XMAT: Modeling and Simulation

Laurent Capolungo

Acknowledgements: Mickael Brady, Yuki Yamamoto, Brandon Wood, Mark Cawkwell, Romain Perriot, Arul Kumar, Aaron Kohnert, Richard LeSar, Youhai Wen, Ricardo Lebensohn, Nghiep Nguyen, Hai Huang, Ben Spencer, Millicent Orondo

GOALS

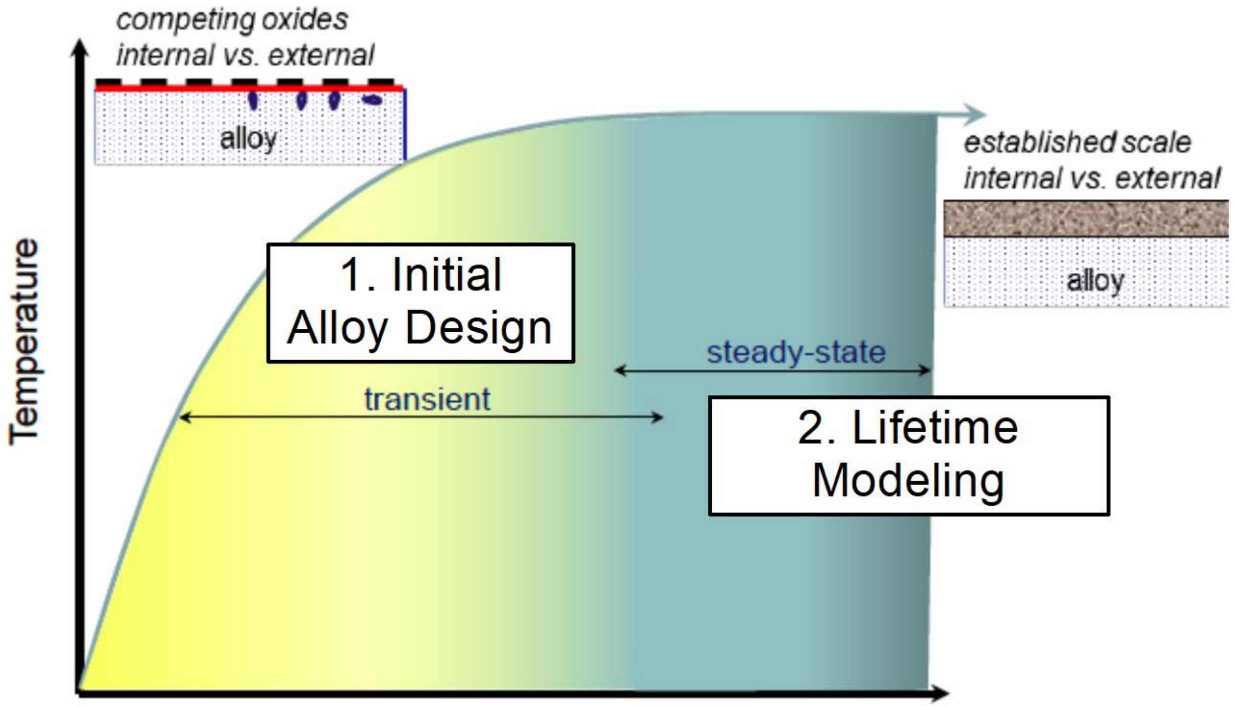
Mod/Sim will deliver a framework for designing metals that fully accounts for metal chemistry, exposure, and cycling.

Generalized rupture life criterion sensitive to chemistry, stress, temperature and for environment.

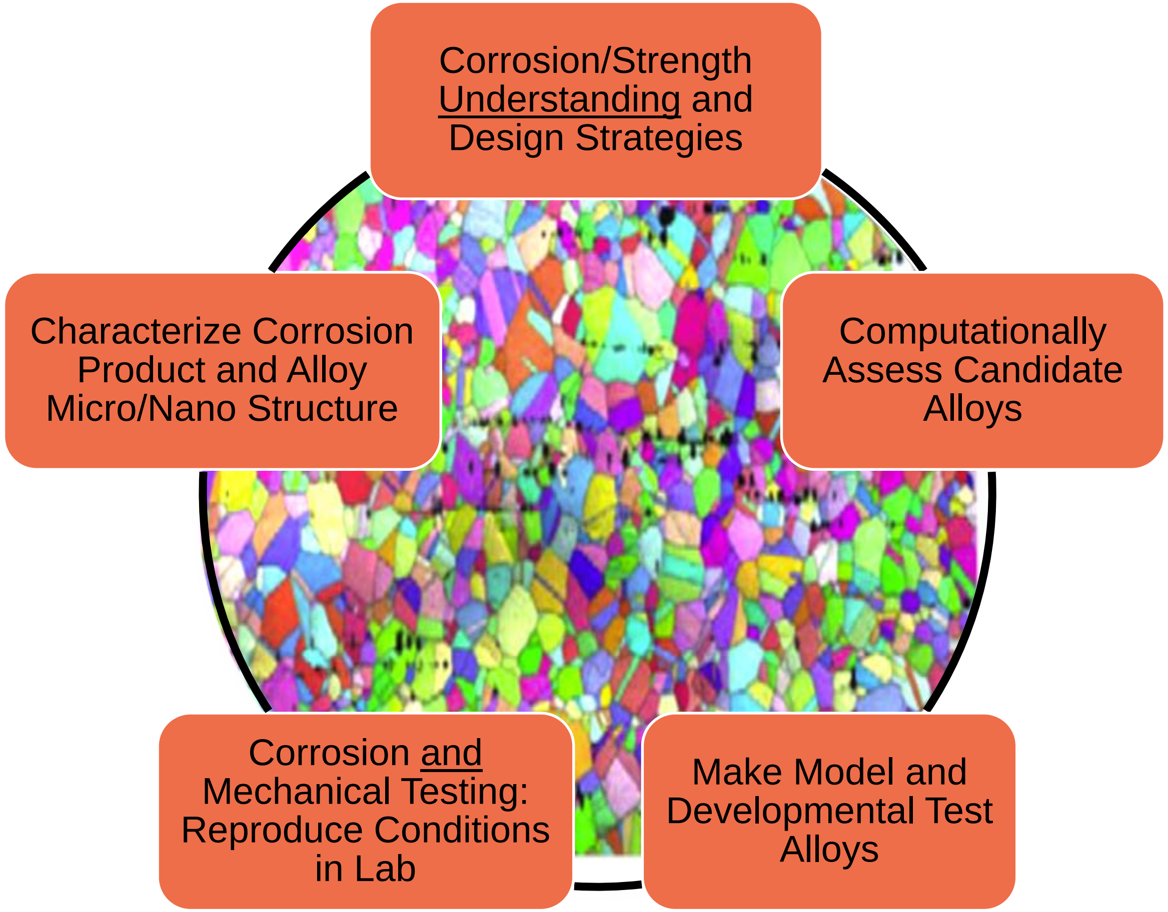
Enhanced thermodynamic and kinetic database.

New alumina forming alloy design guidelines.

Mod/Sim softwares/codes/tools to predict system performance



Design for oxidation and creep resistance



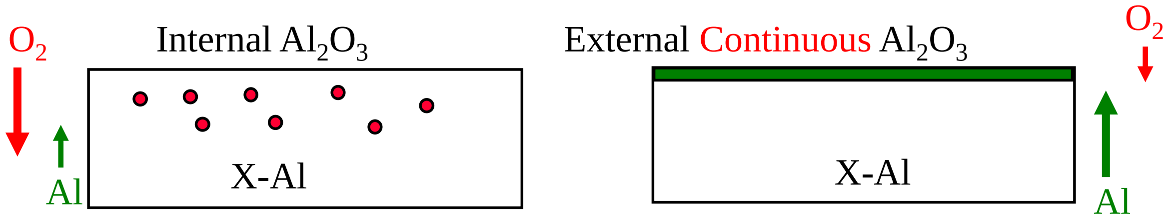
Corrosion/Strength Understanding and Design Strategies

Computationally Assess Candidate Alloys

Make Model and Developmental Test Alloys

Corrosion and Mechanical Testing: Reproduce Conditions in Lab

Characterize Corrosion Product and Alloy Micro/Nano Structure



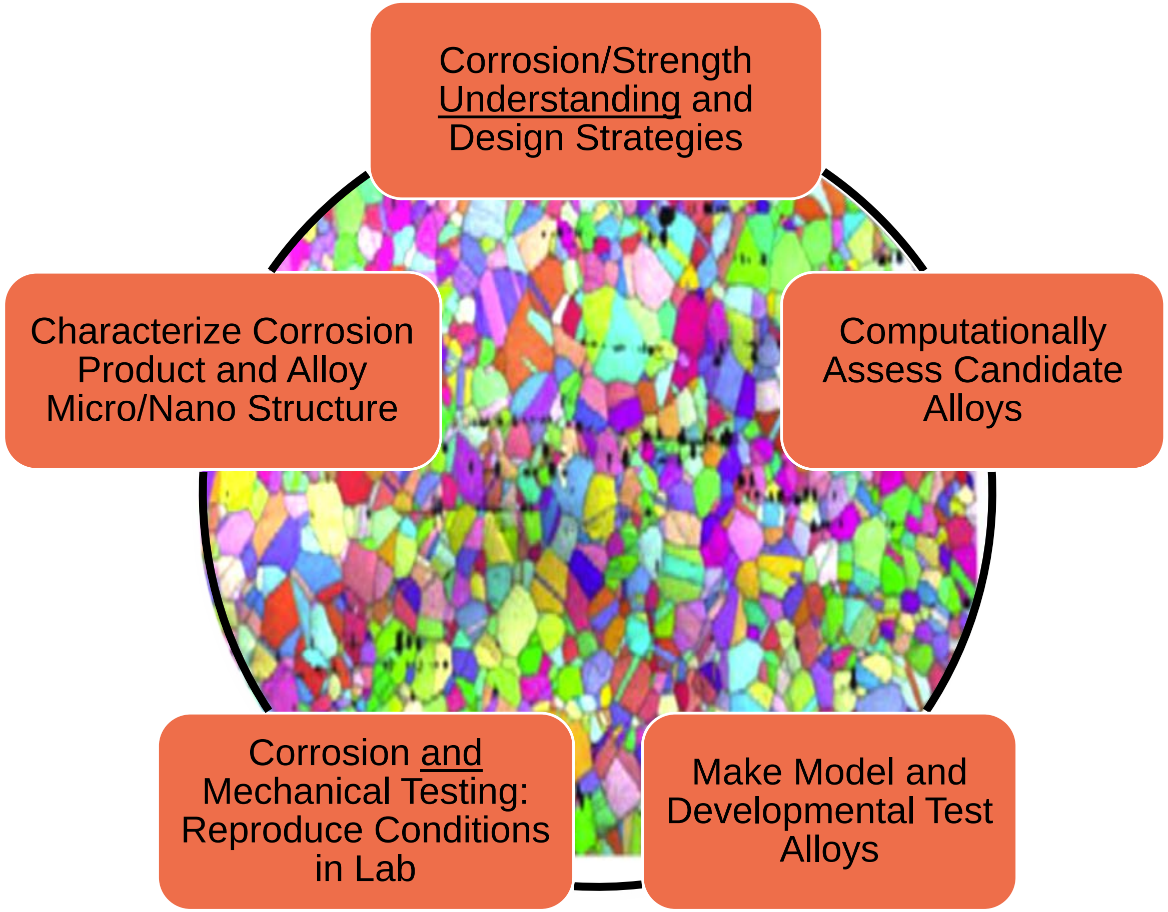
$$\text{Minimum Al for Continuous } Al_2O_3 \propto \left[O_{solubility} * \frac{O_{diffusivity}}{Al_{diffusivity}} \right]^{1/2}$$

Limitations:

Edisonian approaches to material design are reaching their limits

Trace elements and many-body interactions between defects and chemical species can rarely be postulated a priori.

Design for oxidation and creep resistance



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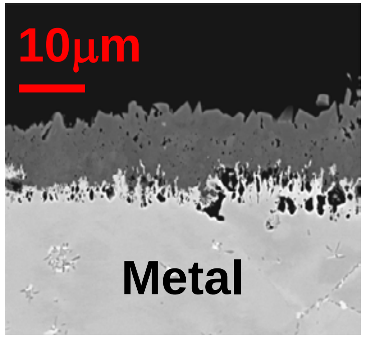
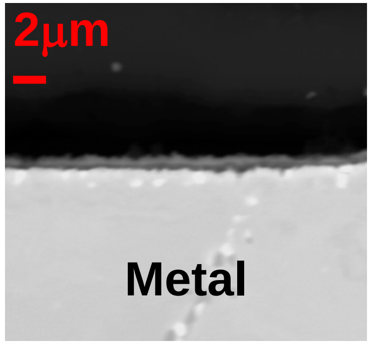


Fe-20Ni-14Cr-2.5Al-0.5V-0.3Ti-0.1C



Fe-20Ni-14Cr-2.5Al-0.9Nb-0.1C

Limitations:

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Trace elements and many-body interactions between defects and chemical species can rarely be postulated a priori.

Lifetime assessment

Empirical laws predicting creep rupture life (example of the Larson Miller law)

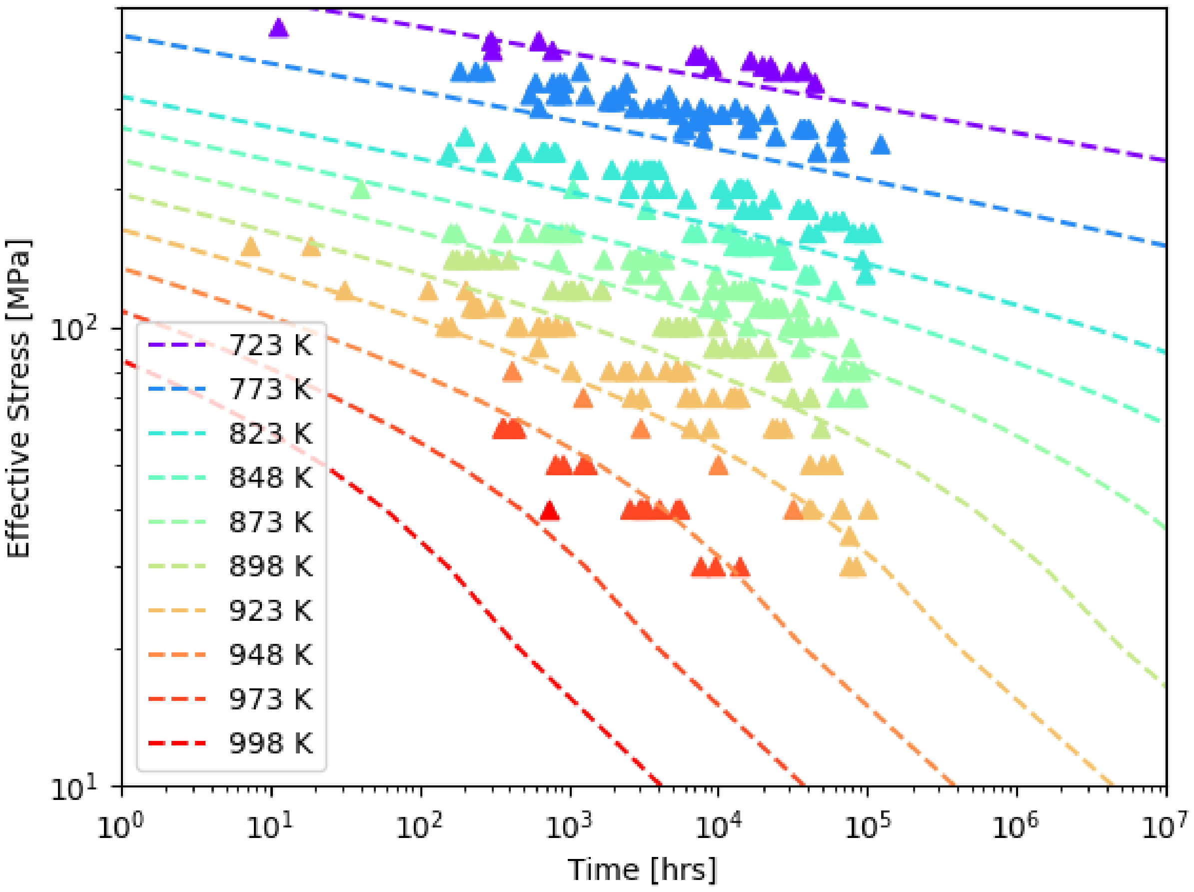
$$P_{LM}(\sigma) = [C_{LM} + \log_{10}(t_R)]T$$

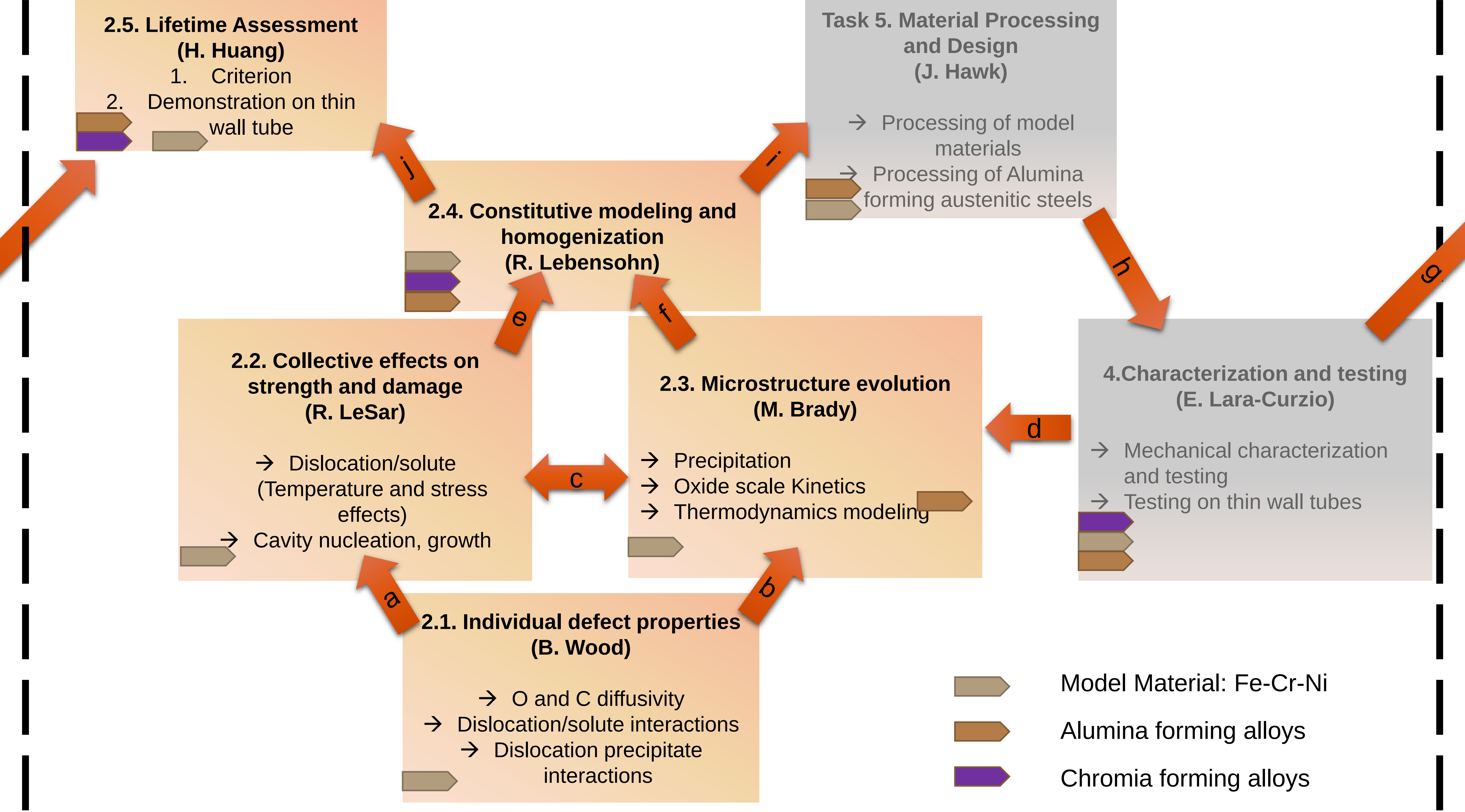
P_{LM}: stress function
C_{LM}: constant
σ: effective stress
T: temperature
t_R: time to rupture

Limitations:

Not valid in all temperature regimes.
Stress dependence is fitted.
No sensitivity to material pedigree, microstructure
Multiaxial loading is approximated (Hayhurst, Huddleston).
Uncertainty quantification
No effect of environment (i.e. oxidation)
No sensitivity to chemistry

Example Grade 91 steels





2.5. Lifetime Assessment
(H. Huang)

1. Criterion
2. Demonstration on thin wall tube

Task 5. Material Processing and Design
(J. Hawk)

→ Processing of model materials
→ Processing of Alumina forming austenitic steels

2.4. Constitutive modeling and homogenization
(R. Lebensohn)

2.2. Collective effects on strength and damage
(R. LeSar)

→ Dislocation/solute (Temperature and stress effects)
→ Cavity nucleation, growth

2.3. Microstructure evolution
(M. Brady)

→ Precipitation
→ Oxide scale Kinetics
→ Thermodynamics modeling

4.Characterization and testing
(E. Lara-Curzio)

→ Mechanical characterization and testing
→ Testing on thin wall tubes

2.1. Individual defect properties
(B. Wood)

→ O and C diffusivity
→ Dislocation/solute interactions
→ Dislocation precipitate interactions

Model Material: Fe-Cr-Ni
Alumina forming alloys
Chromia forming alloys

Lifetime Prediction

Questions:

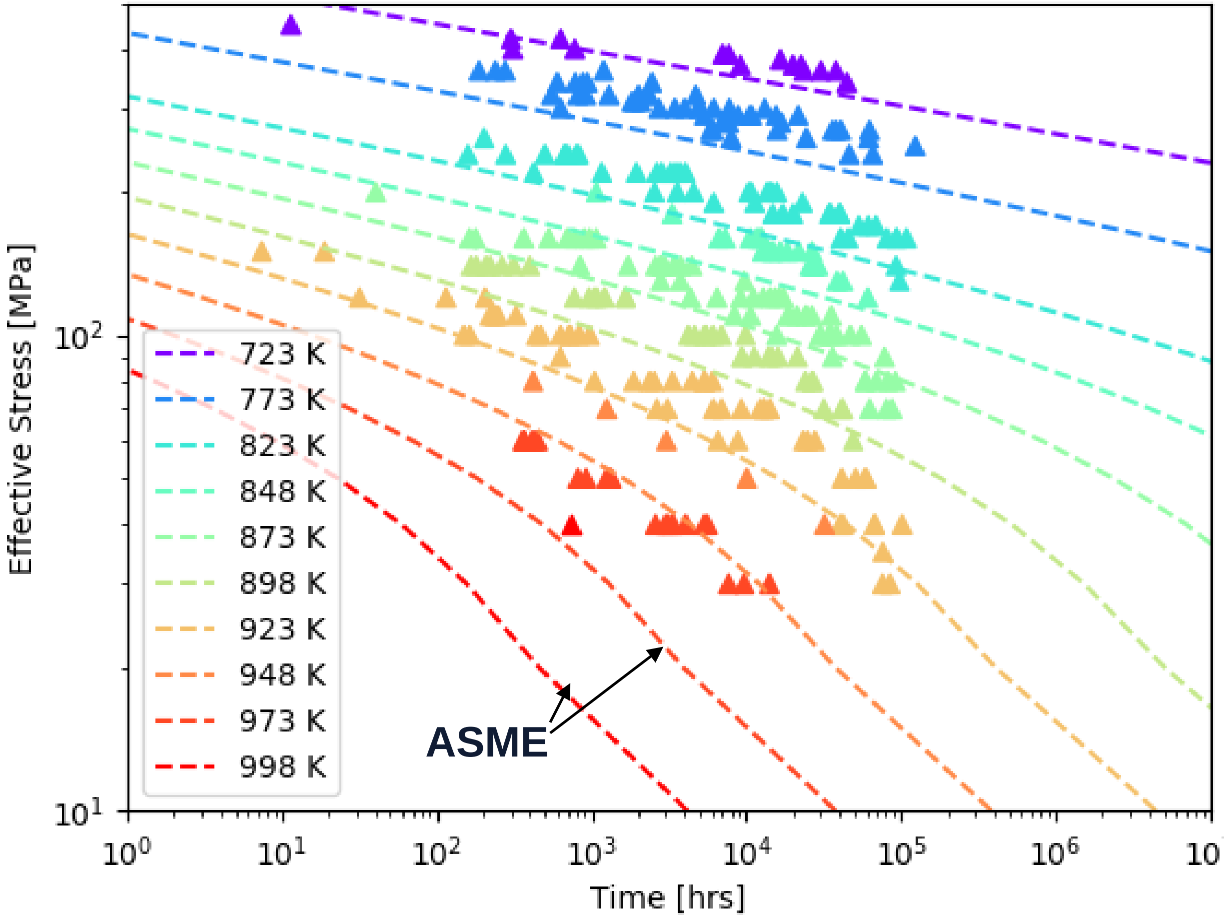
1. Can high fidelity physics based model be used to derive new rupture life model?
2. Can uncertainty be built in the rupture life model?
3. Can short term creep tests be used to extrapolate material lifetime (rapid material assessment)?
4. Can a design of experiment be derived?

e.g. Larson-Miller:

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

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

9Cr-1Mo-V: ASME vs. experimental data



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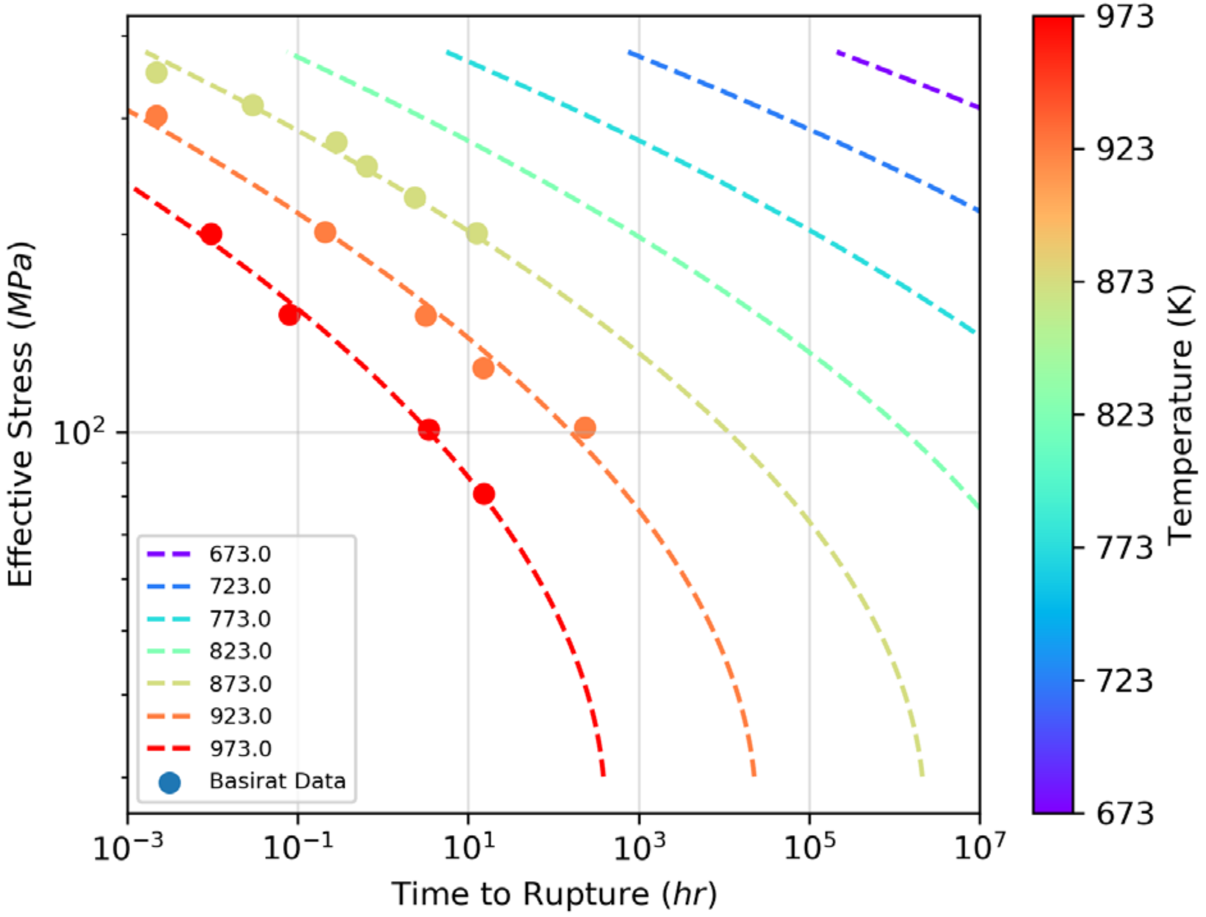


Lifetime Prediction

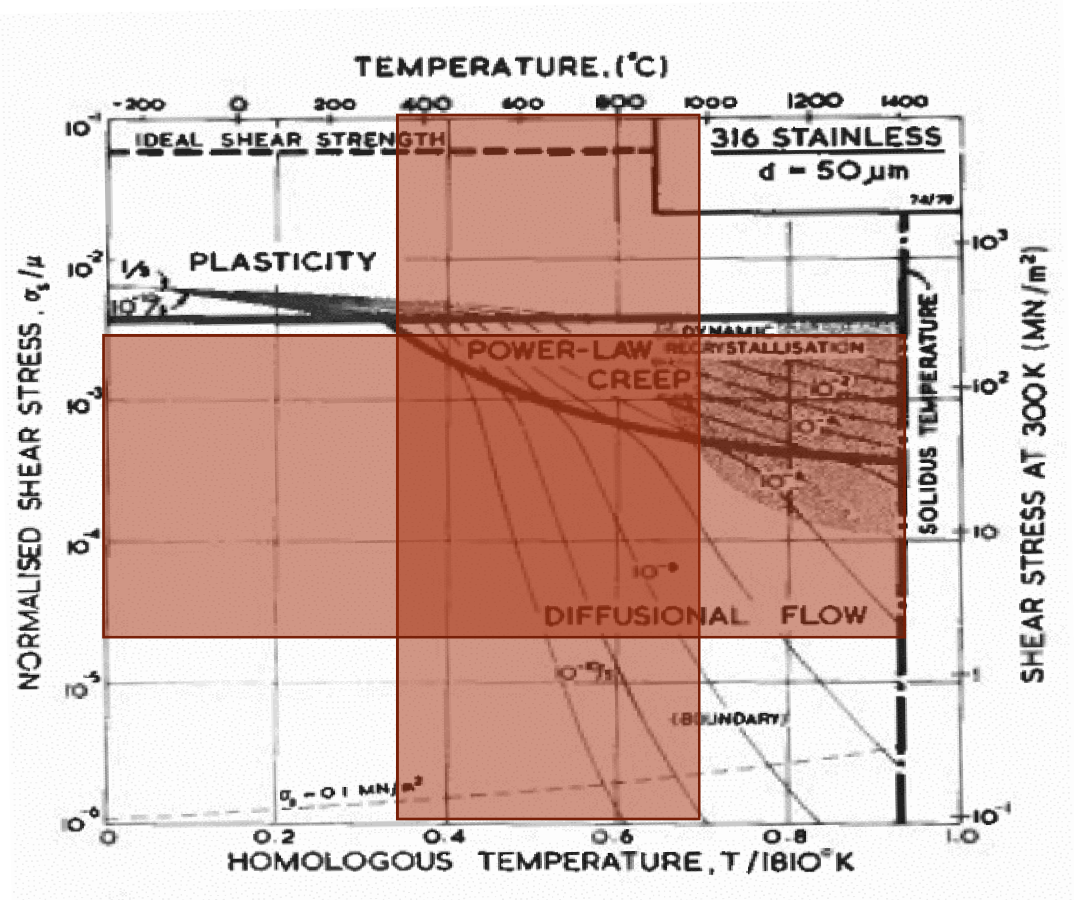
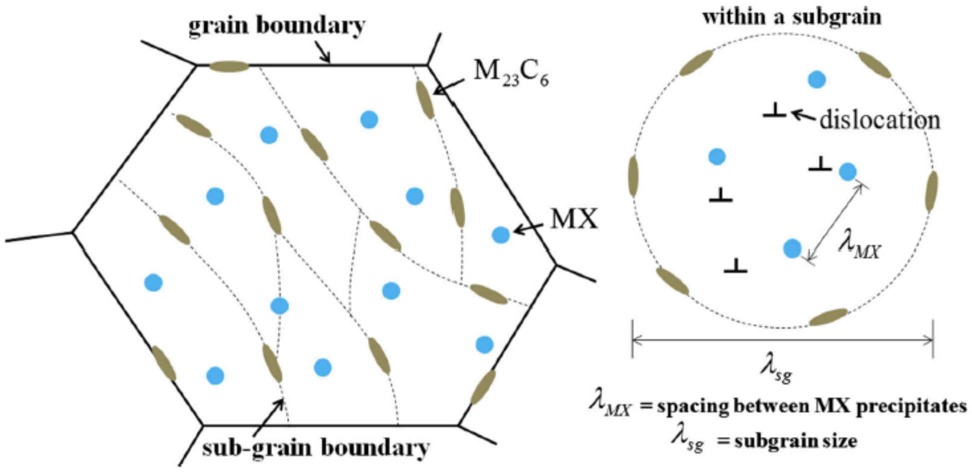


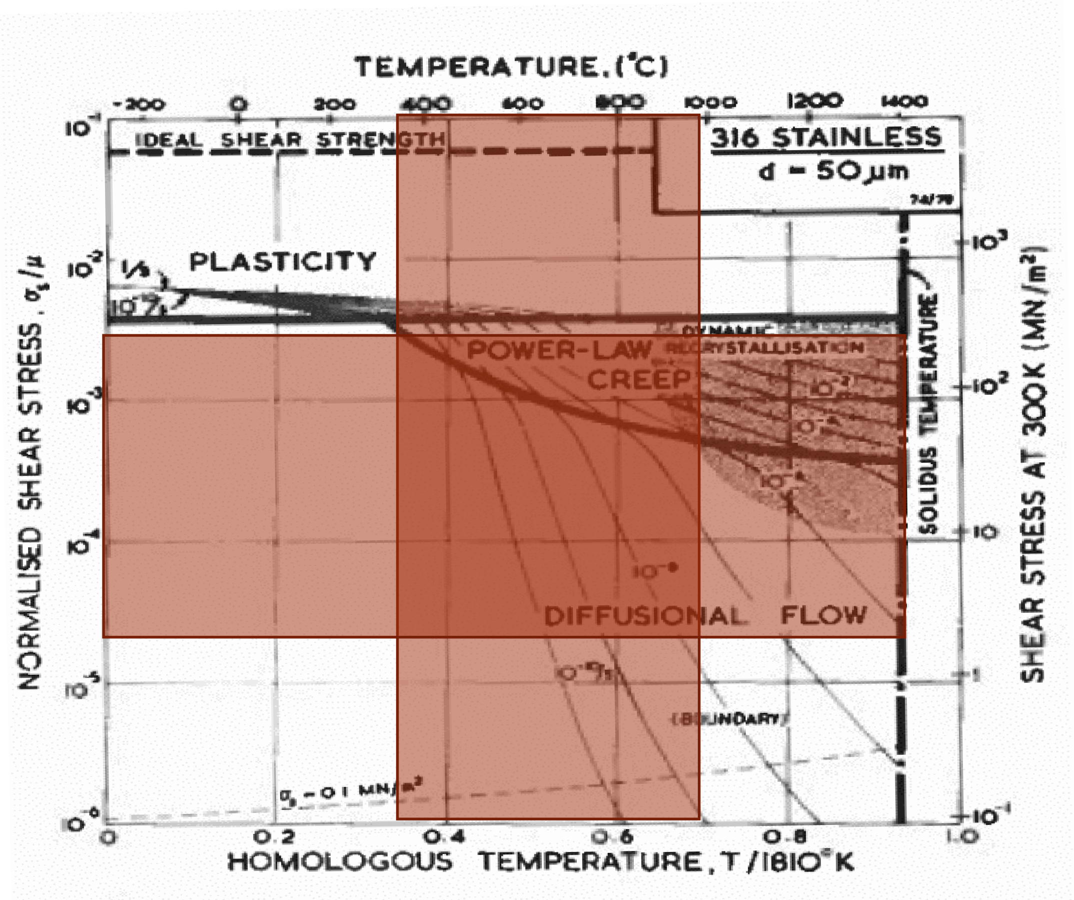
Fig. 8.8. A stress/temperature map for type 316 stainless steel of grain size 50 μm.



Components of crystal plasticity based model

Vacancy diffusion /
Precipitates /
Internal stress distribution /
Dislocation density evolution in cell walls and cell interior /
Loop density evolution
Latent dislocation interactions
Solute strengthening

Lifetime Prediction



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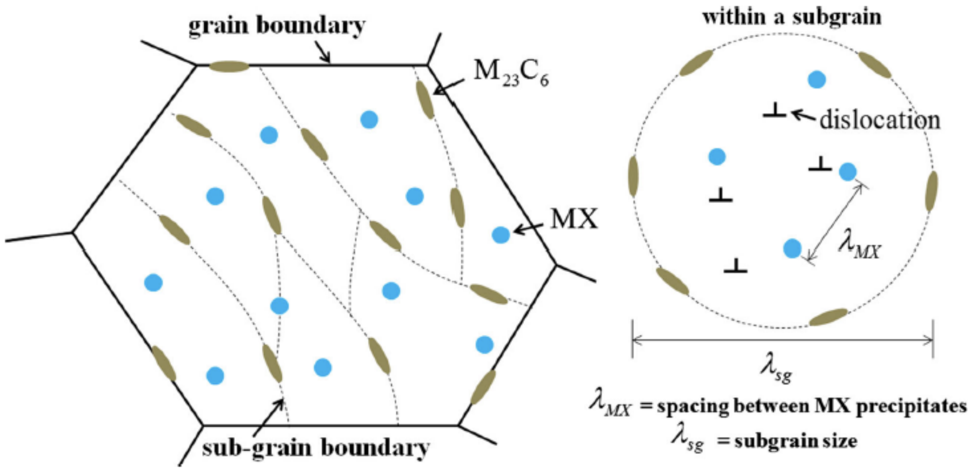
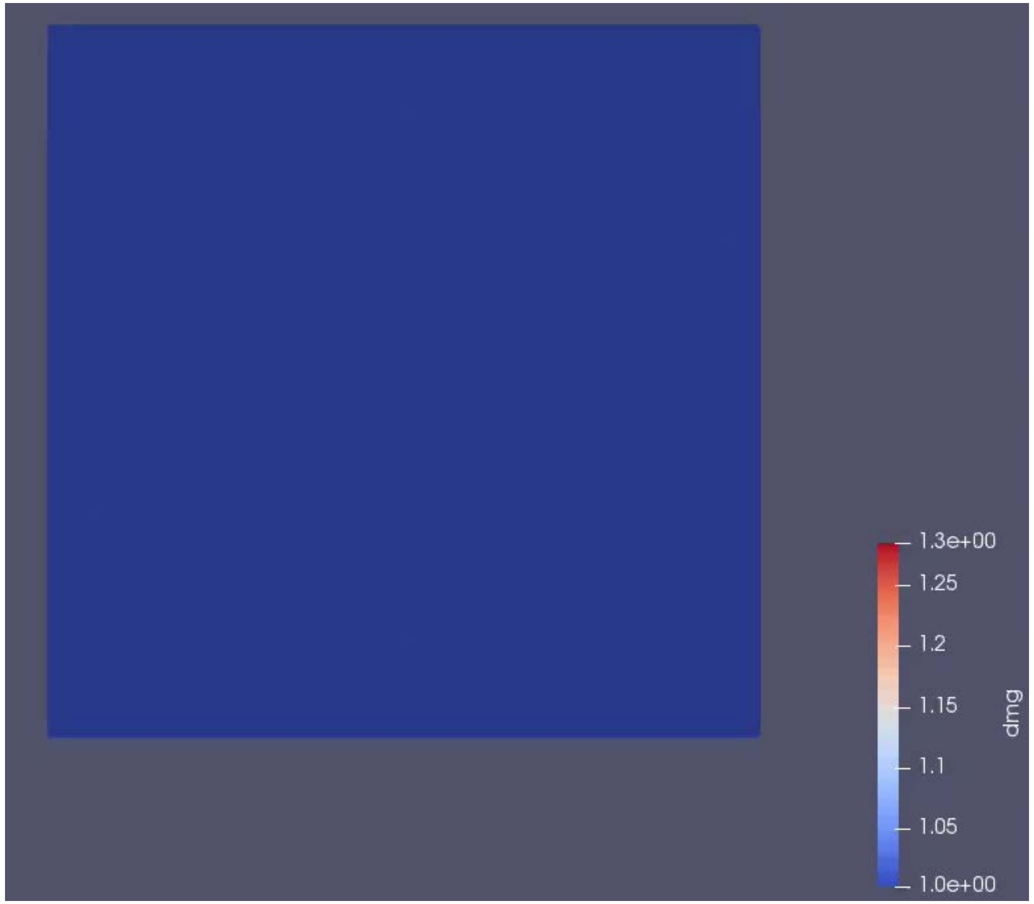


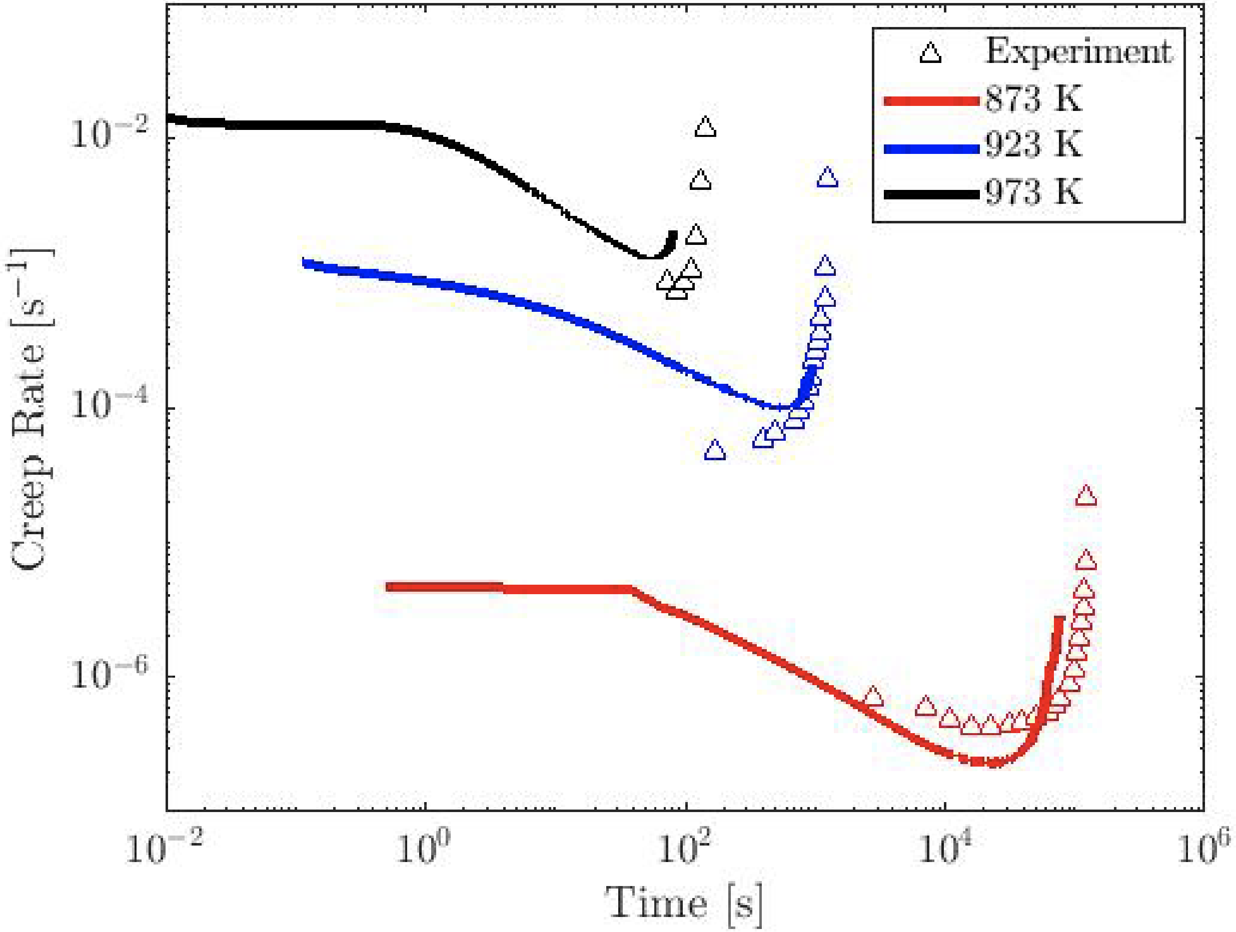
λ_{MX} = spacing between MX precipitates
λ_{sg} = subgrain size

Damage model

Accounts for the statistics of size distributions of cavities
Nucleation is both mediated by stress and accumulated plastic strain
Growth is mediated by plasticity and by diffusive processes at grain boundaries

Lifetime Prediction





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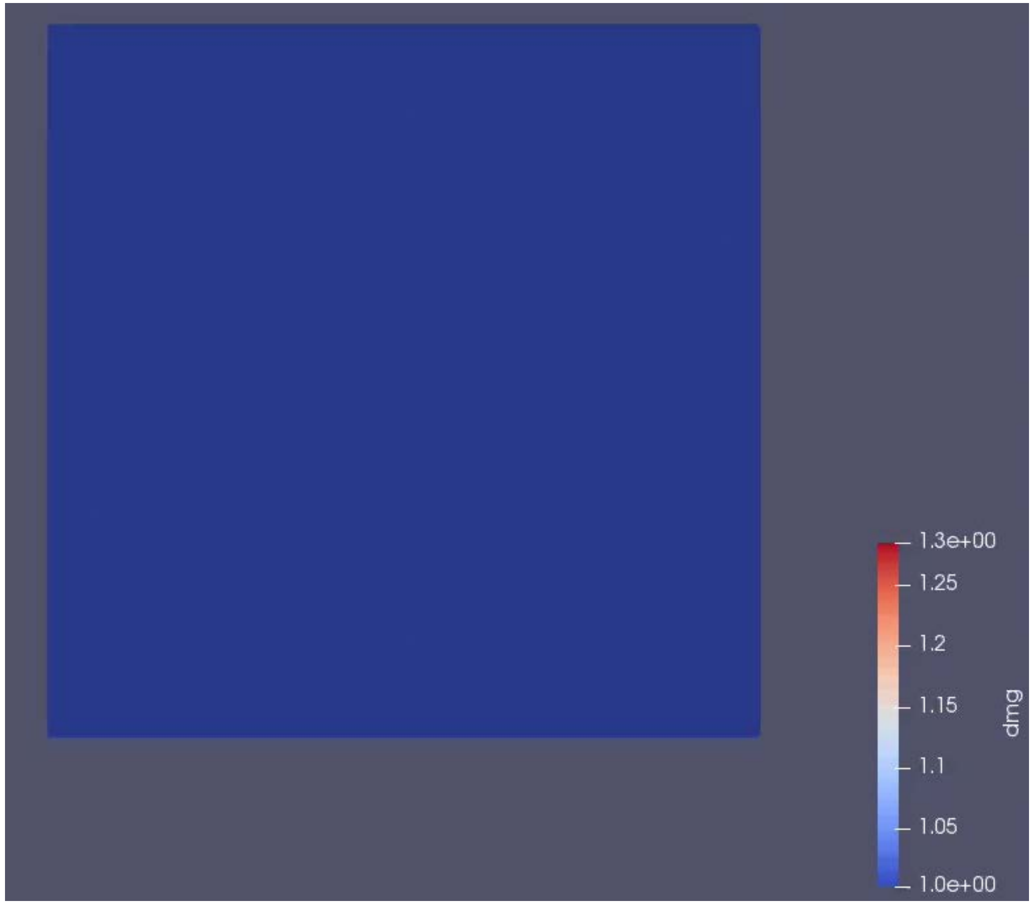

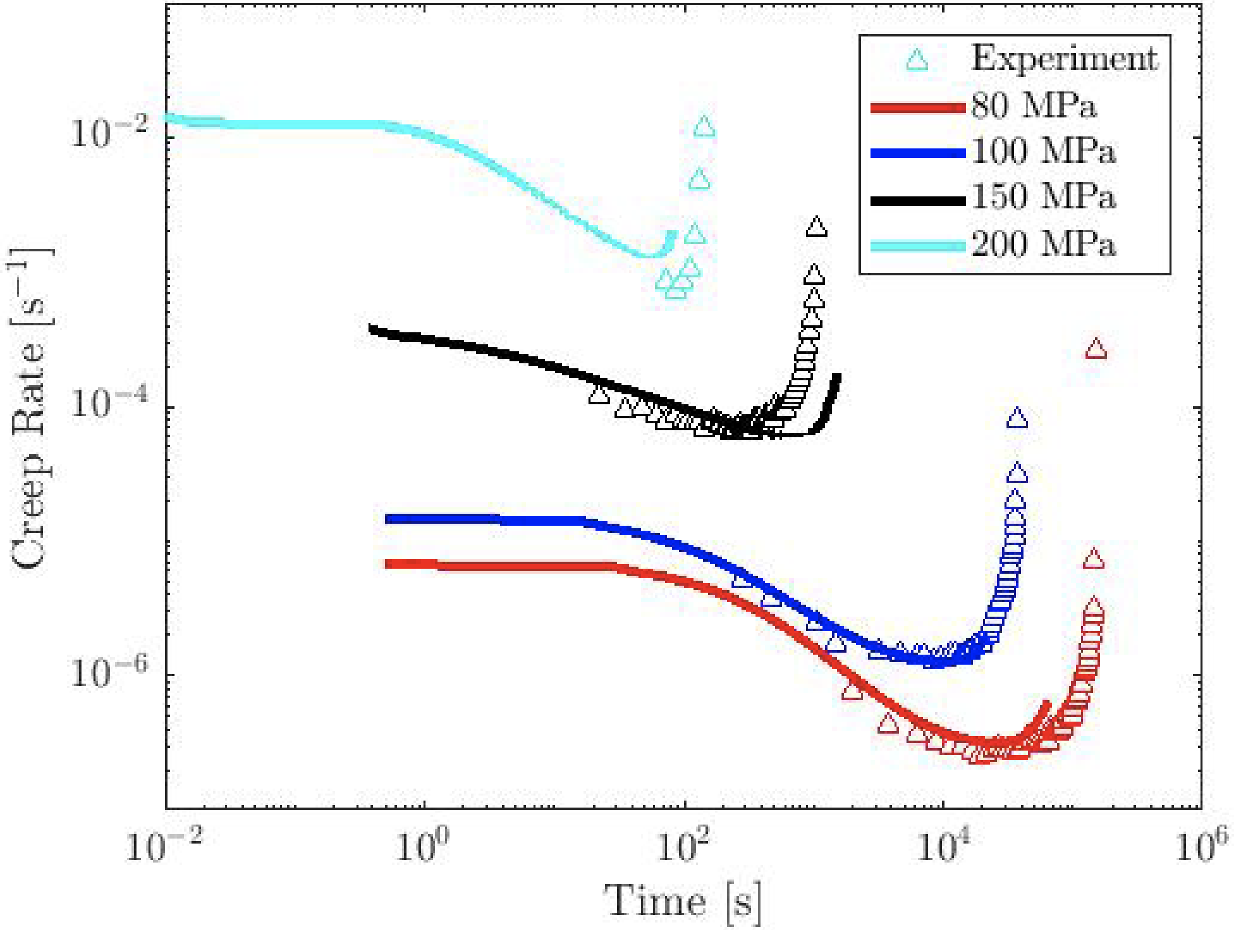

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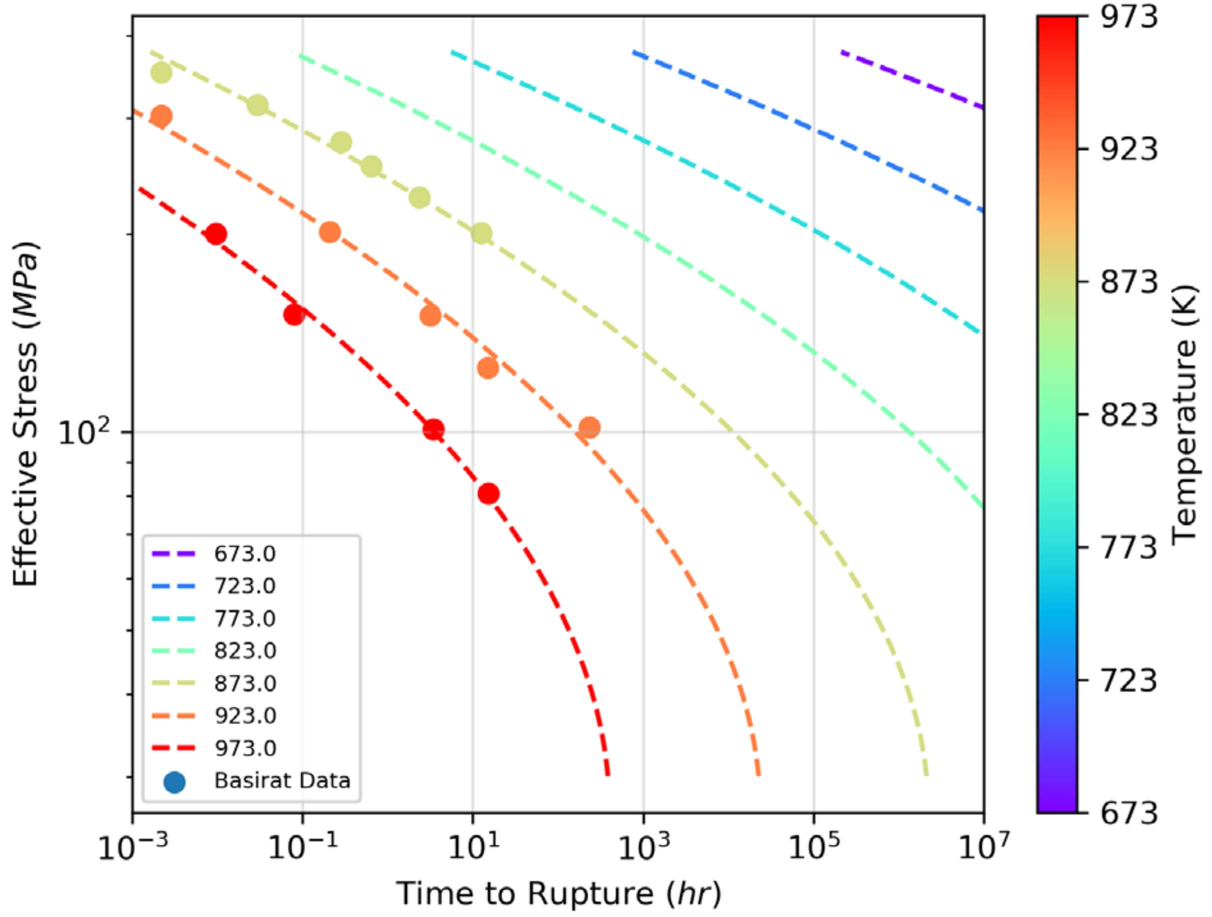

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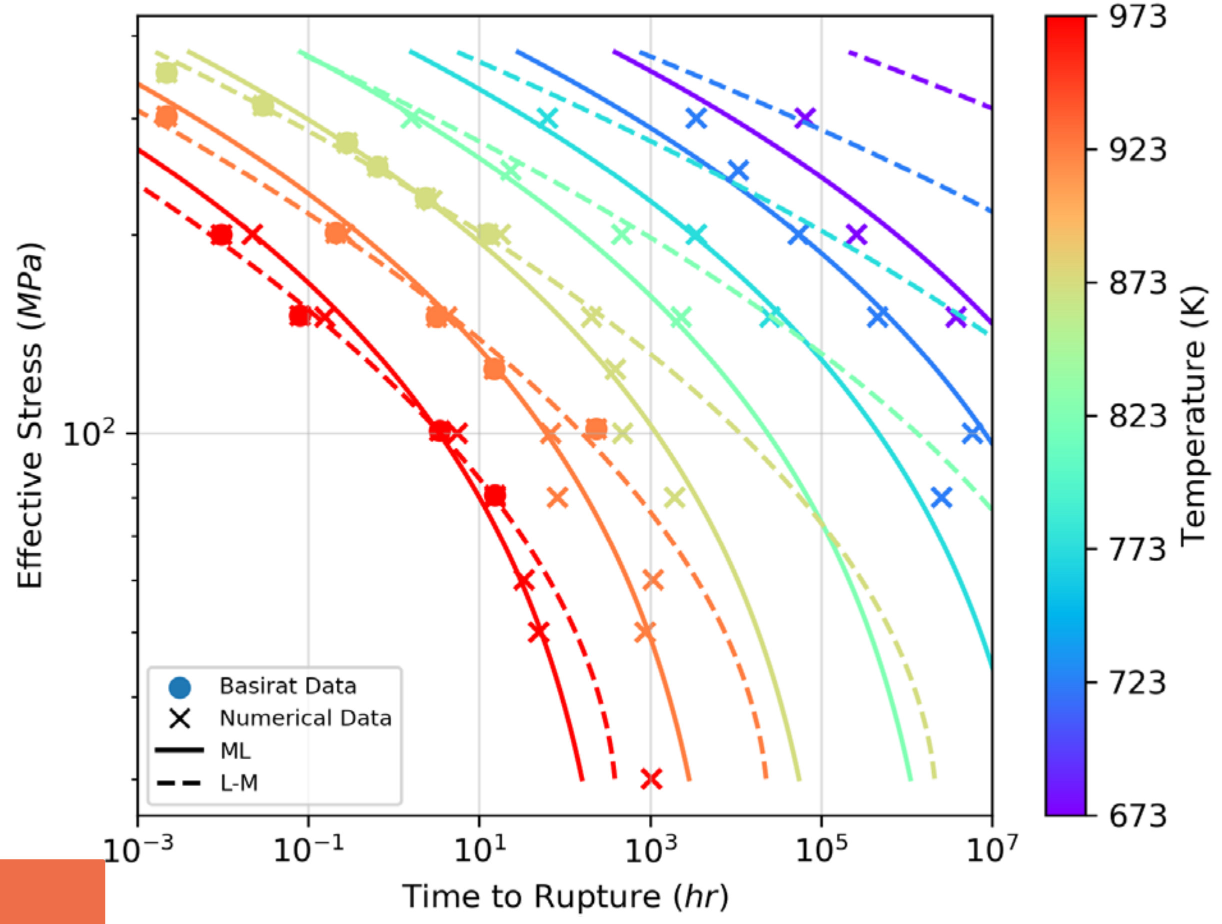
$$P_{LM}(\sigma) = [C_{LM} + \log_{10}(t_R)]T$$

σ: effective stress
T: temperature
t_R: time to rupture

$$\log_{10}(t_R) = -6.7 \times 10^{-2}(\log_{10}(\sigma))^5 - 1.5 \times 10^7 \left(\frac{1}{T}\right)^2 + 5.4 \times 10^4 \left(\frac{1}{T}\right) - 37.3$$



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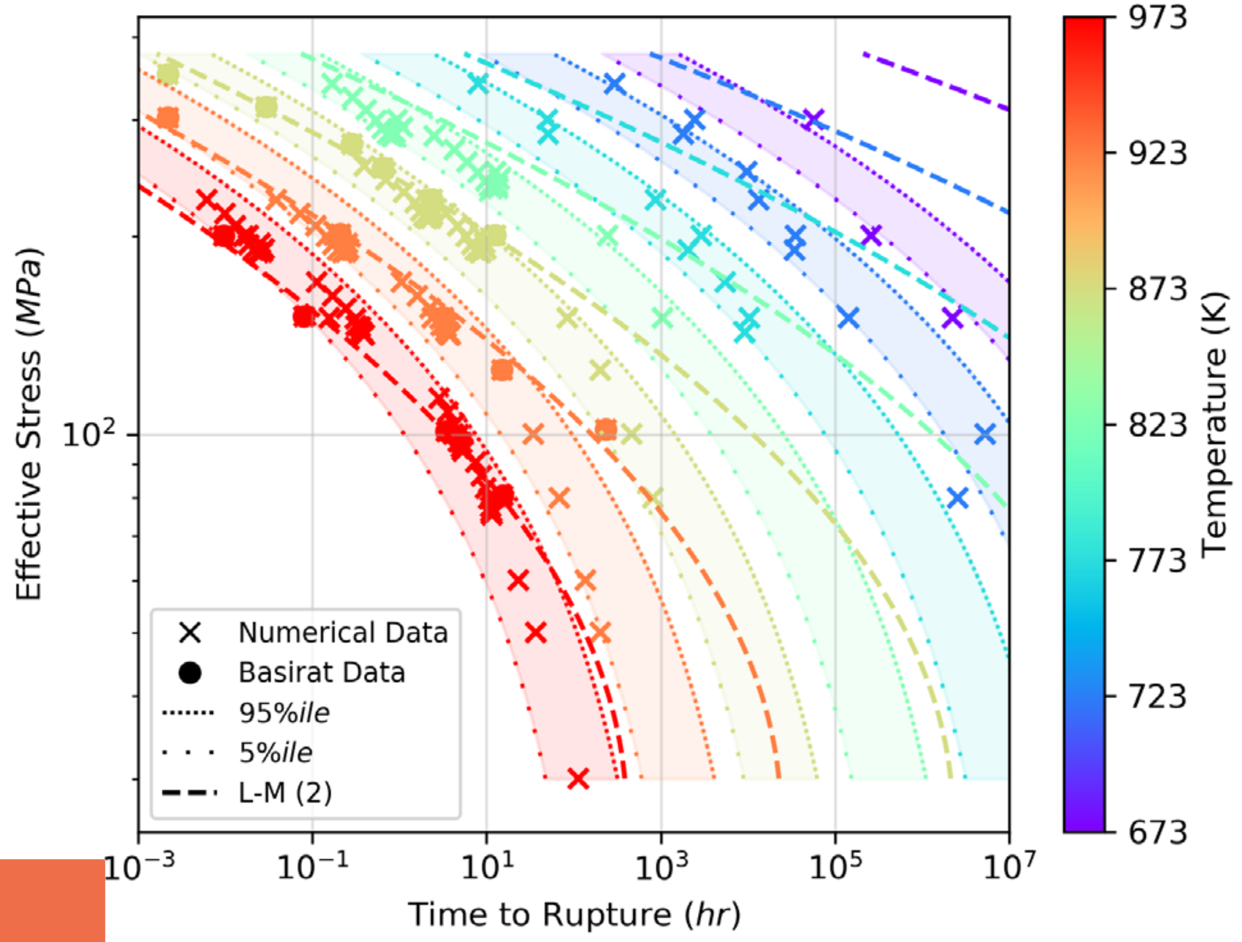

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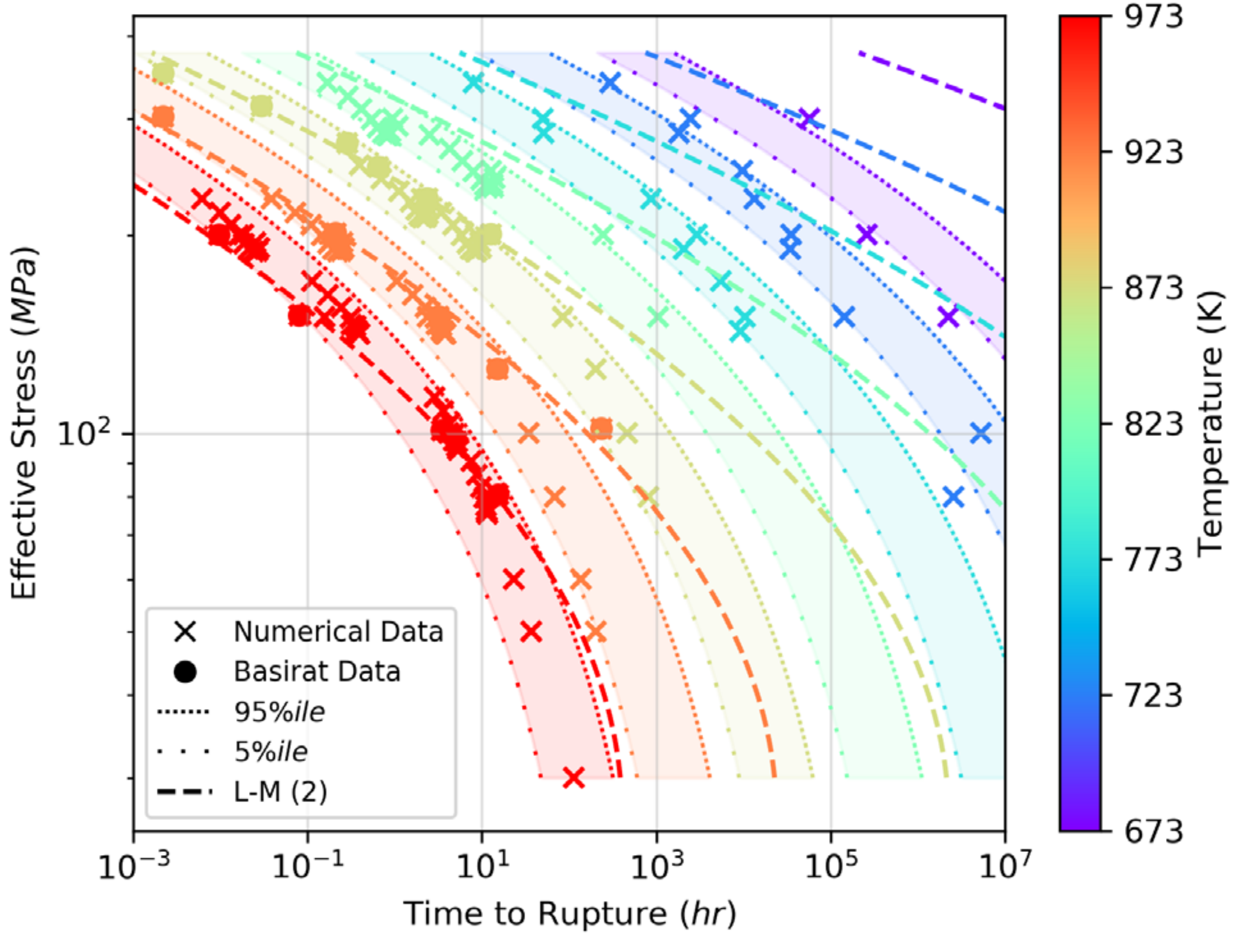
Lifetime Prediction

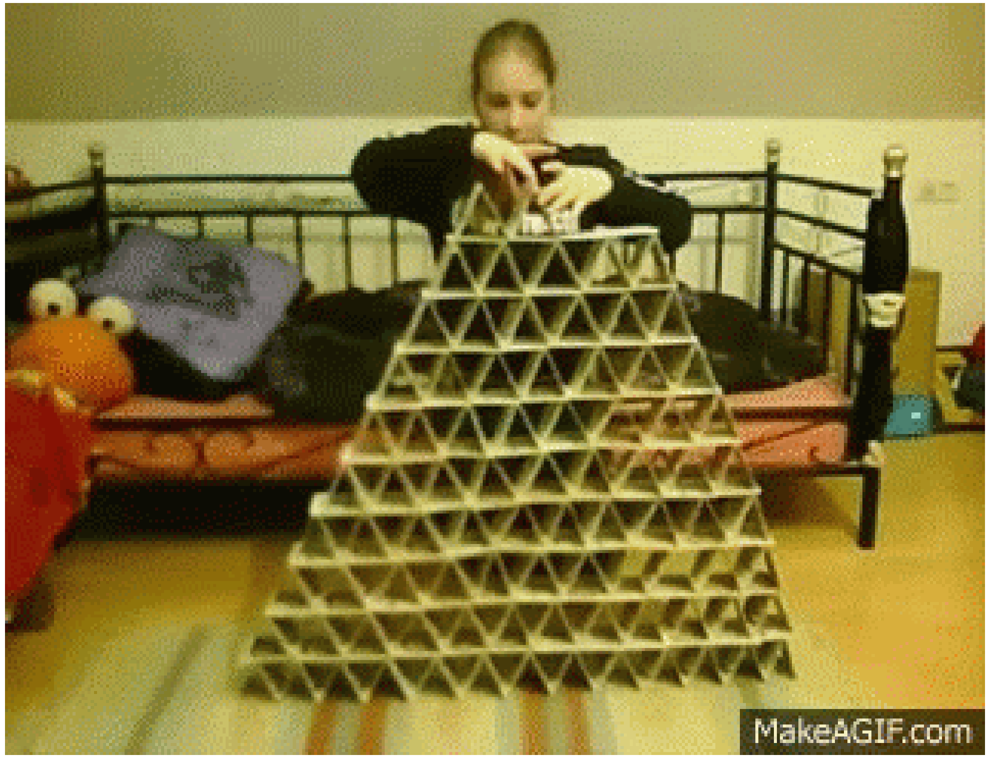
Conclusion:

By combining high fidelity based constitutive models with a mechanistic description of damage with data analytics one can:

- Derive new rupture life criteria applicable to multi-axial stress loading.
- Quantify uncertainty associated with lifetime (pedigree).
- Assist in rapid screening of new materials.
- Design experiments (not shown in this presentation)



Introspection



1. Nucleation model is empirical (Needleman and Chu, Besson etc.).
2. Grain boundary sliding is disregarded.
3. No sensitivity to precipitate type.
4. Poor model for precipitate strengthening (dispersed barrier hardening model. Lack of sensitivity to temperature).

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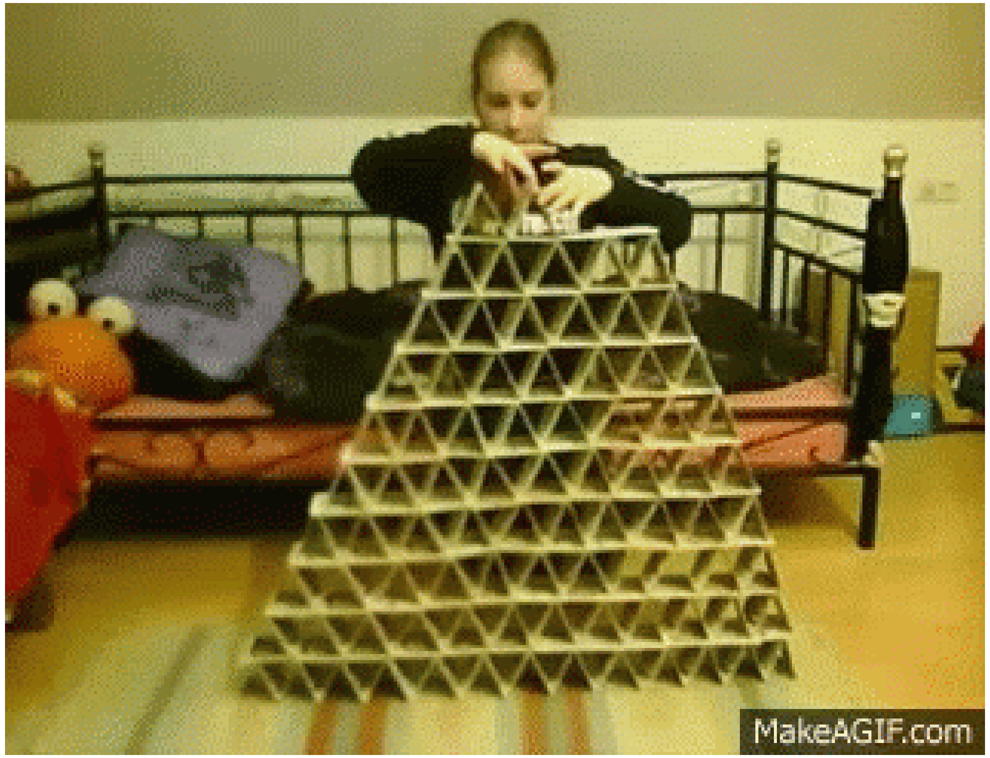

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…

$$\dot{N} = \mathcal{D}\dot{\varepsilon}_p + \mathcal{B}(\dot{\sigma}_e + \dot{\sigma}_h)$$

$$\mathcal{D} = \frac{f_N}{s_N\sqrt{2\pi}}\exp\left(-\frac{1}{2}\left(\frac{\varepsilon_p - \varepsilon_N}{s_N}\right)^2\right)$$

Example Tveergard and Needleman

Cavity nucleation

Question:

Is there a correlation between microstructure and cavity nucleation?

Vacancy distribution

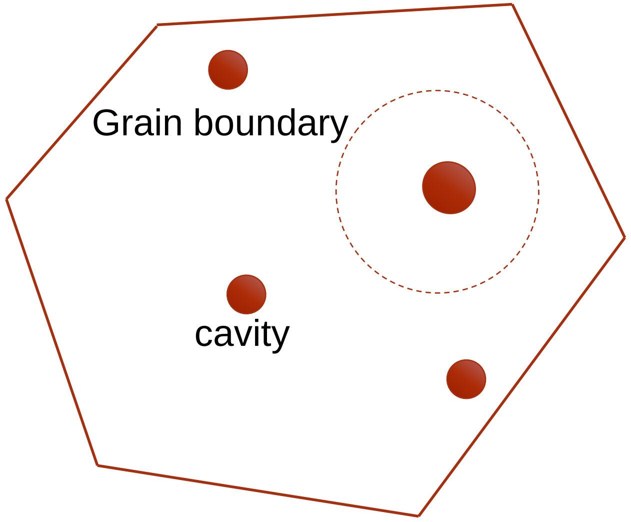
$$J_v = -D_v \nabla c$$

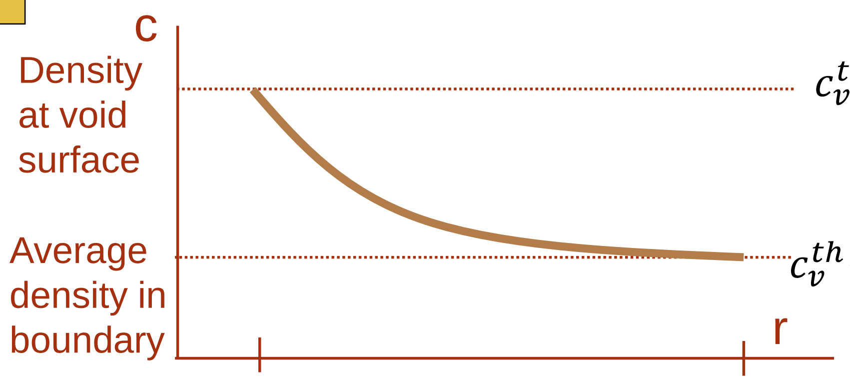
$$\frac{dc}{dt} = 0 = -\nabla \cdot J_v$$

Flux into cavity

$$\dot{n}_v = D_v \oint \nabla c \cdot dA$$

$$\dot{n}_v = \frac{4\pi\delta D'C'}{\log b/a}\left[c_v^{th}(b) - c_v^{th}(a)\right]$$





$$c_v^{th}(a) = \frac{1}{\Omega}\exp\left(\frac{-\Delta G_v(a)}{kT}\right)$$

$$c_v^{th}(b) = \frac{1}{\Omega}\exp\left(\frac{-E_v^f + \Omega\sigma_n}{kT}\right)$$

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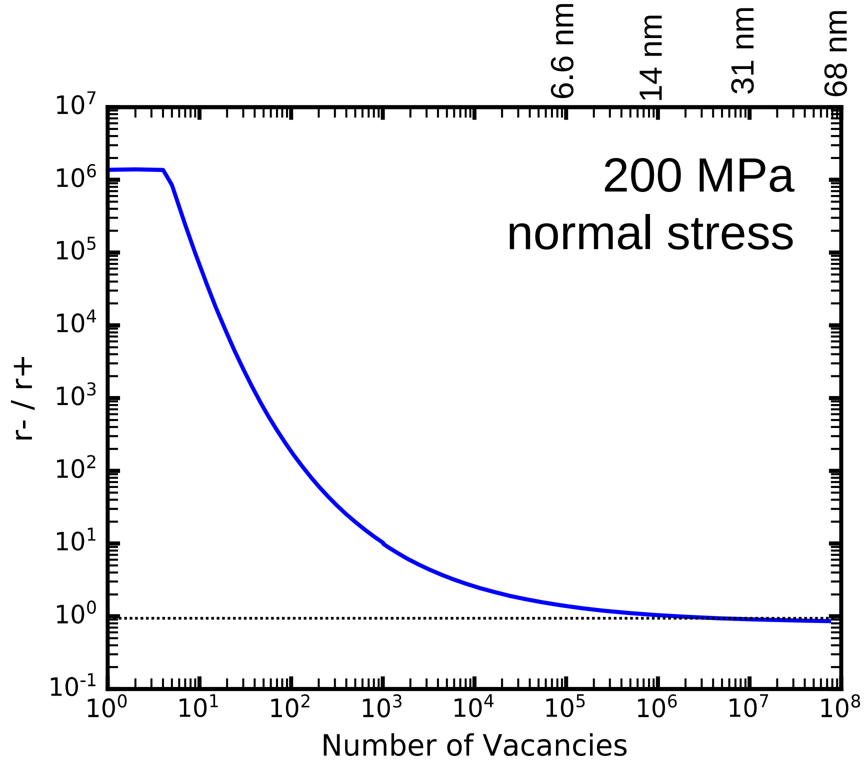


Cavity nucleation

Question:

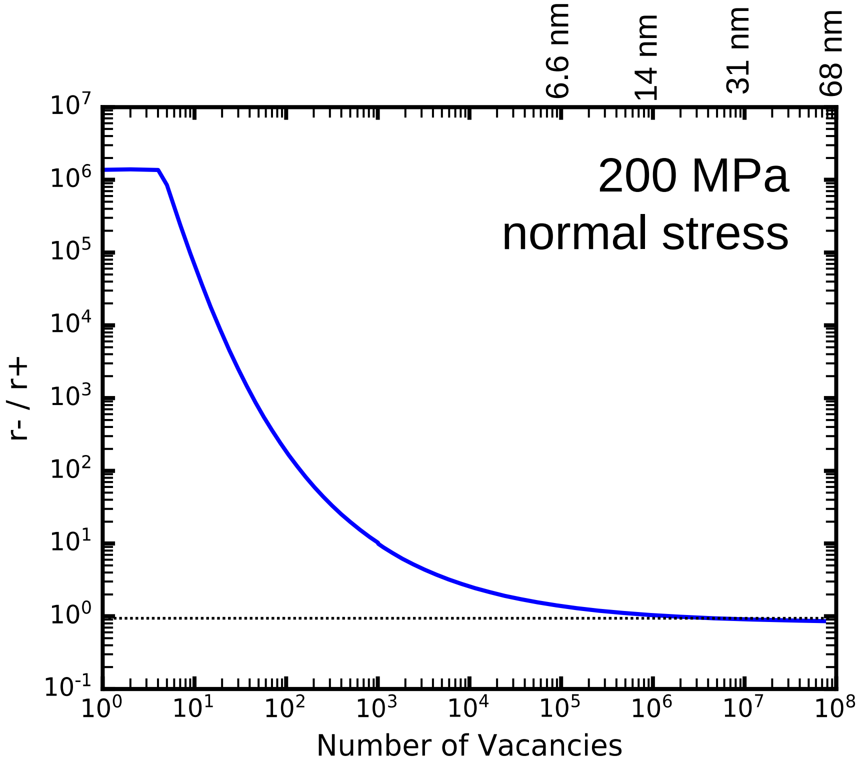
Is there a correlation between microstructure and cavity nucleation?

Conclusion:

Existing physics based models for vacancy condensation mediated cavity nucleation would predict that metals do not fail…

Option 1: Problem solved

Option 2: Thermodynamics should be reconsidered



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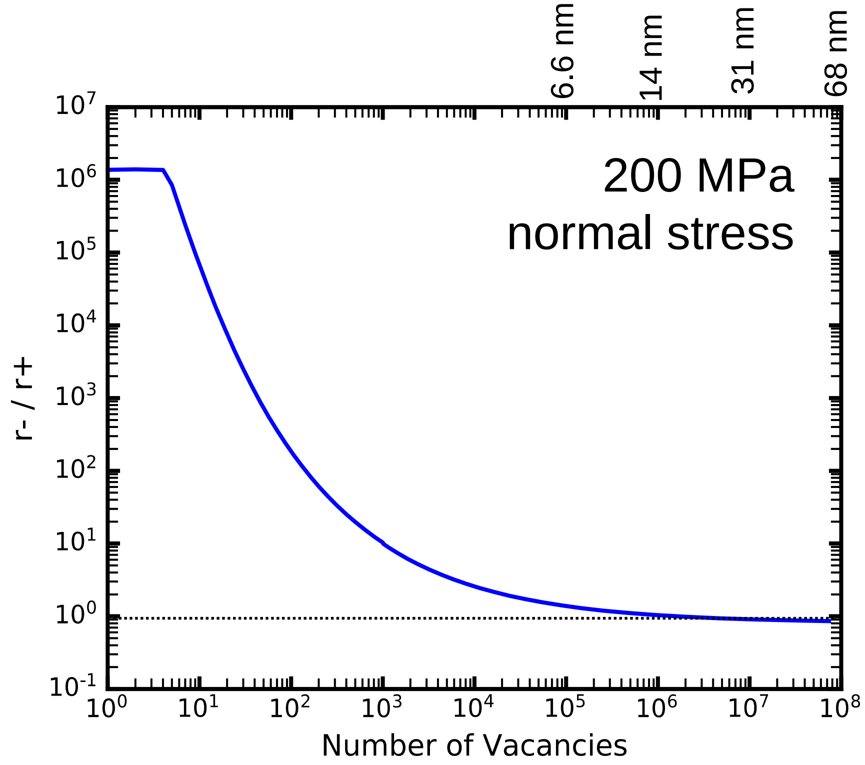

Cavity nucleation

Nucleation Sites

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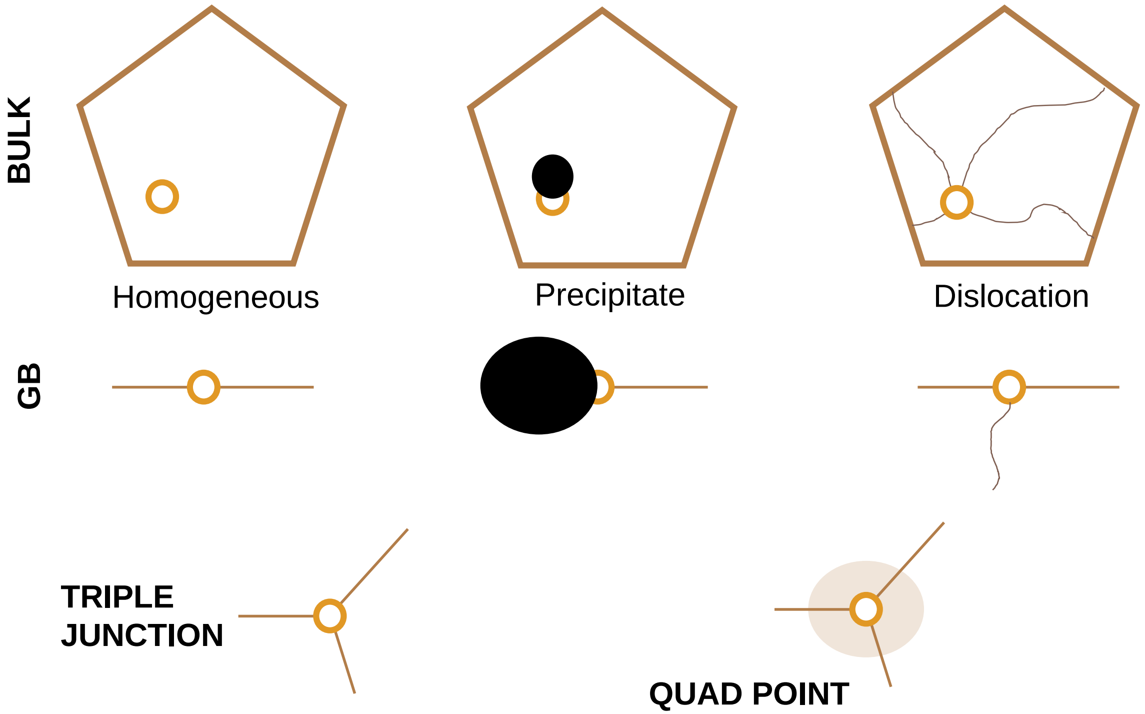

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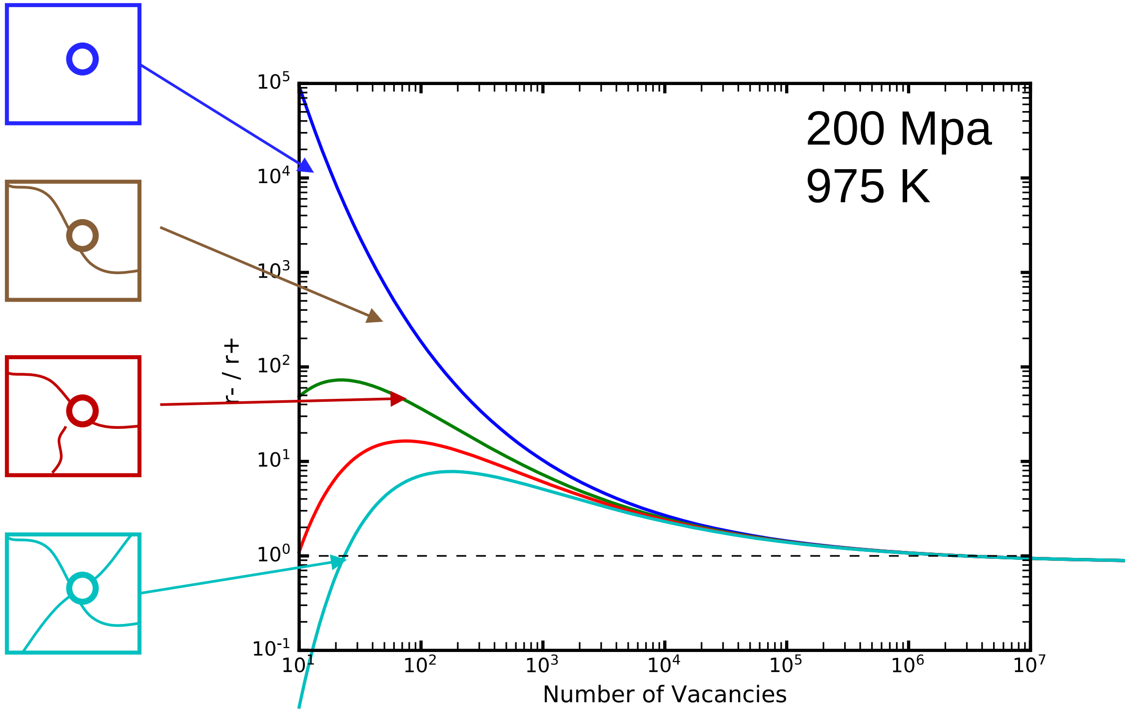
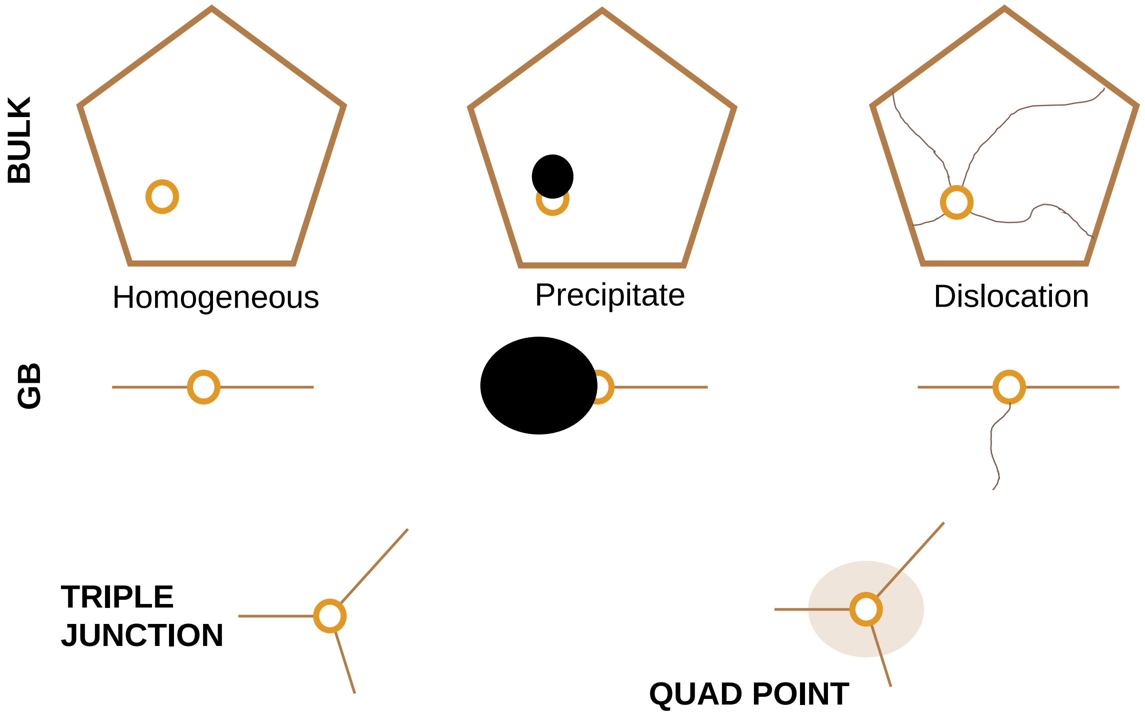




Nucleation Sites

Cavity nucleation

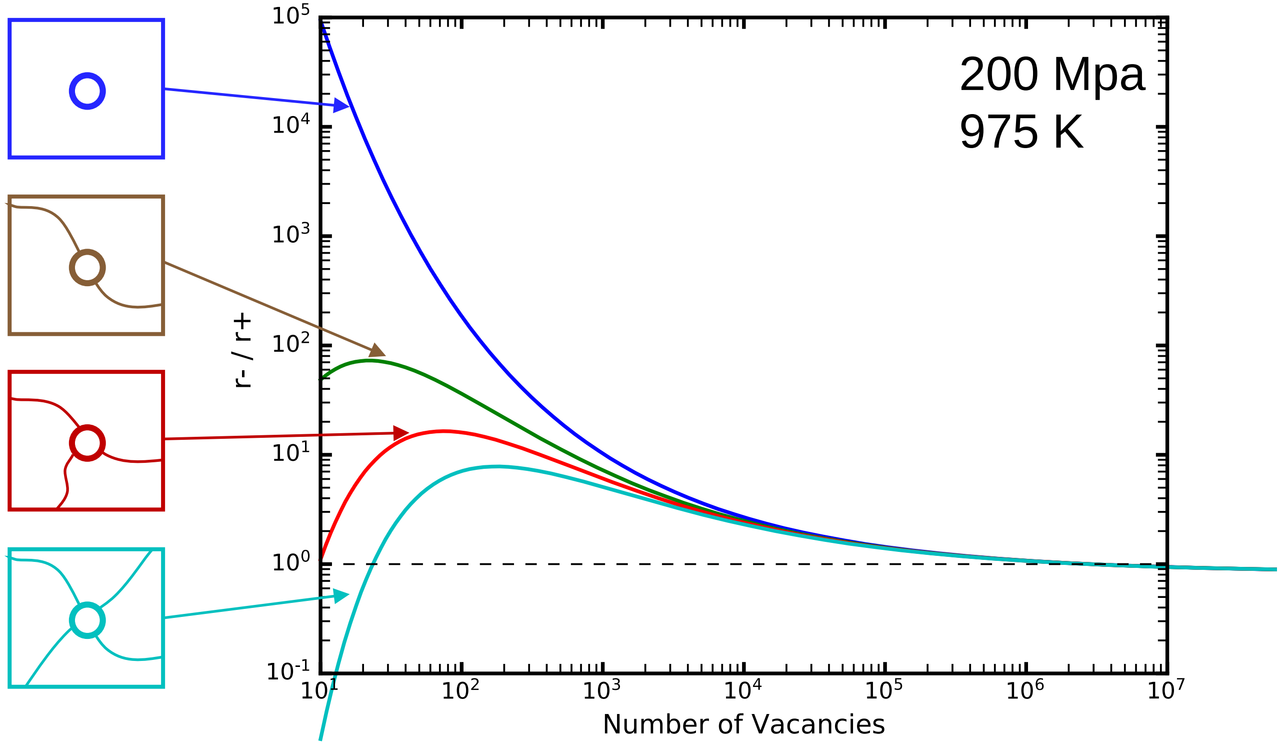
Question:

Is there a correlation between microstructure and cavity nucleation?

Conclusion:

Cavity nucleation rates are strongly biased in the presence of dislocations

Connection with material pedigree?
Derivation of new nucleation models?



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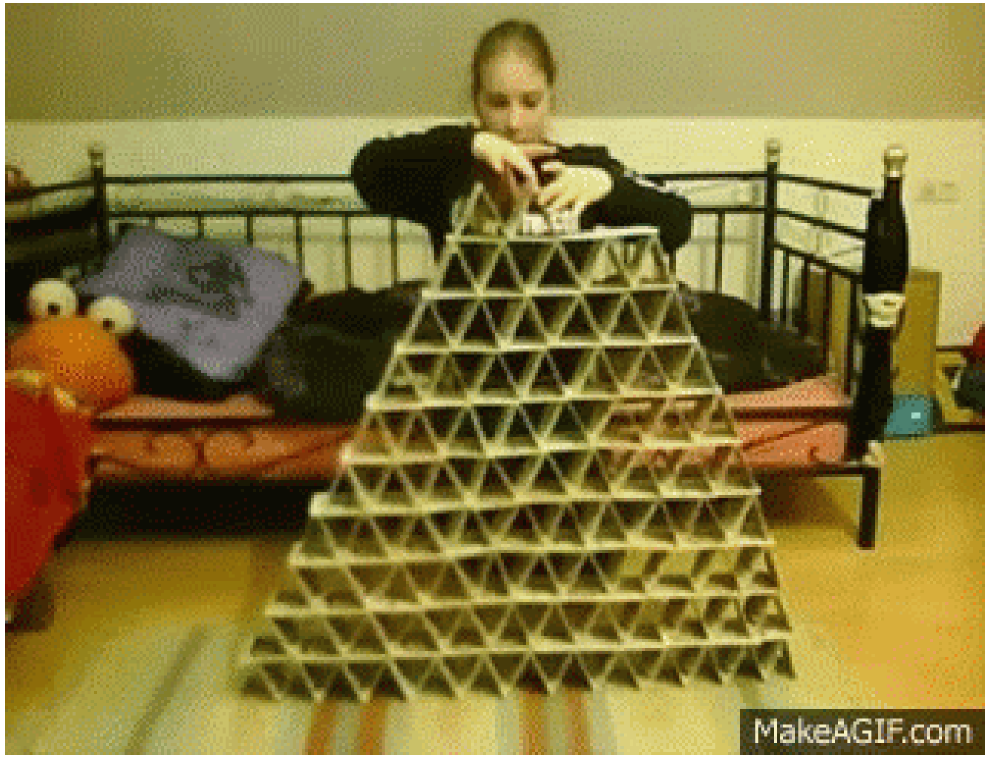

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…

Material Design

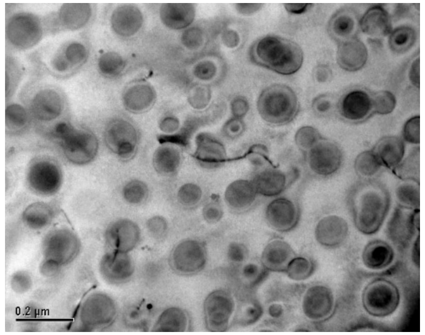
Question:

Can a **model engineering metal** can be designed to improve our understanding of precipitate strengthening?

Alumina forming austenitic steel
Nb stabilizes alumina oxide
Target phase equilibria at 750°C

Al addition tends to favor the formation L12 and B2 Fe2Nb type Laves phase

L12 strengthened AFA
(Fe-32Ni-14Cr-3Al-Nb-Ti base, 750°C/100MPa)

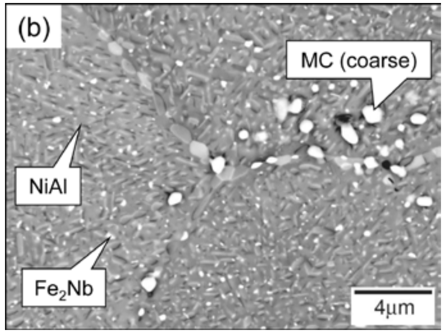


Y. Yamamoto et al. / Scripta Materialia 69 (2013) 816–819

Design 2 types of alloys:

L12 strengthened	Laves+carbide
Similar composition without L12	Similar composition without laves+ carbide

GB decoration by Laves phase
(Fe-25Ni-14Cr-3Al-Nb-C base, 750°C/100MPa)



Y. Yamamoto et al. / Met.Mate.Trans.A 42A (2011) 922-931

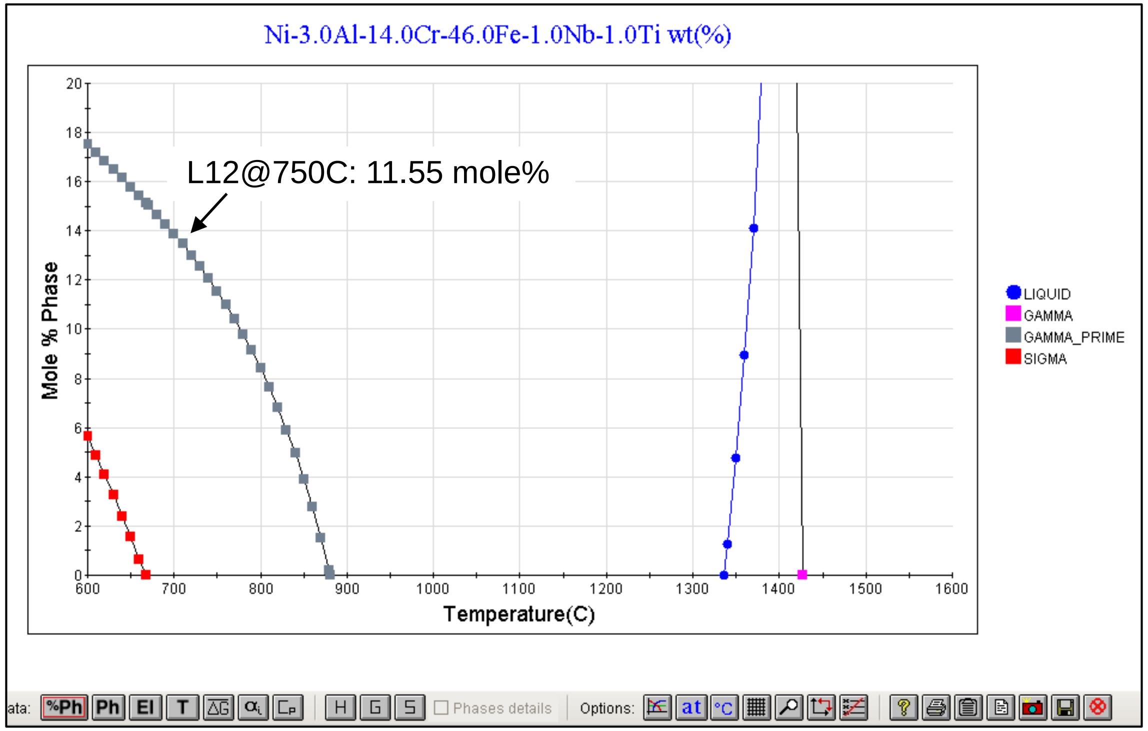
Fe-14Cr-3Al-(25-40)Ni + Nb, Ti (wt.%)

Starting point

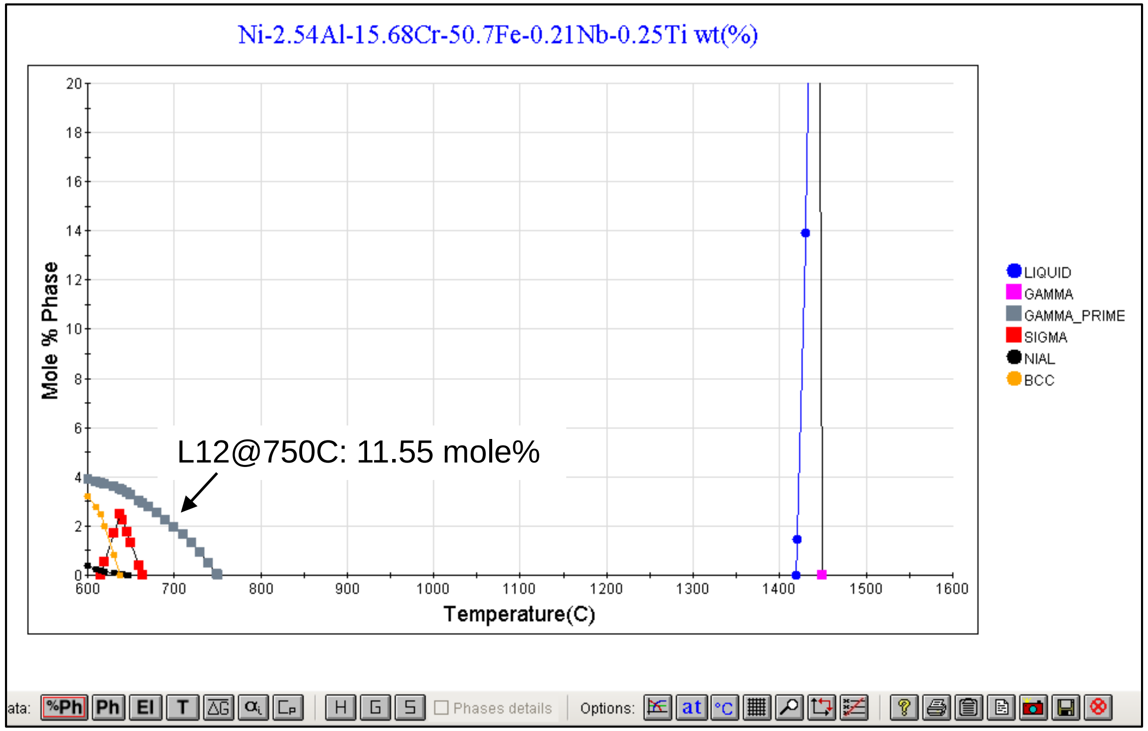
Fe-14Cr-3Al-20Ni + Nb, Ti, Mo, W, and C (wt.%)

Starting point

Design for L12 strengthening



L12@750C: 11.55 mole%



L12@750C: 11.55 mole%

#01: Fe-14Cr-3Al-35Ni-1Nb-1Ti

($L1_2$ strengthening)

- **FCC solvus: 881.4°C**
- **$L1_2$ at 750°C: 11.55 mole%**

#02: Fe-15.68Cr-2.54Al-30.63Ni-0.21Nb-0.25Ti

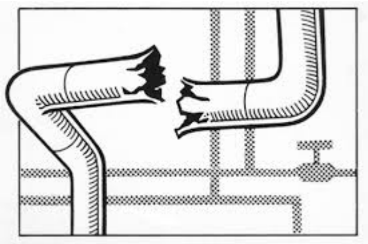
(FCC only at 750C)

- **Calculated FCC composition of 35Ni-1Nb-1Ti alloy at 750C**
- **FCC solvus: 750°C**
- **L12 at 750°C: 0 mole%**

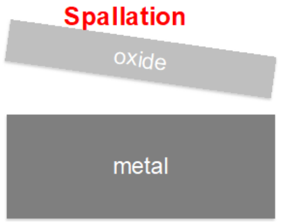
eXtremeMAT Challenges

Accelerating the Development of Extreme Environment Materials

U.S. DEPARTMENT OF ENERGY



CHEMISTRY



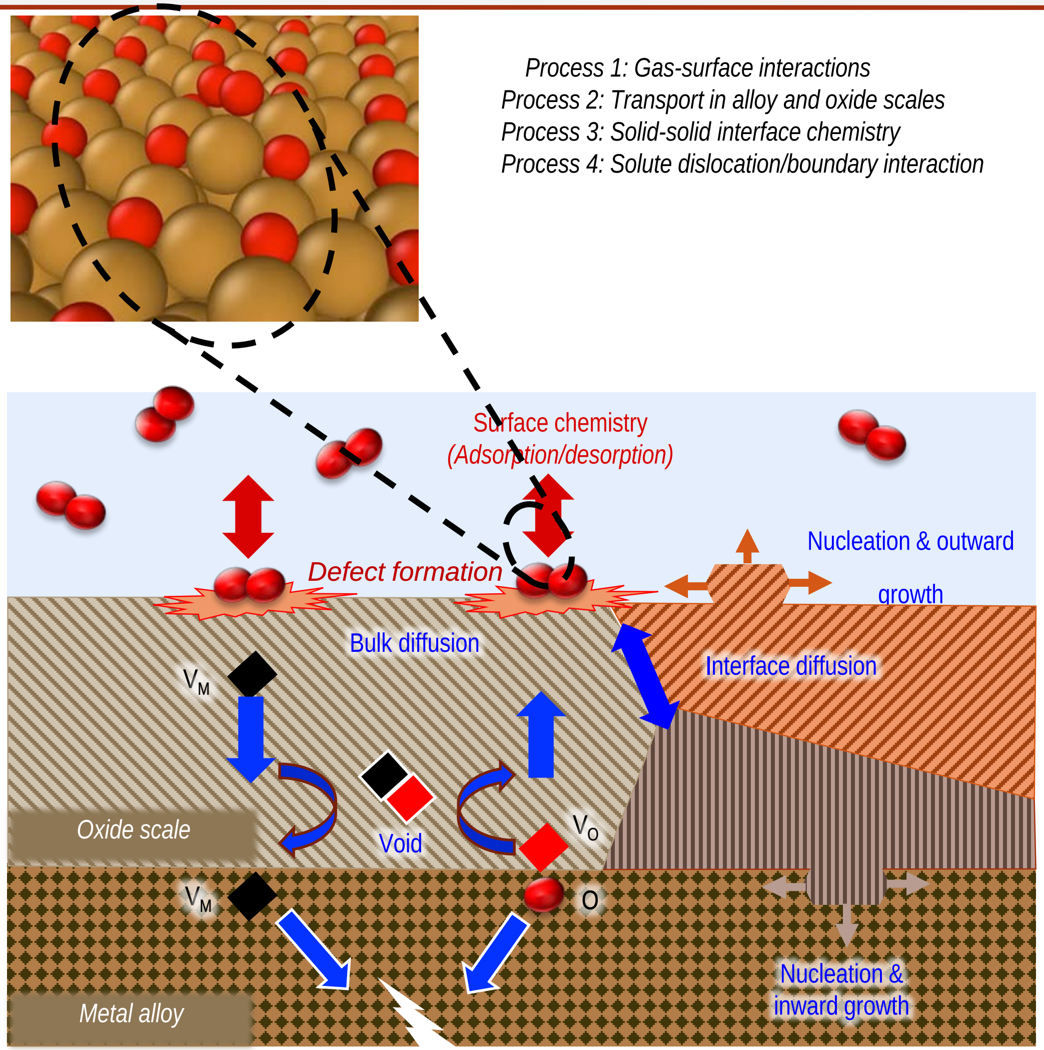
Mechanical Response as a function of microstructure and chemistry

Failure due to damage evolution as a function of composition, stress, temperature

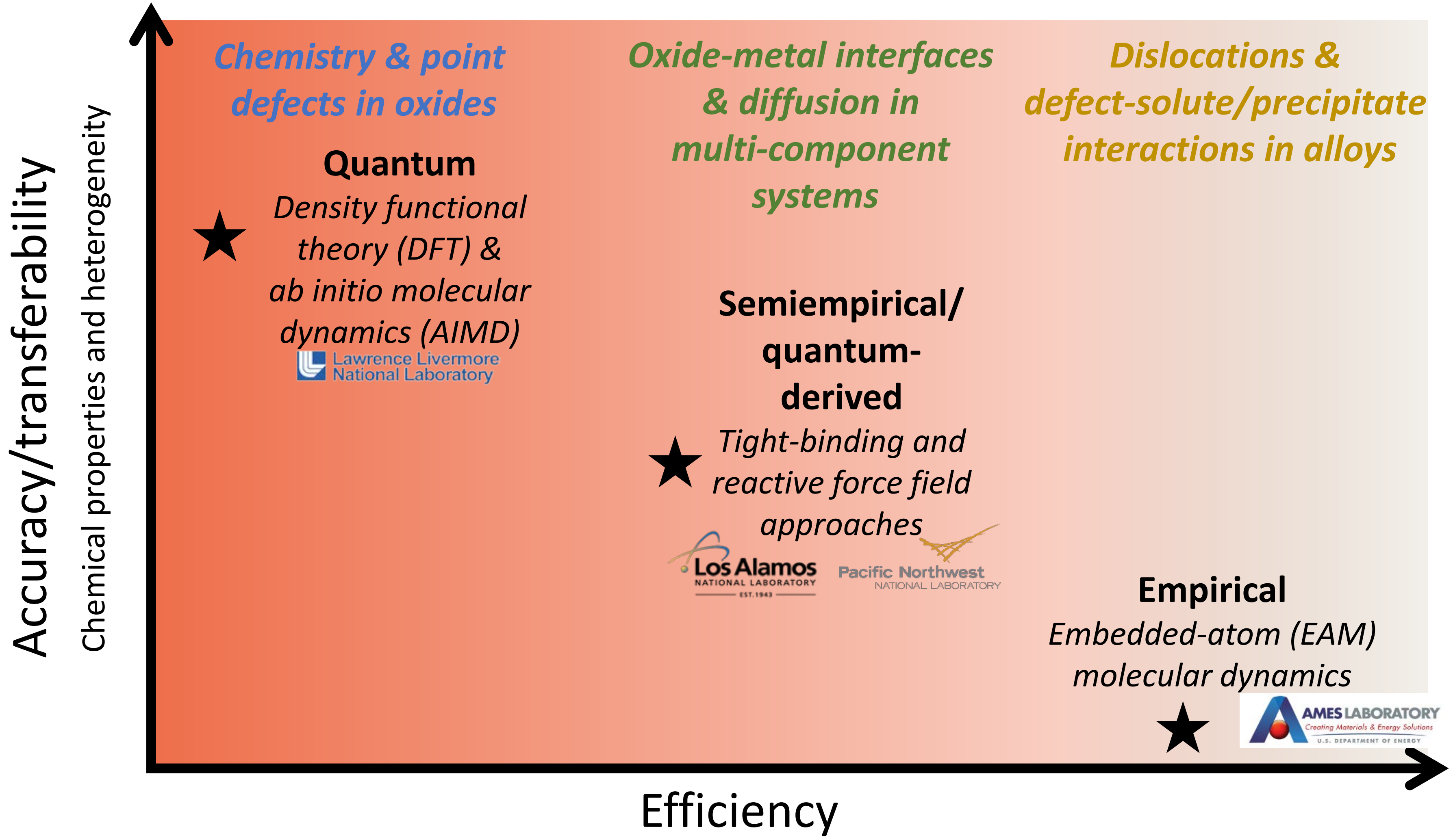
Formation oxide scale (transient, steady state)

Breakaway oxidation
(Intrinsic Chemical Failure, Mechanically Induced ChemicalFailure)

Process 1: Gas-surface interactions
Process 2: Transport in alloy and oxide scales
Process 3: Solid-solid interface chemistry
Process 4: Solute dislocation/boundary interaction



Methods



Chemistry & point defects in oxides

Oxide-metal interfaces & diffusion in multi-component systems

Dislocations & defect-solute/precipitate interactions in alloys

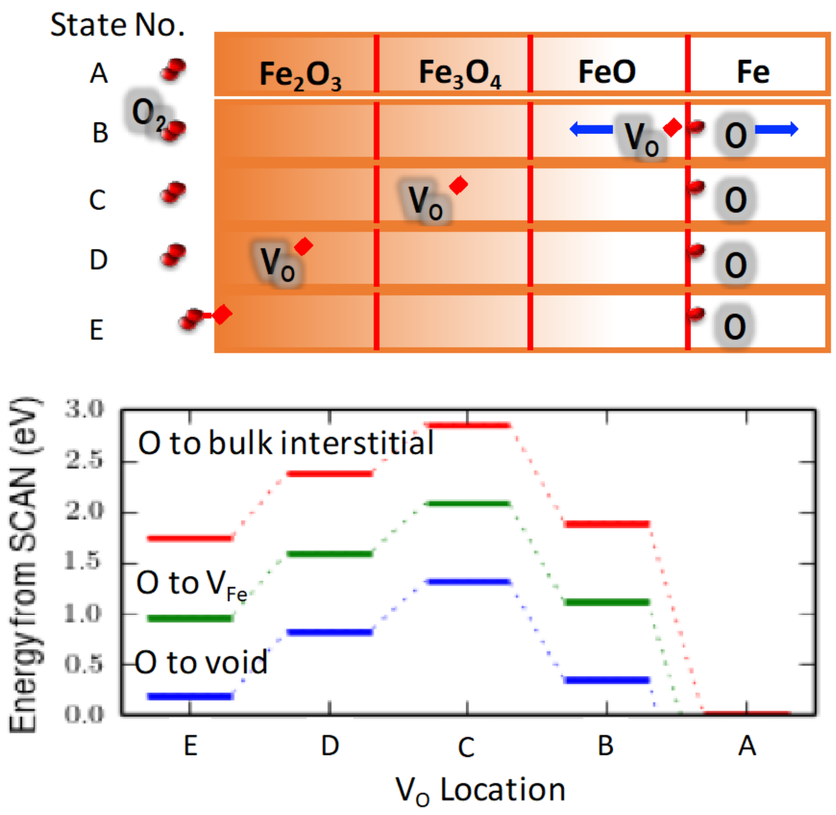
★ **Quantum**
Density functional theory (DFT) & ab initio molecular dynamics (AIMD)
Lawrence Livermore National Laboratory

★ **Semiempirical/ quantum-derived**
Tight-binding and reactive force field approaches
Los Alamos National Laboratory
Pacific Northwest National Laboratory

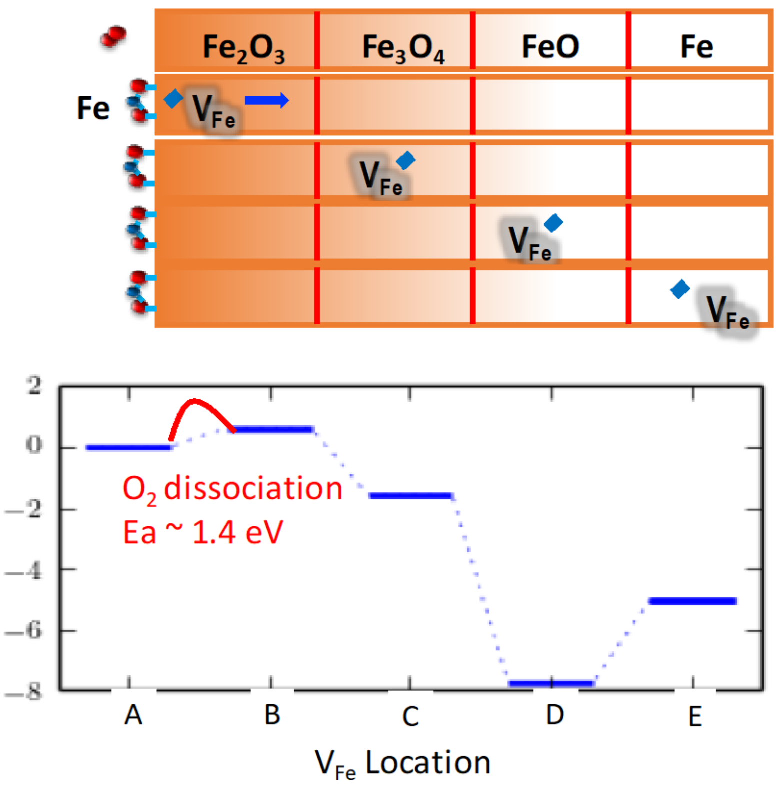
★ **Empirical**
Embedded-atom (EAM) molecular dynamics
Ames Laboratory

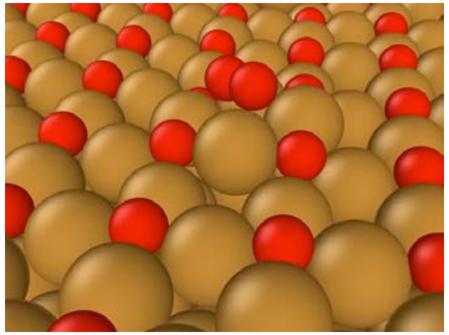
Density functional theory

O inward growth



Fe outward growth





Conclusion:

Using SCAN potentials, DFT was used to compute the thermodynamics of O_2 dissociation at different oxides.

Inward growth is not dominant at the onset of the oxidation process

Density functional theory: NOTB

Accuracy/transferability

Chemical properties and heterogeneity

Chemistry & point defects in oxides

- Surface oxygen dissocation barrier
- Oxygen and metal vacancy diffusion in oxide

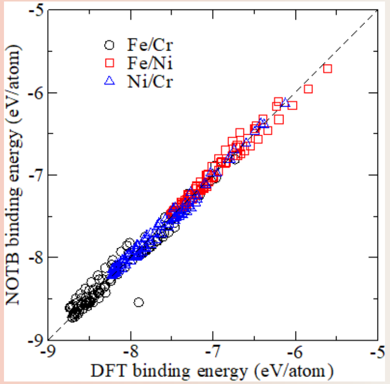
★

Oxide-metal interfaces & diffusion in multi-component systems

- DFT-NOTB potential parameterized for FeCrNi
- O, C diffusivity ?

★

Dislocations & defect-solute/precipitate interactions in alloys



- EAM potential for FeCrNi

★

Efficiency

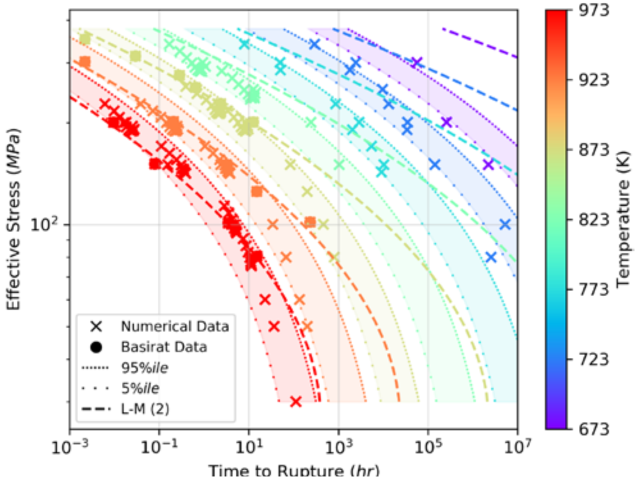
Conclusion:

A Density functional theory based non-orthogonal (i.ehandling paramangetism) tight-binding potential was derived for FeCrNi systems.

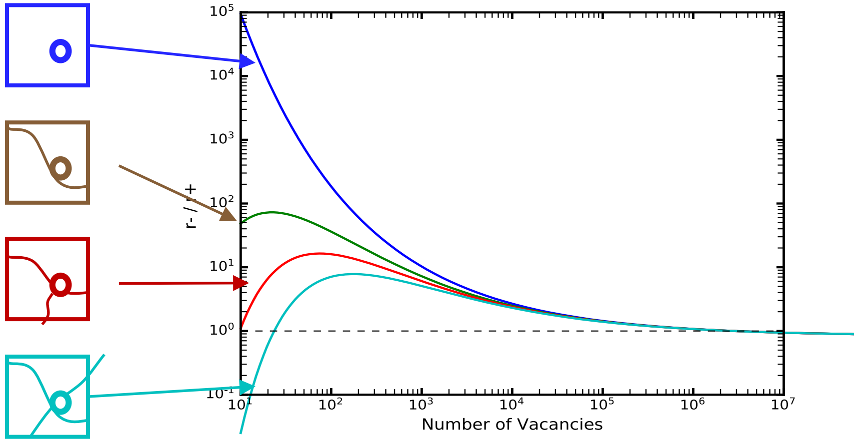
It provides the tool to numerical compute O and C diffusivities over a large compositional space

CONCLUSION

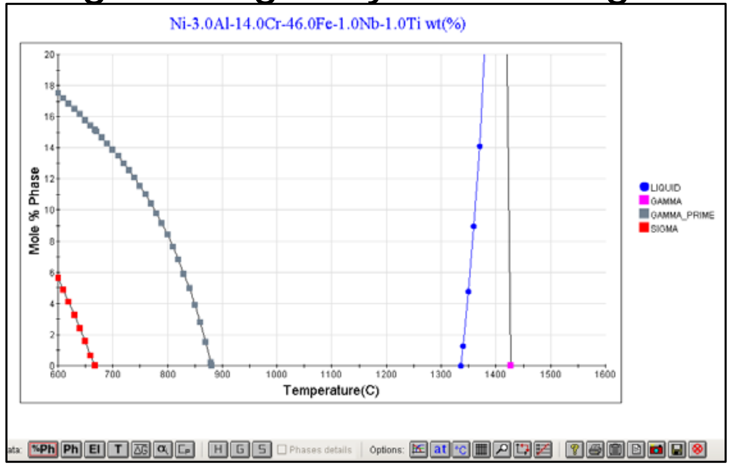
Rupture life model

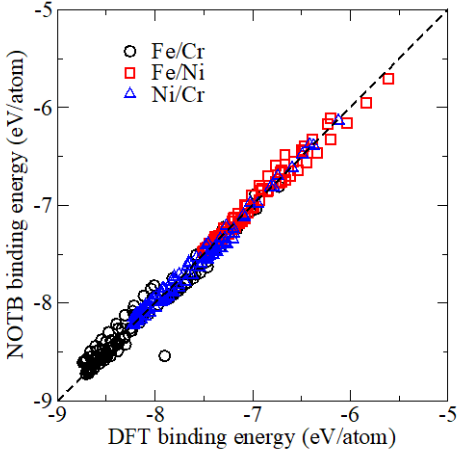


Cavity nucleation model

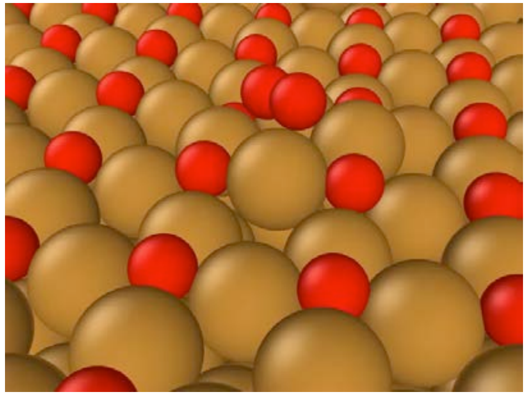


Engineering alloys for strength

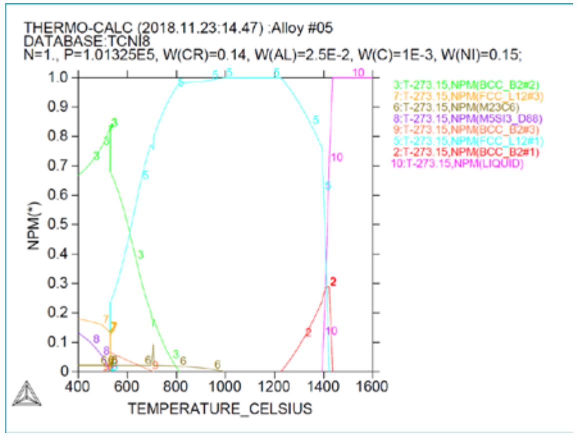

Ni-3.0Al-14.0Cr-46.0Fe-1.0Nb-1.0Ti wt(%)



DFT TB for Fe Cr Ni



DFT for Oxidization

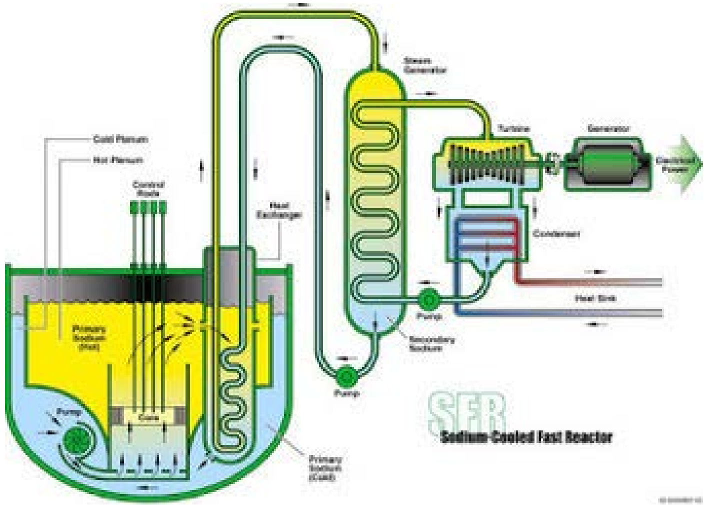

THERMO-CALC (2018.11.23:14.47) :Alloy #05
DATABASE:TCNI8
N=1., P=1.01325E5, W(CR)=0.14, W(AL)=2.5E-2, W(C)=1E-3, W(NI)=0.15;

O diffusivity

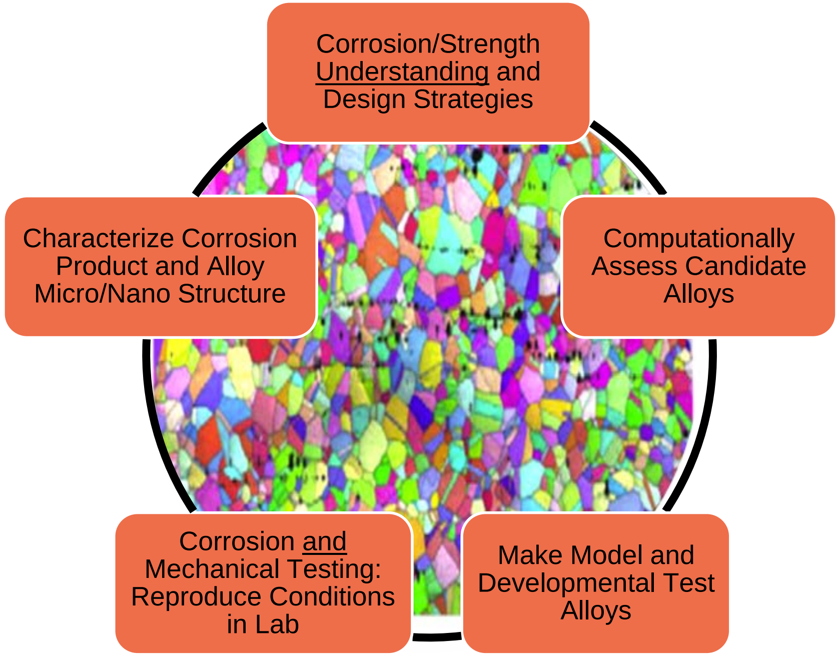
Grand challenge

Grand challenge:

Can mod/sim be used to accelerate the design and certification of existing and future alloys subjected to extreme environments?



Design cycle



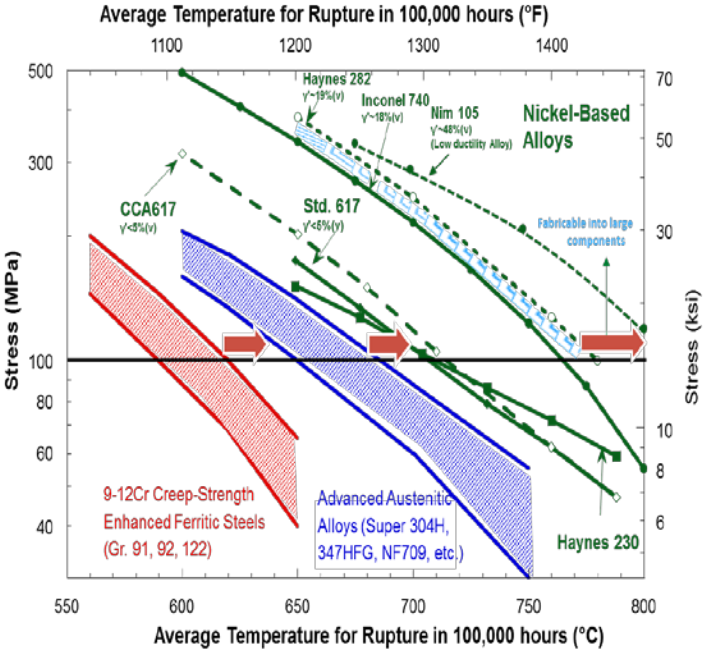
Corrosion/Strength Understanding and Design Strategies

Computationally Assess Candidate Alloys

Make Model and Developmental Test Alloys

Corrosion and Mechanical Testing: Reproduce Conditions in Lab

Characterize Corrosion Product and Alloy Micro/Nano Structure



Design for L12 strengthening

- Calculated with JMatPro v.9 + "Ni database"

  Available "$L1_2$-gamma-prime" and "B2-NiAl"

- Ni content is a strong factor to stabilize $L1_2$ phase

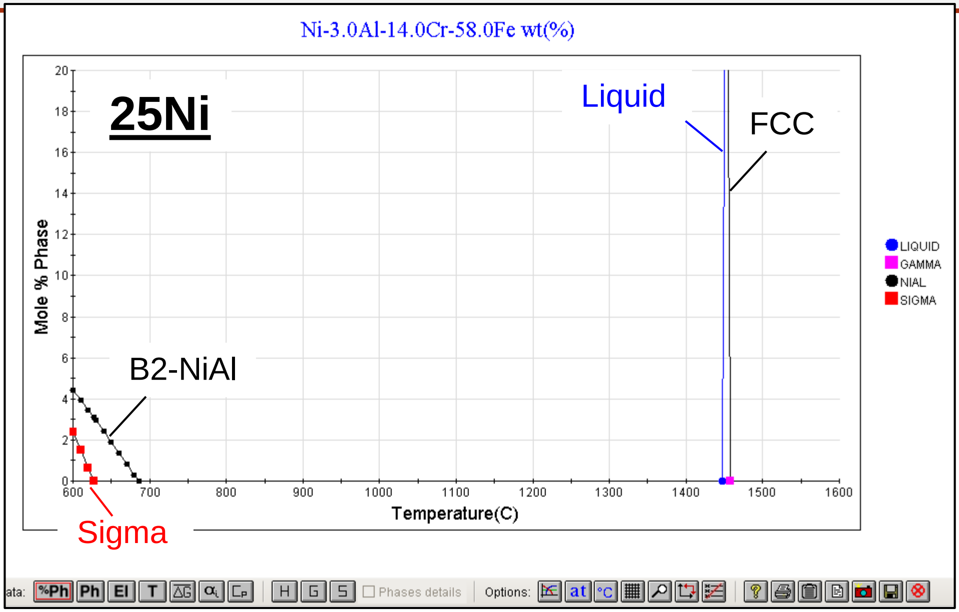
  Evaluate 25, 30, 35, and 40 wt.% Ni

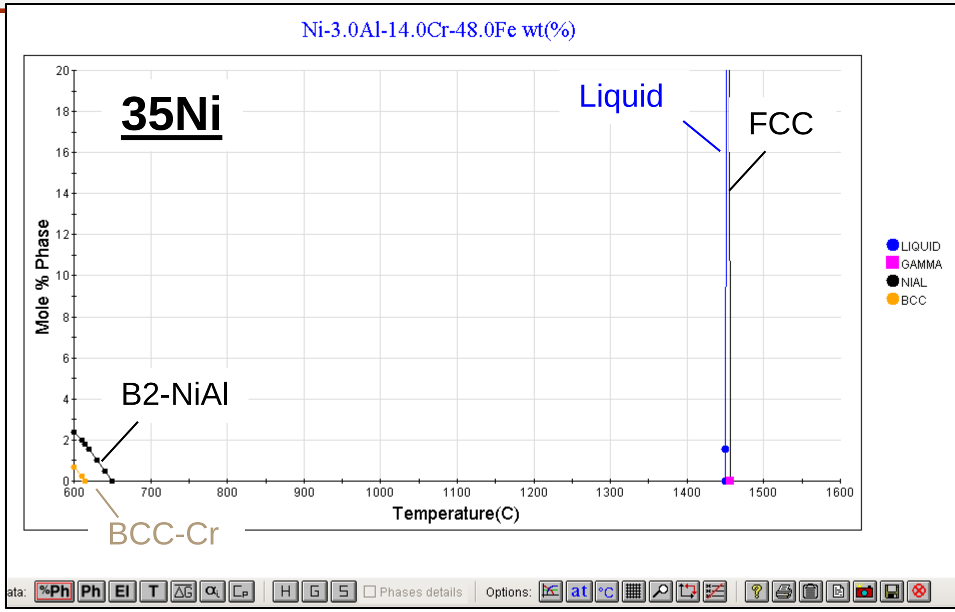
- Nb is required for stabilizing alumina scale and $L1_2$ phase

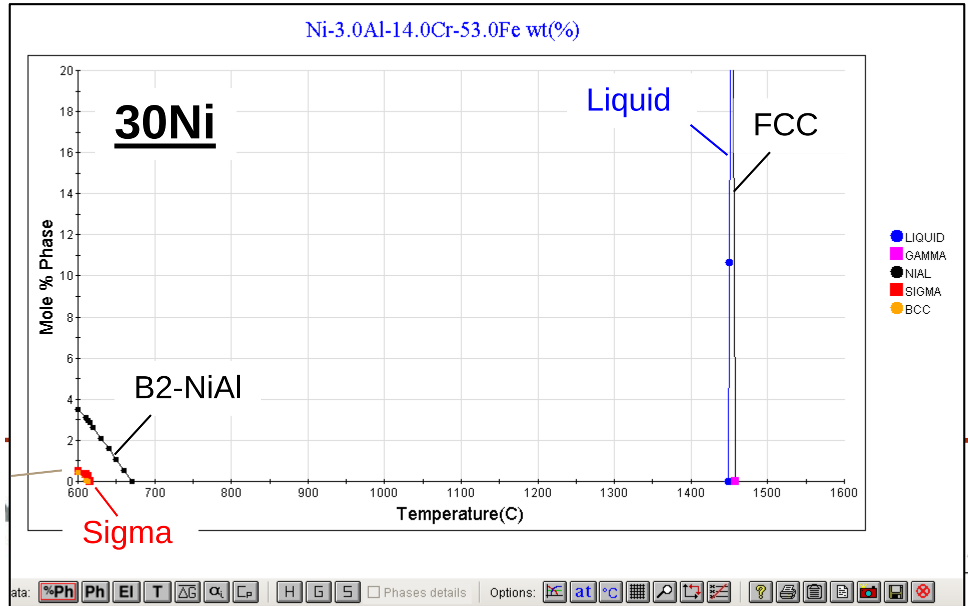
  Up to 1 wt.% to minimize the formation of other phases

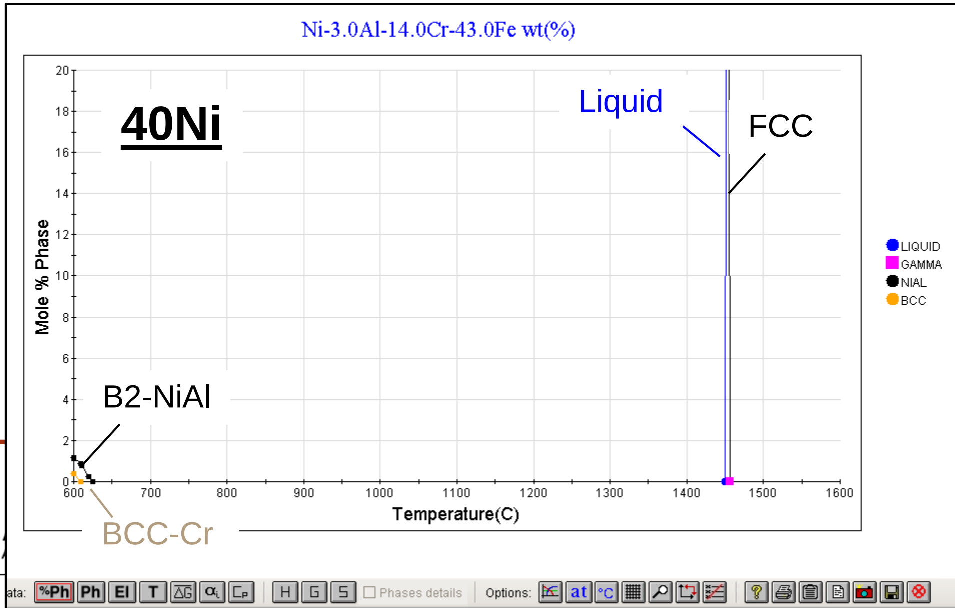
- Ti is required for stabilizing $L1_2$ phase

  Up to 1 wt.% to avoid Ni_3Ti eta phase formation









Design for L12 strengthening

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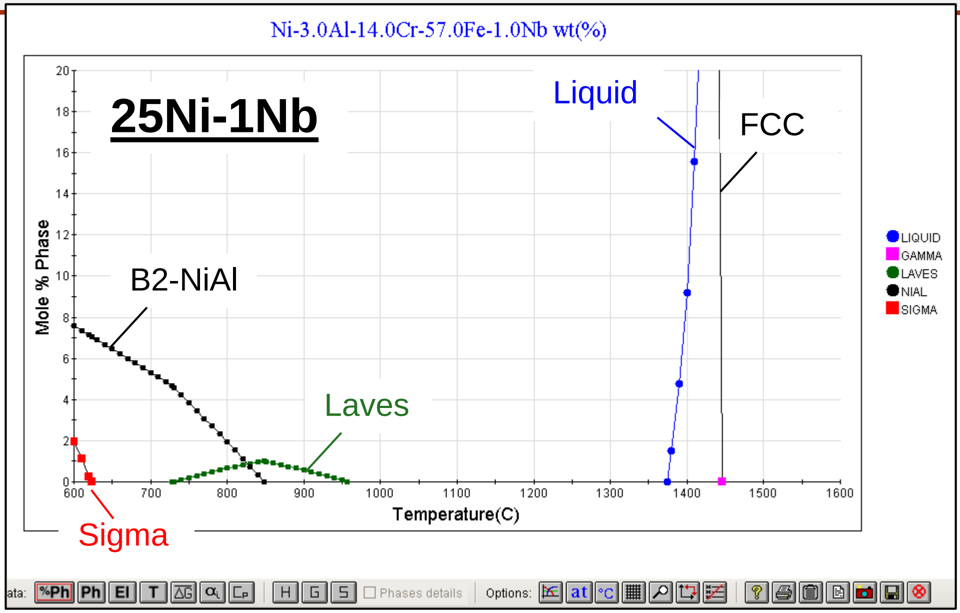
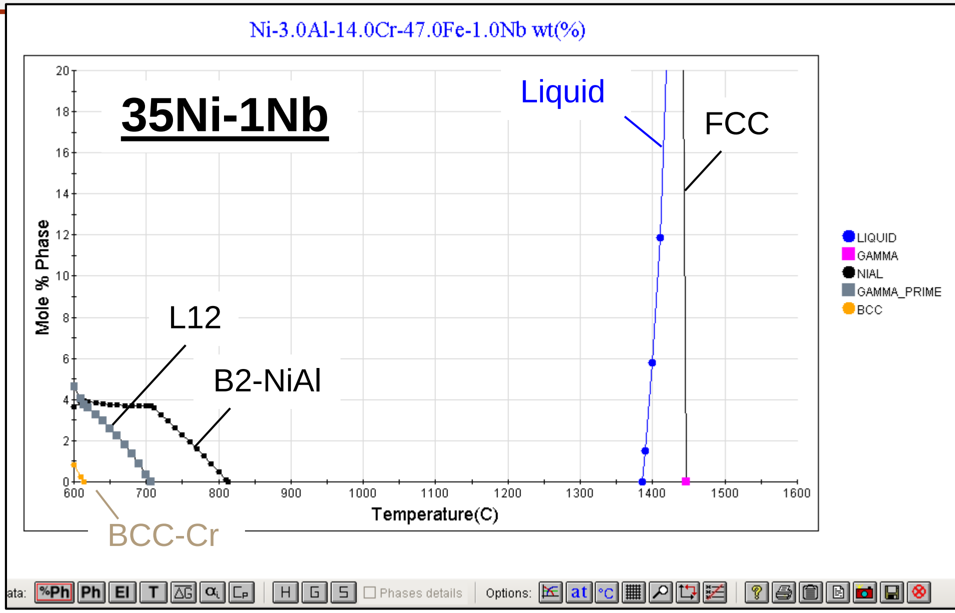
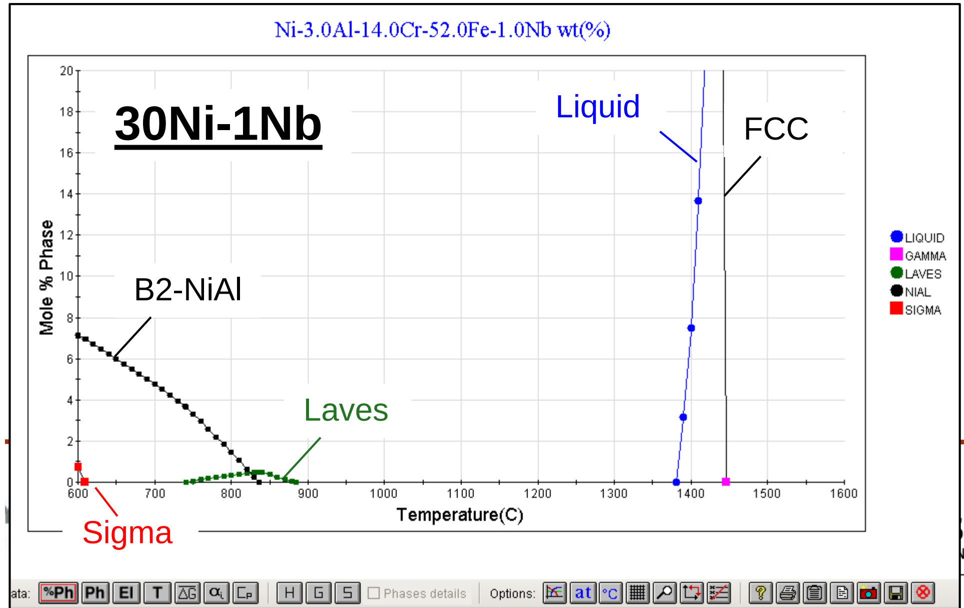
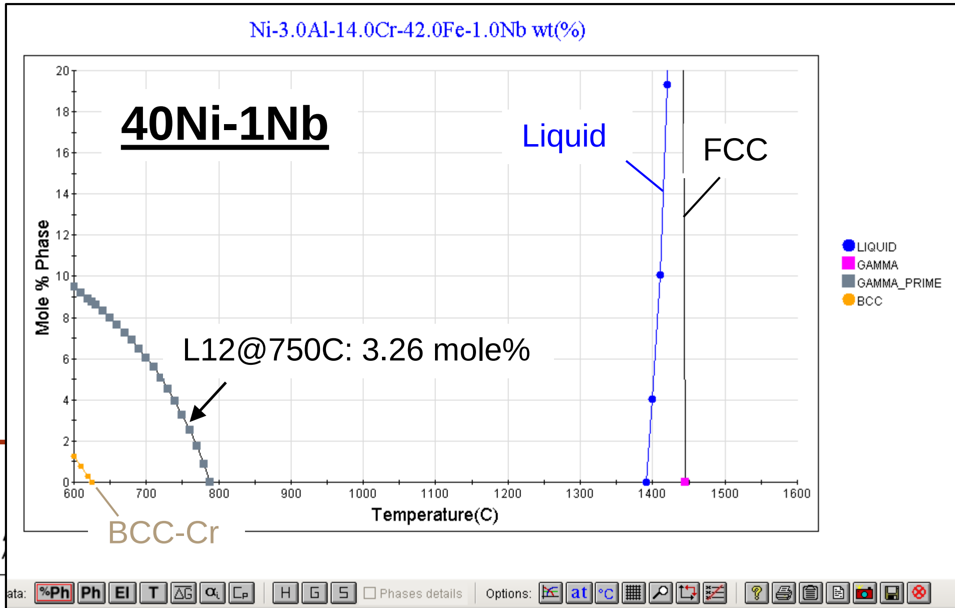

25Ni-1Nb


35Ni-1Nb


30Ni-1Nb


40Ni-1Nb

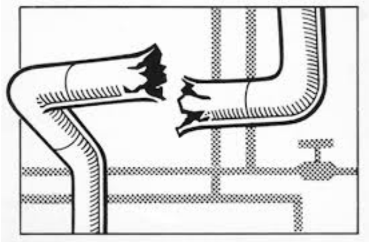
L12@750C: 3.26 mole%

eXtremeMAT Challenges

Accelerating the Development of Extreme Environment Materials

U.S. DEPARTMENT OF ENERGY

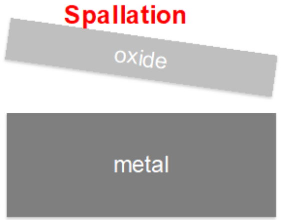
Mechanical Response as a function of microstructure and chemistry



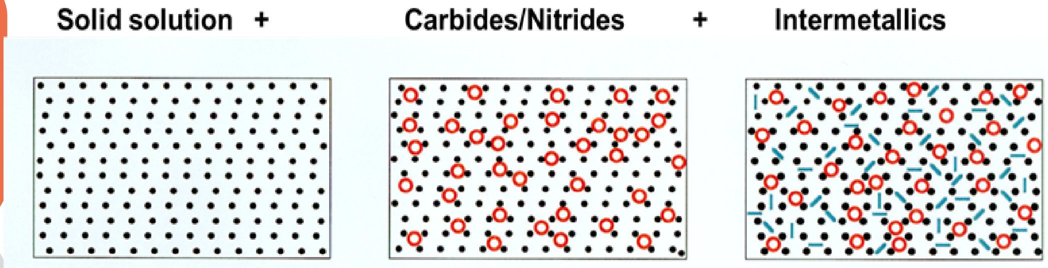
Failure due to damage evolution as a function of composition, stress, temperature

CHEMISTRY

Formation oxide scale (transient, steady state)



Breakaway oxidation (Intrinsic Chemical Failure, Mechanically Induced ChemicalFailure)



Carbides, nitrides, carbonitrides:

M(C,N): M = Ti, Zr, Hf, V, Nb, Ta (cubic); a good size stability, low super-saturation (= less availability of nano-scale precipitation in FCC matrix)

$M_{23}C_6$: M = mainly Cr (cubic); formed in the grain interior and on the grain boundary with ~100nm-1μm range

M_6C: M = Fe, Cr, Ni, Mn, V, Mo, W, Si (cubic); typically observed on grain boundary

M_2C: M = V, Nb, Ta, Mo, W (hexagonal); typically observed in low alloy steels

Z-phase: Cr(V,Nb)N compound (cubic); formed in N-rich steel with Cr and Nb

Intermetallic compounds:

(Fe,Ni)Al: AB compound (B2, ordered BCC); formed in Al (+Ni) containing steel, typically coupled with Laves-phase precipitates when Nb exists

Laves: A_2B compound (hexagonal or cubic), A = Fe, Cr, B = Ti, Zr, Mo, Nb, W, Ta, Hf; typically equilibrated directly with Fe solid solution (BCC/FCC)

γ'-Ni_3Al: A_3B compound ($L1_2$, ordered FCC); formed as coherent precipitates in FCC matrix of Ni-rich alloy with Al, Ti, Nb

γ''-Ni_3Nb: A_3B compound ($D0_{22}$, ordered FCT); formed as semi-coherent, meta-stable phase precipitates in FCC matrix of Ni-rich alloy with Nb, Fe, V

eXtremeMAT Challenges

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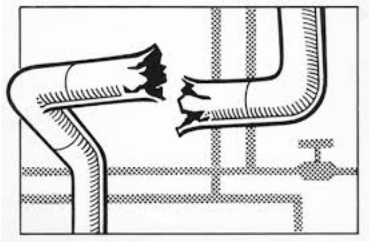
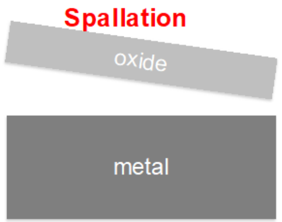
U.S. DEPARTMENT OF ENERGY



CHEMISTRY

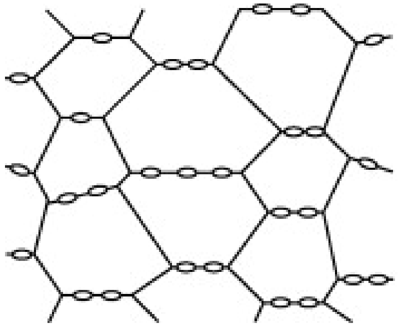


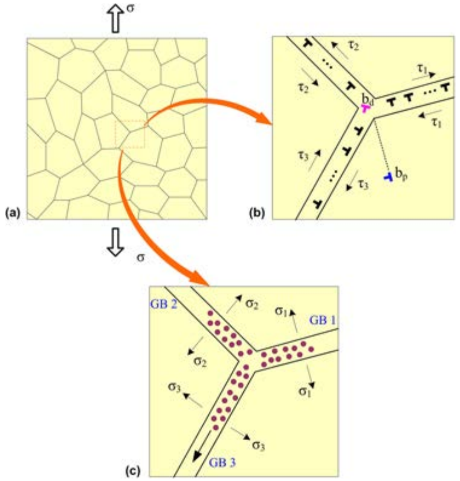
Mechanical Response as a function of microstructure and chemistry

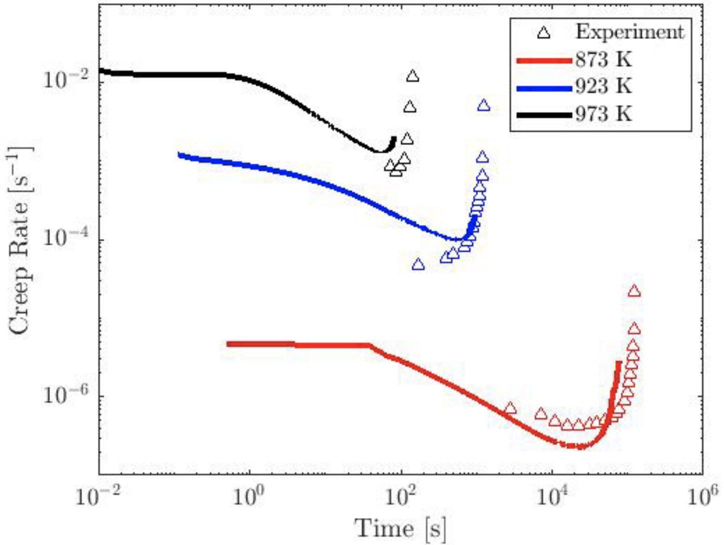
Failure due to damage evolution as a function of composition

Formation oxide scale (transient, steady state)

Breakaway oxidation (Intrinsic Chemical Failure, Mechanically Induced ChemicalFailure)







eXtremeMAT Challenges

Accelerating the Development of Extreme Environment Materials

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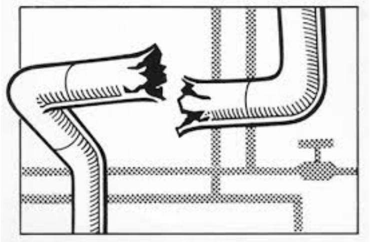

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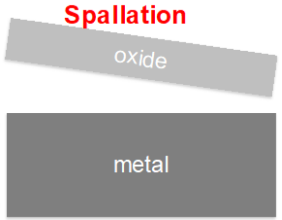
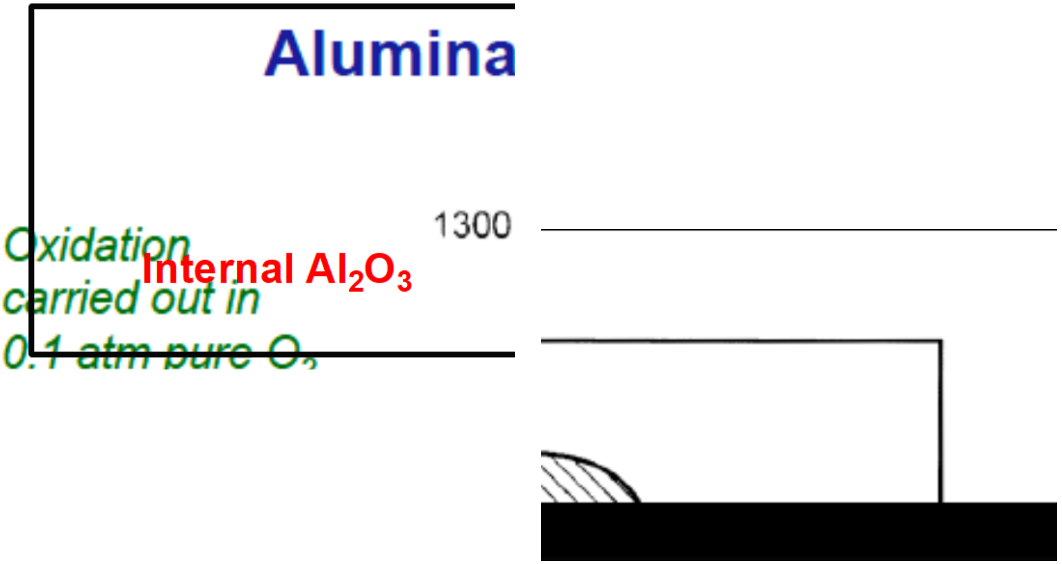


Breakaway oxidation (Intrinsic Chemical Failure, Mechanically Induced ChemicalFailure)

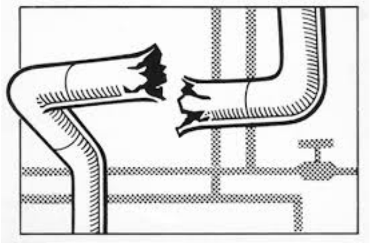


- Internal vs external oxidation
- Dynamics competition between rapid transient base metal oxidation and establishment of a continuous protective layer (Cr_2O_3, Al_2O_3, SiO2)
- Effect of of alloying on O/N/C permeability?

eXtremeMAT Challenges

Accelerating the Development of Extreme Environment Materials

U.S. DEPARTMENT OF ENERGY



Mechanical Response as a function of microstructure and chemistry

Failure due to damage evolution as a function of composition

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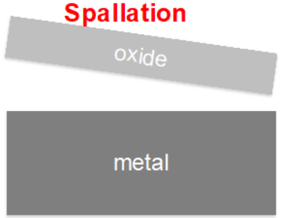

Breakaway oxidation
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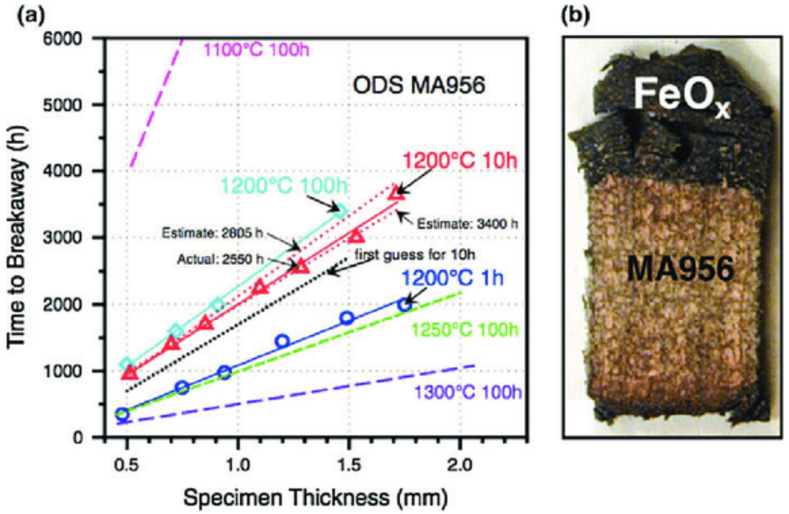

Not considered this year