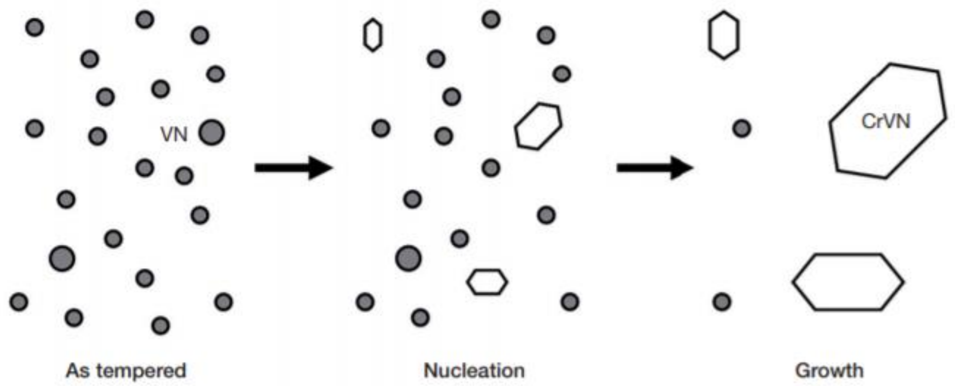
[2] H. K. Danielsen and J. Hald, *Mater. Sci. Eng. A*, vol. 505, no. 1–2, pp. 169–177, 2009.

Modeling of heterogeneous nucleation

- Heterogeneous nucleation dependent on the size of MX precipitate
- Cut-off radius defined as the minimum radius required for nucleation



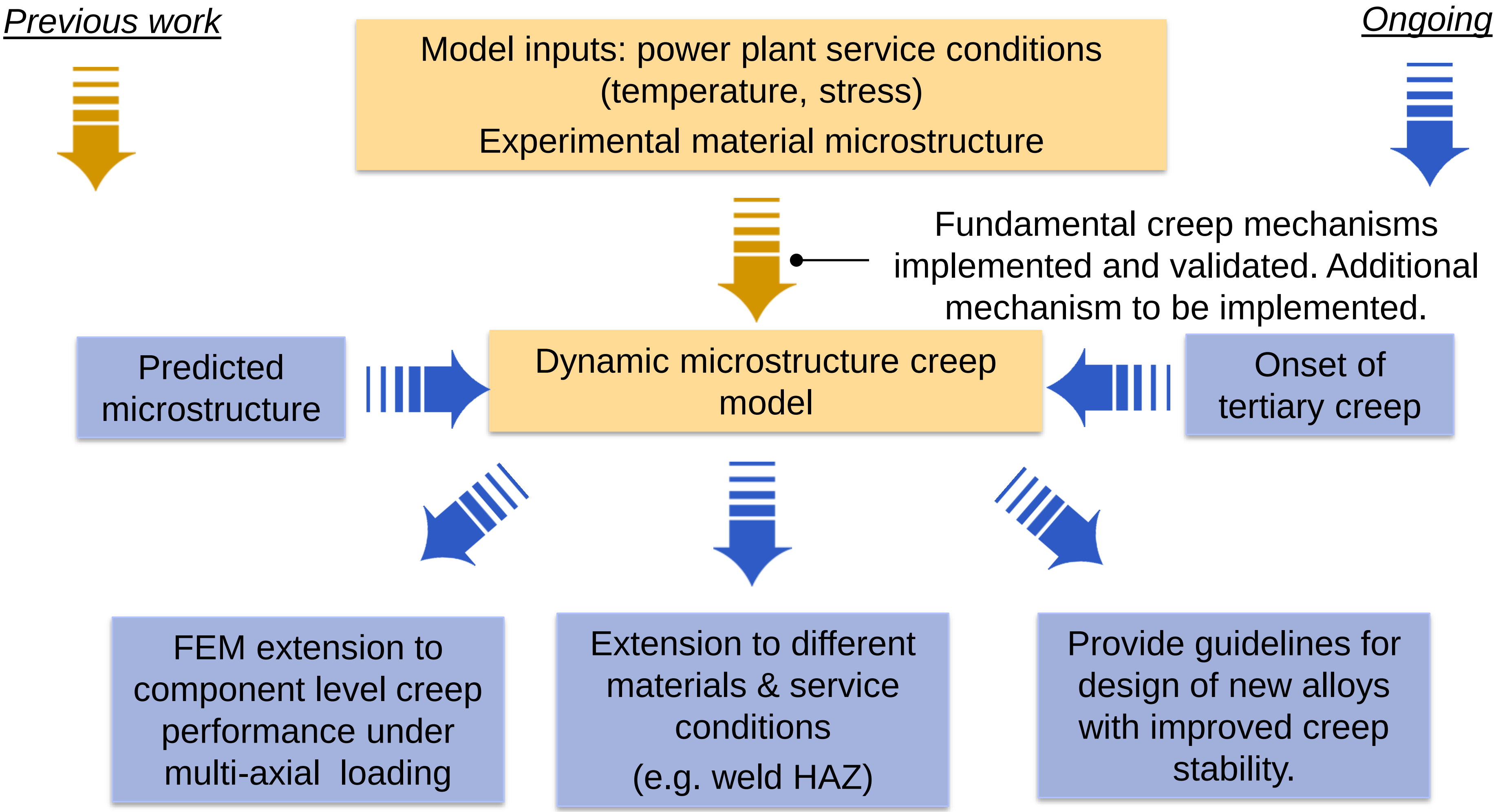
Microstructures from Sawada et al



$J_{ss} = Z\beta^* N_{sites} exp(-\frac{W_r f_{het}}{k_B T})$	$R_{MX} > R_{cut-off}$ $N_{sites} = N_{MX}(R > R_{cutoff})$	Z nucleates on MX particles
$J_{ss} = Z\beta^* N_{sites} exp(-\frac{W_r}{k_B T})$	$R_{MX} < R_{cut-off}$	Homogeneous nucleation of Z

Sawada, K., et al. "Microstructural degradation of Gr. 91 steel during creep under low stress." Materials Science and Engineering: A 528.16 (2011): 5511-5518.

Conclusion and future work



Previous work

Ongoing

Model inputs: power plant service conditions (temperature, stress)

Experimental material microstructure

Fundamental creep mechanisms implemented and validated. Additional mechanism to be implemented.

Predicted microstructure

Dynamic microstructure creep model

Onset of tertiary creep

FEM extension to component level creep performance under multi-axial loading

Extension to different materials & service conditions

(e.g. weld HAZ)

Provide guidelines for design of new alloys with improved creep stability.

Thank you for your attention

Abhinav Saboo
Materials Engineer
QuesTek Innovations LLC
Evanston, IL USA
847.425.8244, asaboo@questek.com
www.questek.com

Acknowledgements

NETL, U.S Department of Energy (DOE)

Appendix

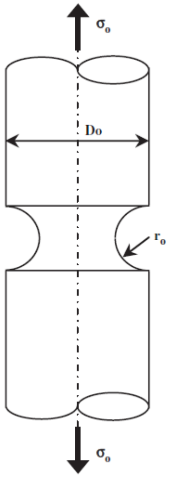
Finite element modeling (preliminary results)

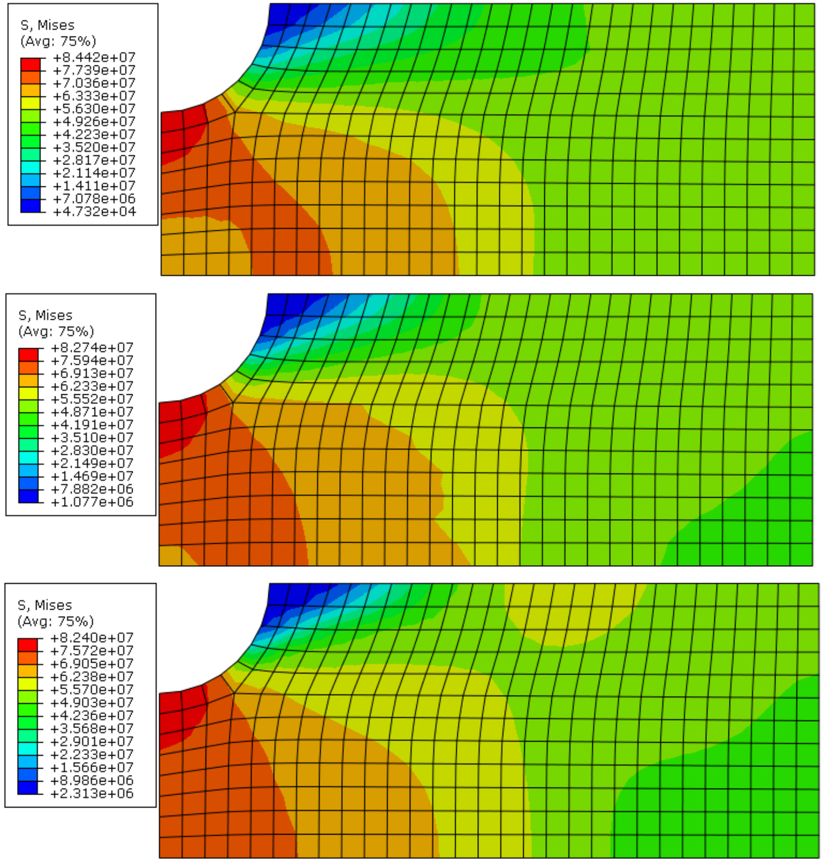
- Creep model as a function of temperature, stress, microstructure is implemented in FEM.
- Currently stress-independent microstructure is taken as the input:
    - Ideally FEM will take *PrecipiCalc predicted* microstructure information.

D_0 =12.5 mm

r_0 =2.5 mm

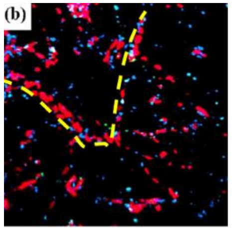
$\sigma_0 = 50$ MPa



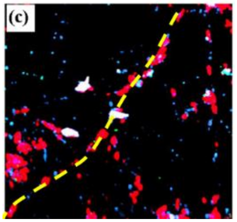


Microstructures from Sawada et al

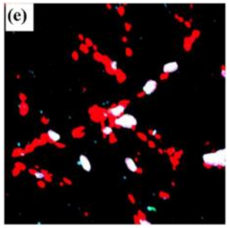
Time =



10,000h



30,000h



50,000h

Sawada, K., et al. "Microstructural degradation of Gr. 91 steel during creep under low stress." Materials Science and Engineering: A 528.16 (2011): 5511-5518.