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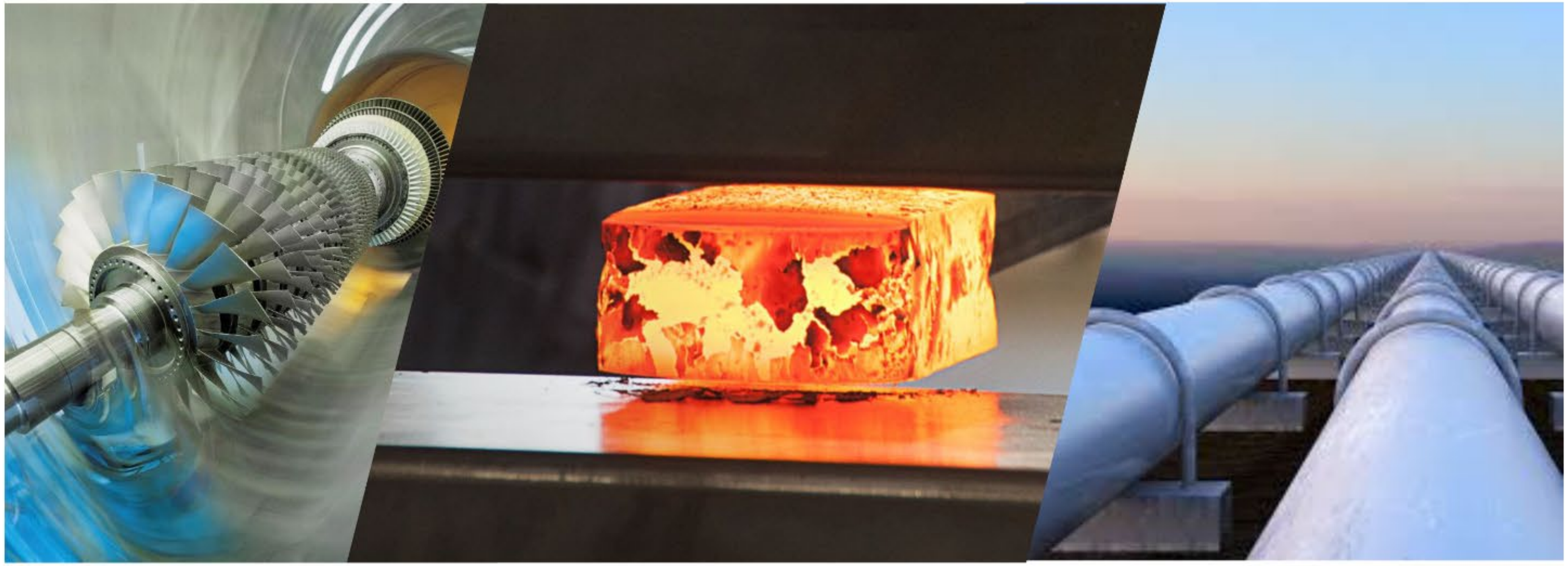
Guidelines for Alloy Development

Crosscutting Research & Advanced Energy Systems Project Review Meeting, High Performance Materials Program Virtual Session (06/15/2021)



Yukinori Yamamoto, Mike Brady, Edgar Lara-Curzio (ORNL) & Jeffrey Hawk (NETL)

Thrust 4 (FWP 1022433) Extreme Environment Materials (eXtremeMAT)

XMAT: Project Team & Other Acknowledgements

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XMAT Thrust 4 Project Team

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Acknowledgement

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XMAT: Project Outline

eXtremeMAT

Accelerating the Development of Extreme Environment Materials

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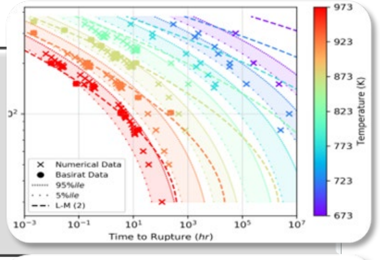
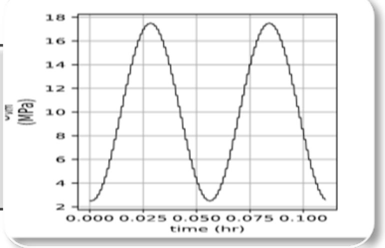
Thrust 1: Material Lifetime and Performance Predictors

- Physics-based mechanistically derived material lifetime prediction
- Microstructure characterization and creep deformation parameters of 347H steel & developmental alumina-forming austenitic (AFA) stainless steels



Thrust 2: Component Lifetime and Performance Predictors

- Finite element models predicting the performance and lifetime of 347H components under multi-axial loading (validate with tube form, multi-axial creep studies)



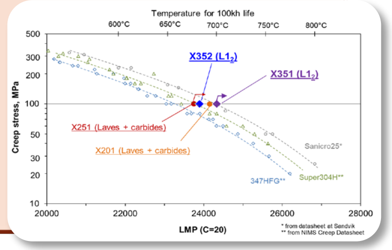
Thrust 3: Materials Database and Analysis Tools

- Management of database and analysis tools for new alloy development and performance assessment

EDX Energy Data eXchange

Thrust 4: Guidelines for the Discovery of New Alumina Forming Alloys

- **Guidelines for the design of next generation alumina-forming austenitic (AFA) alloys**
- **Model microstructures to optimize creep resistance via multi-scale precipitates**
- **Insights for establishment of alumina via experimental and modeling approaches**



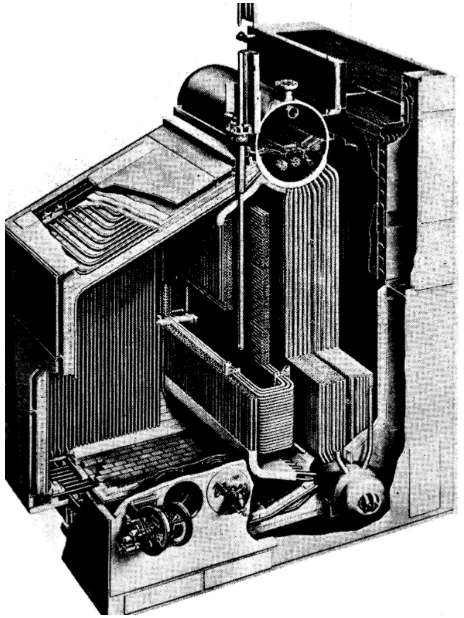
Major Target of "Alloy Development (Thrust 4)" under eXtremeMAT Project

Objective: model alumina-forming austenitic (AFA) steels to guide/validate new computational tools for the design of higher-performing alloys

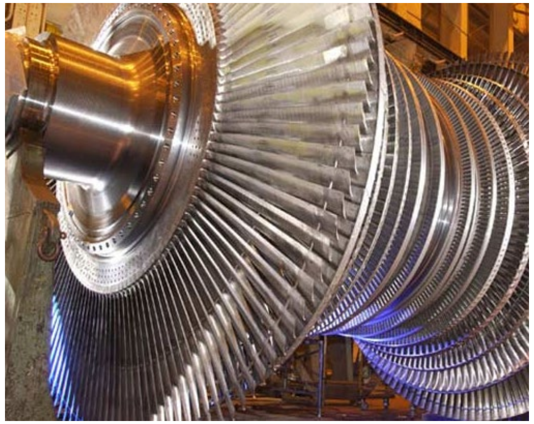
Approaches:

- Thermodynamics/kinetics: phase stability prediction, strengthening second-phase precipitation
- DFT: major element bonding, O permeation/diffusion
- Phase-field: initial establishment of protective alumina
- Experimental validations: selection of model AFA alloys, evaluation of oxidation resistance and creep-rupture performance, characterization of microstructure evolution, measurement of oxygen permeation

Boiler



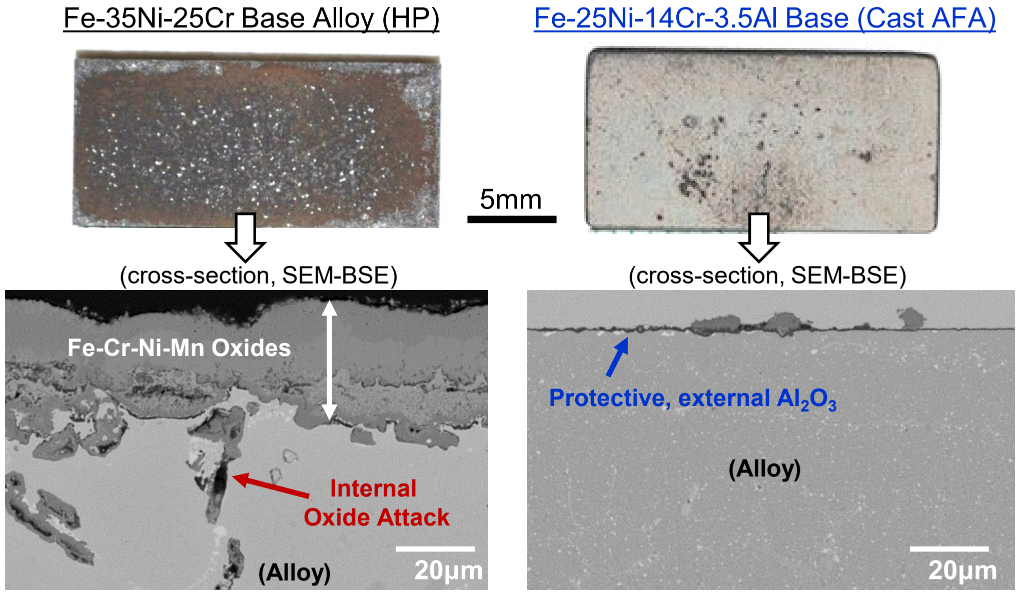
Turbine



Philosophy of AFA Alloy Development

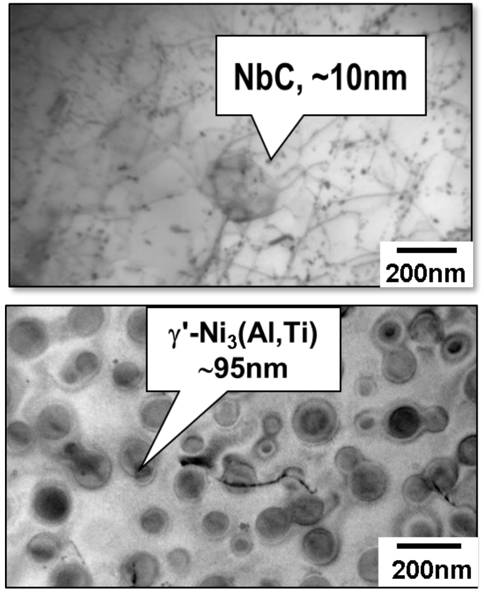
- Oxidation resistance: protective alumina-scale formation (>chromia-scale when water vapor exists)
- Creep performance: austenitic single-phase matrix + precipitation strengthening
- Inexpensive material cost: Fe-base (compared to Ni-base alloys)

Example: 5000 h at 800°C in Air + 10% H_2O



Brady et al, Oxidation of Metals, 2014: joint paper with Cummins

Example: Microstructure after creep-rupture testing at 750°C



Fe-(20-30)Ni-(12-15)Cr-(2.5-4)Al-(1-3)Nb base, wt.%
- Laves (GB) and carbide (GI) strengthening
- High Ni + Nb with rare earth additions will raise the upper temperature limit for oxidation resistance

Fe-(30-35)Ni-(14-19)Cr-(2.5-3.5)Al-3Nb base, wt.%
- $L1_2$-Ni_3(Al,Ti) strengthening
- Target higher strength at elevated temperatures

Brady et al. JOM, 60 (2009) 12-18
Yamamoto et al. Scripta Mat. 69 (2013) 816-819

Downselection of Model AFA Alloys Through Computational Guidance

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- Selected total 7 model AFA alloys:
  - Two different strengthening mechanism alloys
  - Used thermodynamic calculation (ThermoCalc w/TCFE9 and JMatPro v.9) for phase prediction
- Subjected property evaluation:
  - Oxidation tests
  - Creep-rupture tests
  - Microstructure characterization

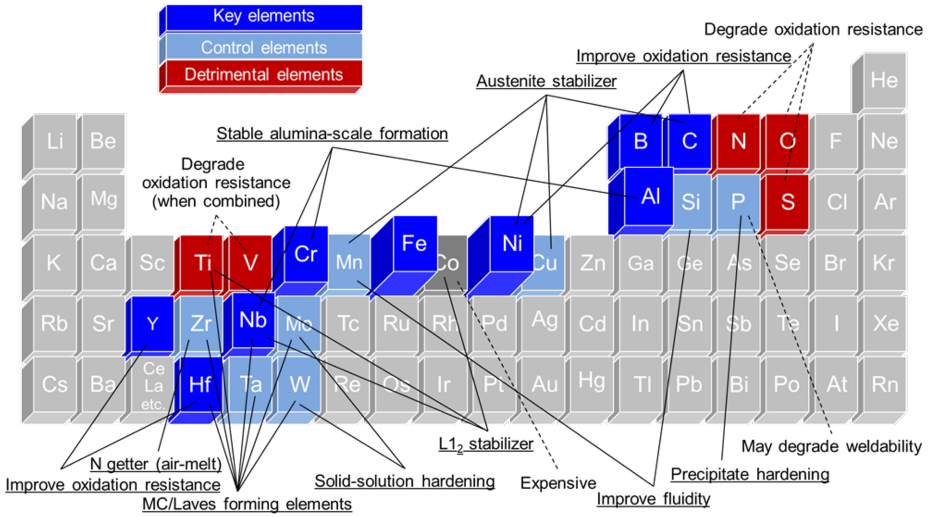
❑ "Laves + carbide" strengthened alloys

wt.%	Fe	Cr	Mn	Ni	Cu	Al	Si	Nb	V	Ti	Mo	W	Zr	C	B	Remarks
X201	56.14	14	2	20	0.5	3	0.15	0.8	0.05	0.05	1	2	0.1	0.2	0.01	20Ni
X221	53.14	15	2	22	0.5	3	0.15	0.9	0.05	0.05	1	2	0	0.2	0.01	22Ni
X251	51.14	14	2	25	0.5	3	0.15	0.8	0.05	0.05	1	2	0.1	0.2	0.01	25Ni

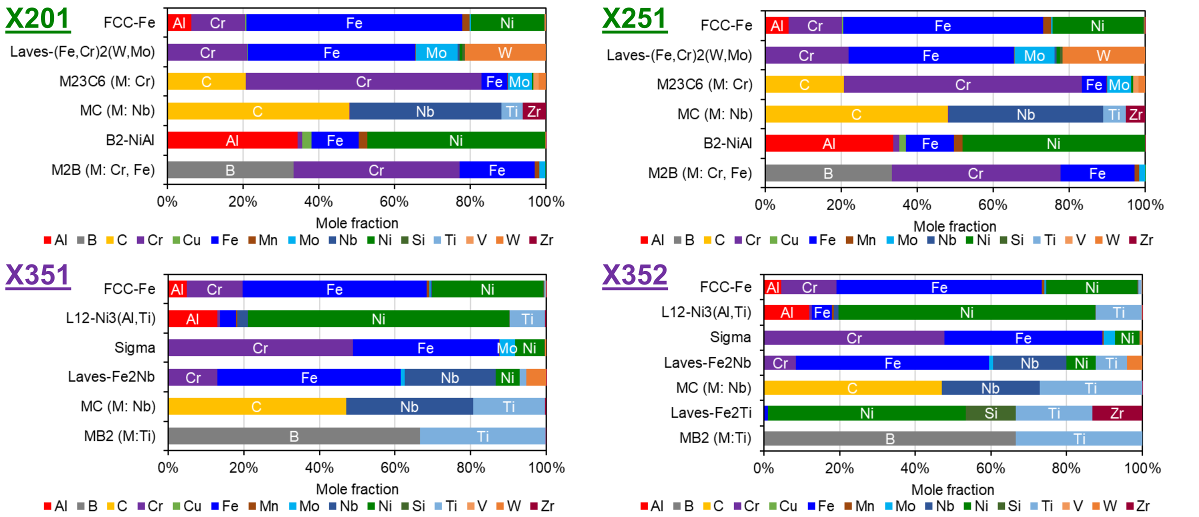
❑ "$L1_2$" strengthened alloys

wt.%	Fe	Cr	Mn	Ni	Cu	Al	Si	Nb	V	Ti	Mo	W	Zr	C	B	Remarks
X351	41.41	14	0.5	35	0	3	0.15	2.5	0.05	2	1	0.5	0.1	0.08	0.01	35Ni
X352	40.11	14	0.5	35	0	3	0.15	1.5	0.05	4	1	0.5	0.1	0.08	0.01	35Ni
X353	39.64	15	0.5	35	0	3	0.15	3	0.05	2	1	0.5	0.1	0.05	0.01	35Ni
X354	40.64	15	0.5	35	0	3	0.15	3	0.05	1	1	0.5	0.1	0.05	0.01	35Ni

Role of elements on AFA alloy development



Predicted phase composition of model AFA alloys (at 750°C, by ThermoCalc)



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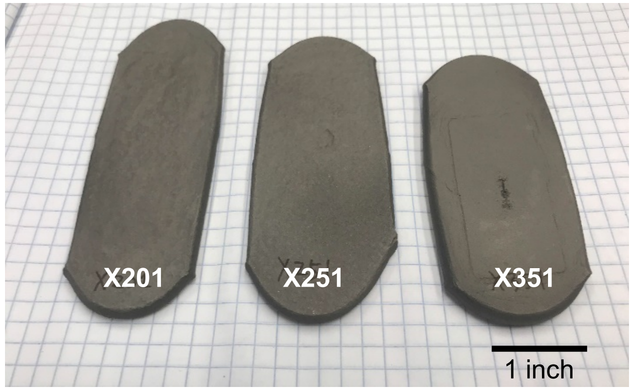
Lab-scale Heat Production and As-processed Microstructure Characterization

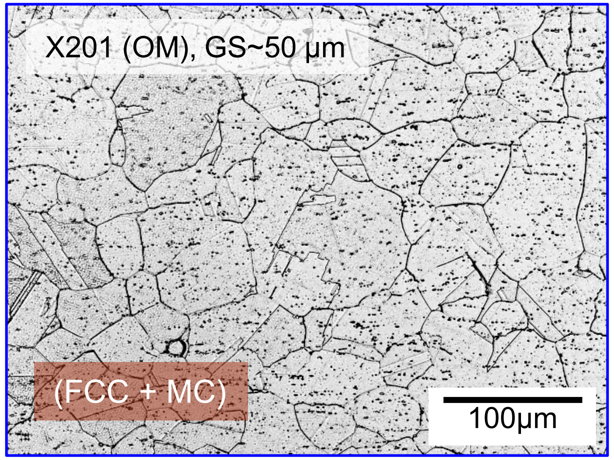
- Prepared lab-scale heats (~700g for each) at ORNL:
  - Arc-melted ingots (25 x 25 x 150 mm)
  - Homogenized, forged, rolled, and annealed at 1200/1150°C
  - X352 showed poor deformability (lots of cracks) ➔ due to partial melt (= lower melting point than the prediction)

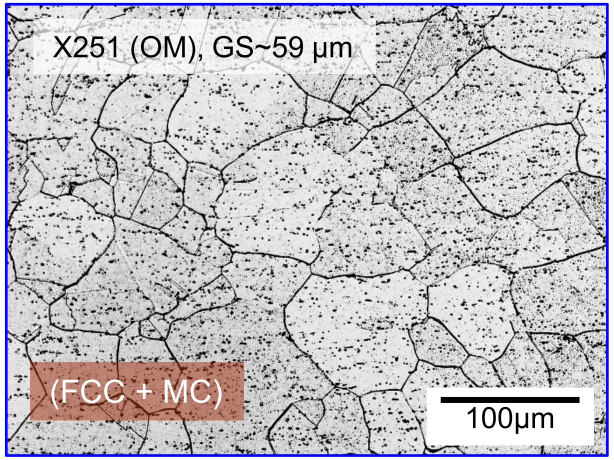
Processed successfully



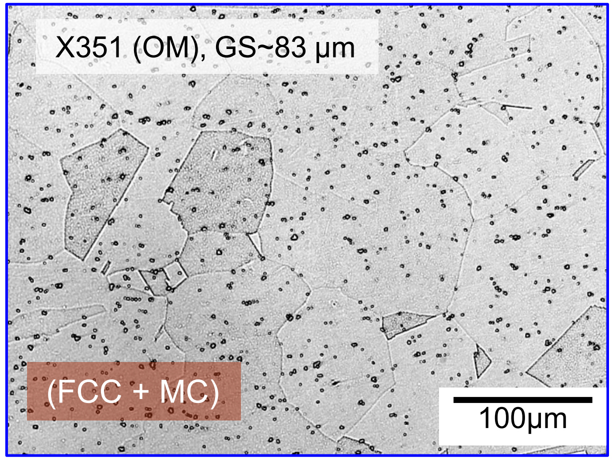
Process failed

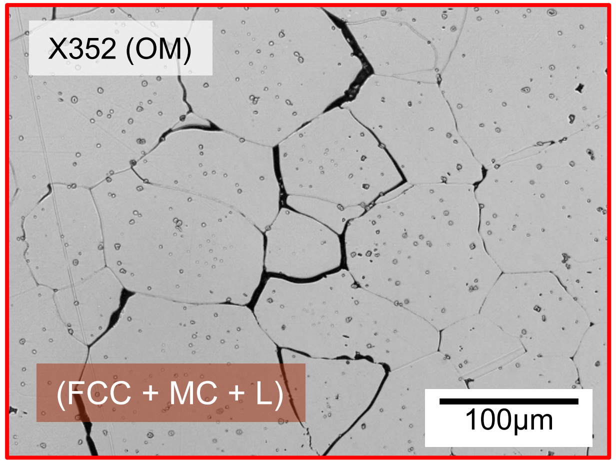
TMT + Annealed at 1200°C





TMT + Annealed at 1150°C





(↑ melted at 1150°C; a gap from the prediction)

Oxidation Tests at 750°C Revealed Borderline Alumina Formation in Fe-35Ni γ′ Alloys

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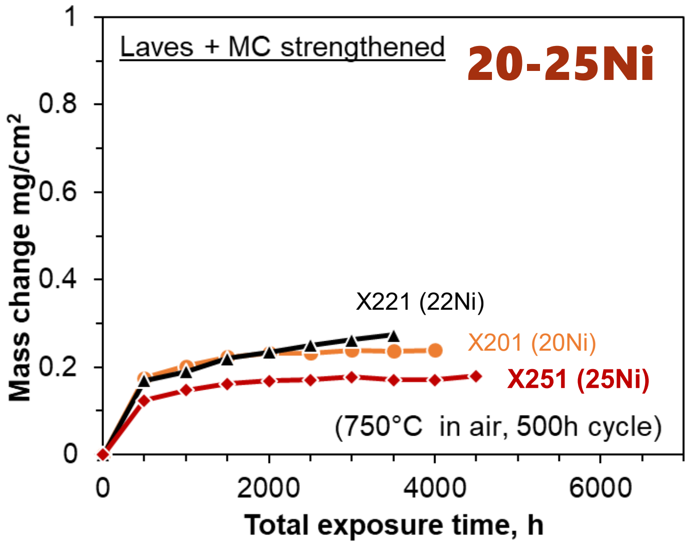
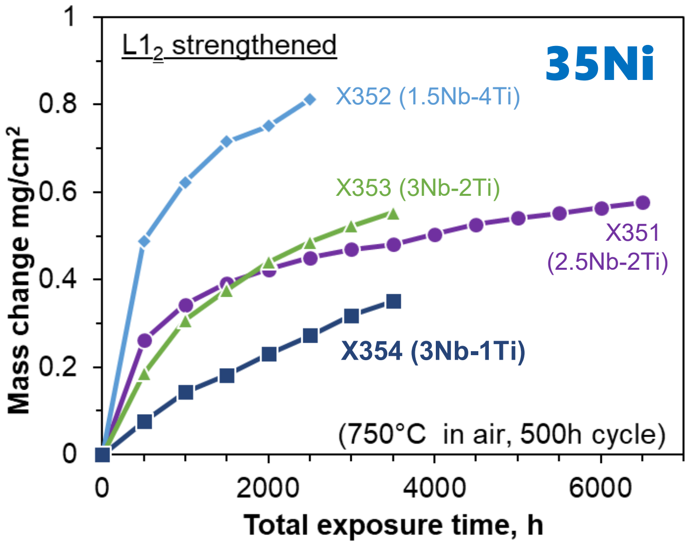
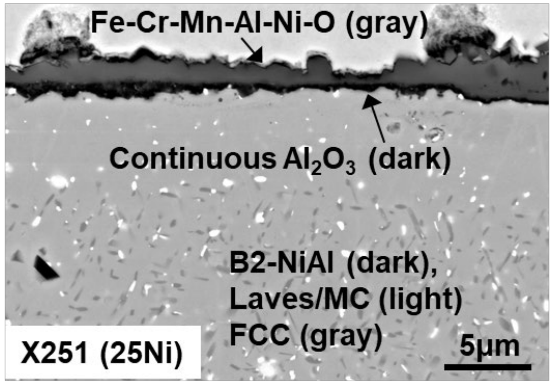
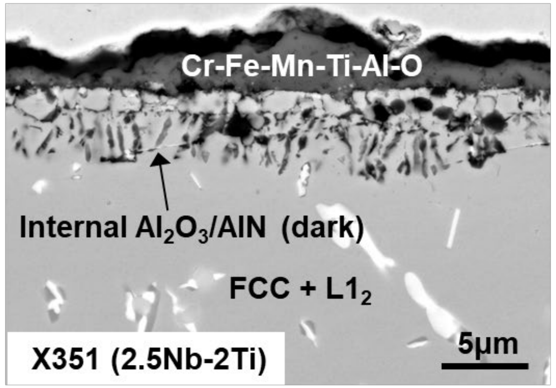
Mass changes at 750°C exposure

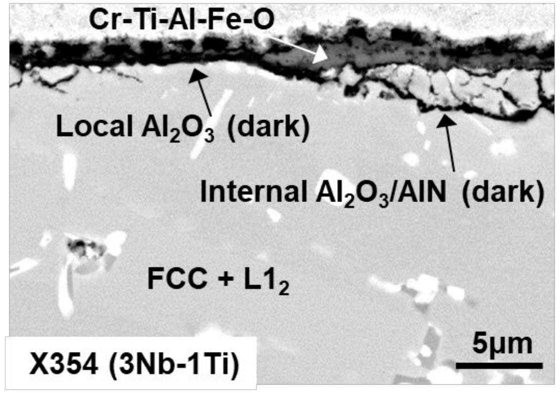




Cross-sectional SEM-BSE images







All alloys showed promising oxidation resistance through protective alumina scale formation

X354 exhibited lowest mass gain among the series of 35Ni alloys due to lower Ti content

Promising Creep-Rupture Performance in X251/X351 Comparable to Benchmarks

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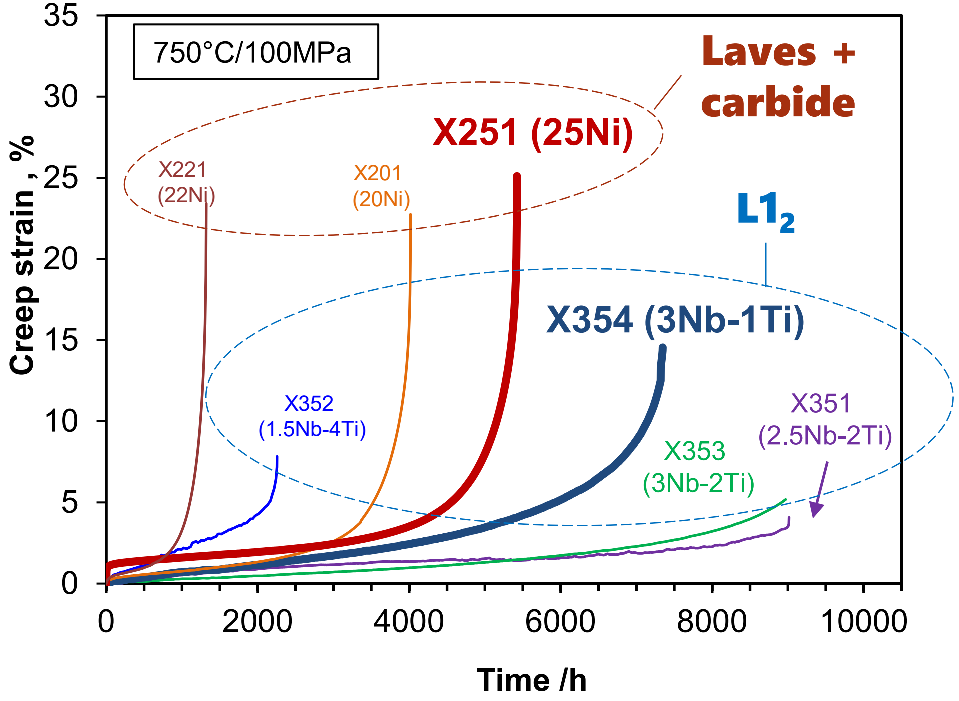
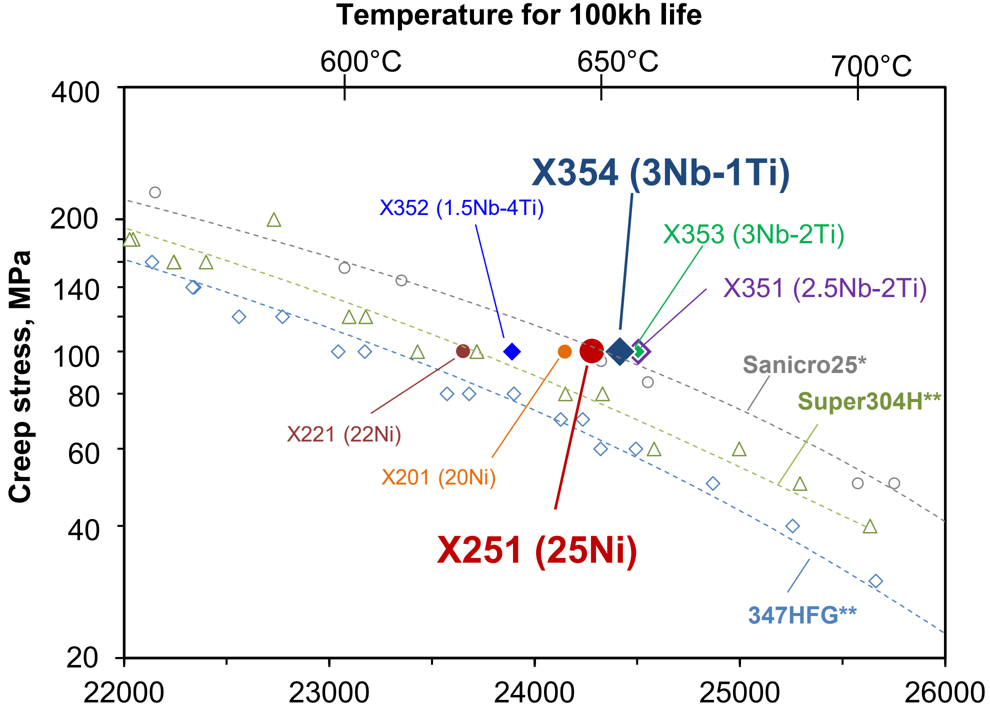
Creep-Rupture Curves



Larson-Miller Parameter Plot



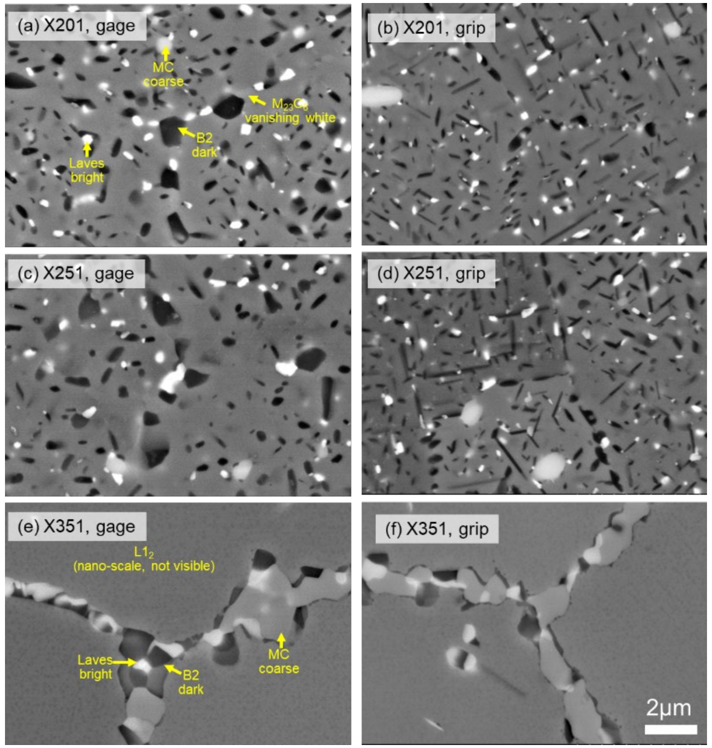
* from datasheet at Sandvik
** from NIMS Creep Datasheet

Model Laves + Carbide X251 and L1$_2$ X354 already achieved comparable creep to state-of-art Cr_2O_3-forming Sanicro 25 but with oxidation advantages of alumina
(Note: These AFA alloys also showed ~2x better creep-rupture performance than 1st generation AFA)

Detailed Characterization Conducted for Life-prediction Modeling and Gap Analysis

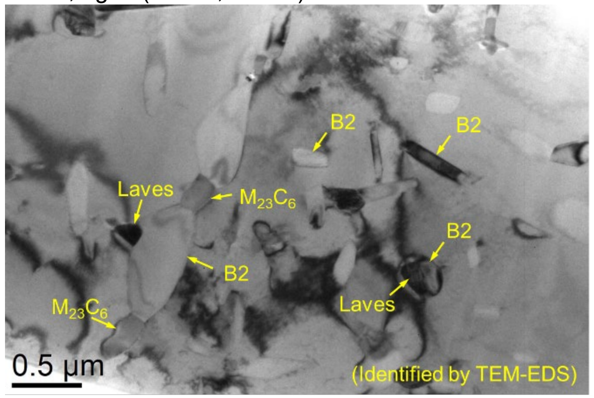
- Applied multi-scale characterization (SEM, TEM, APT):
  - Second-phase precipitate types, size, distribution, and chemistry
  - To be used for life-prediction / gap analysis

SEM-BSE: Creep-ruptured specimens

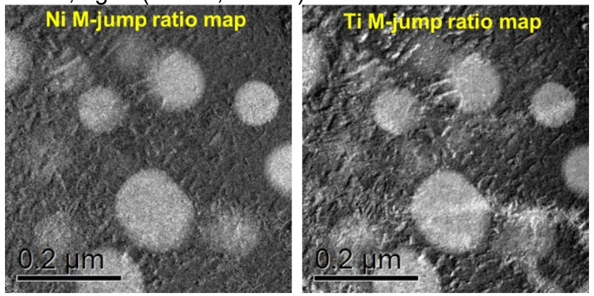


TEM-BF/EFTEM: Aged specimens

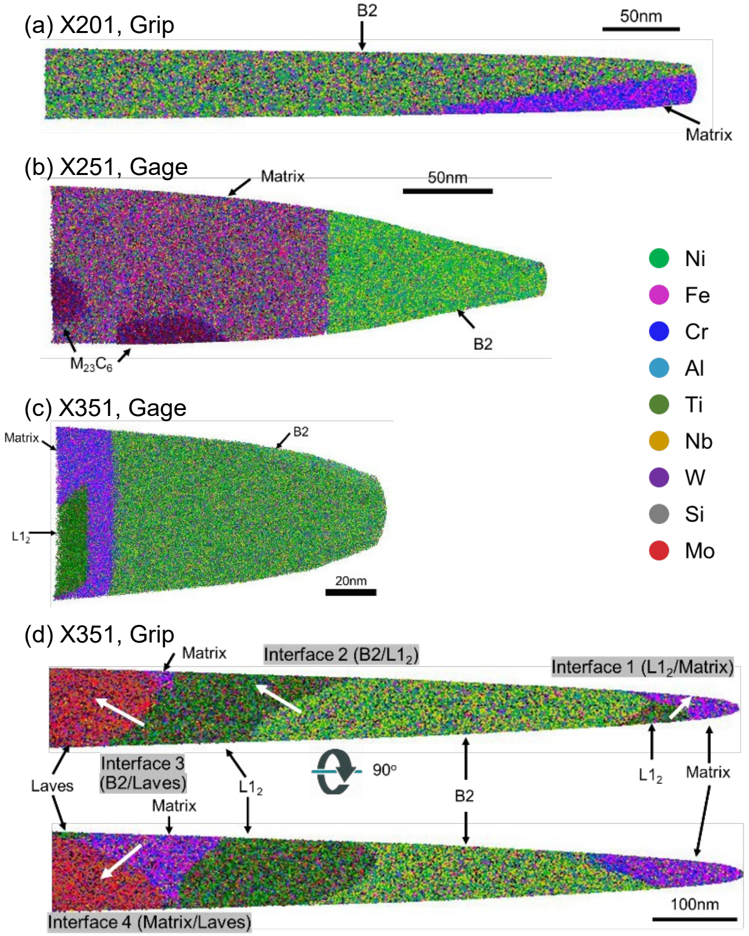
X201, aged (750°C, 1500h)



X351, aged (750°C, 1500h)



APT: Creep-ruptured specimens



Summary and Future Direction

- Computational thermodynamic tools guided downselection of model AFA alloys to be evaluated
  - Phase equilibrium
  - Oxidation/Creep performance
  - Microstructure
- Two AFA alloys (X251/X354) demonstrated balanced properties of oxidation resistance and creep-rupture performance
  - **Already 2x better creep performance than 1st generation AFA**
  - Further evaluation is currently in progress
- Development of new tools to provide insights into initial establishment of continuous alumina scales (one key aspect for long-term oxidation resistance)
  - Phase-field modeling supported by experimental O permeation measurements and simulations of O transport in Fe/Ni/ ± Cr or Al (not presented)

Thanks

Phase Field Modeling: Internal to External Oxidation Transition for Continuous Alumina

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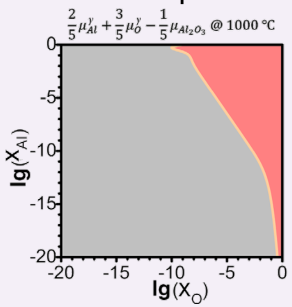
Input

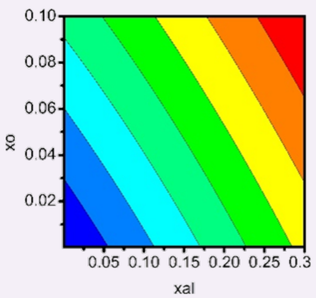
E.g. oxidation in Ni-Al

- Thermodynamic and kinetic databases

Chemical potentials

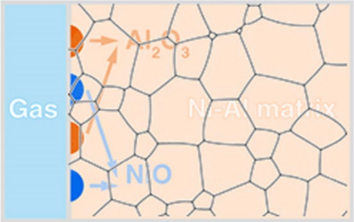


Interdiffusivity



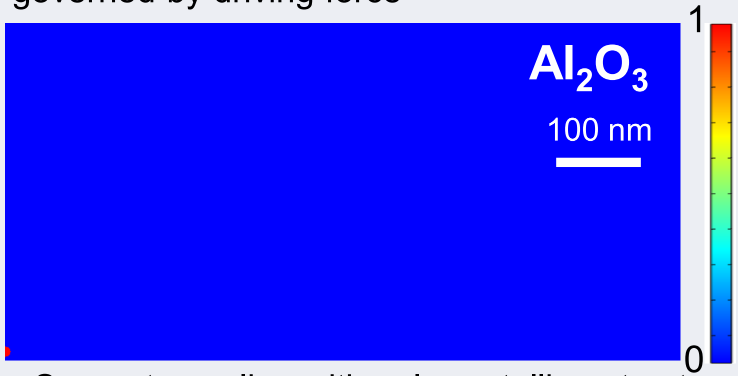
- Parameters: T, composition, p_{O2}, γ, …

- User defined initial microstructure & oxide nuclei morphology

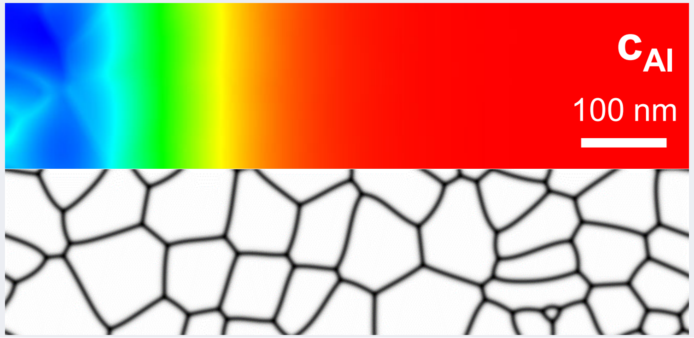


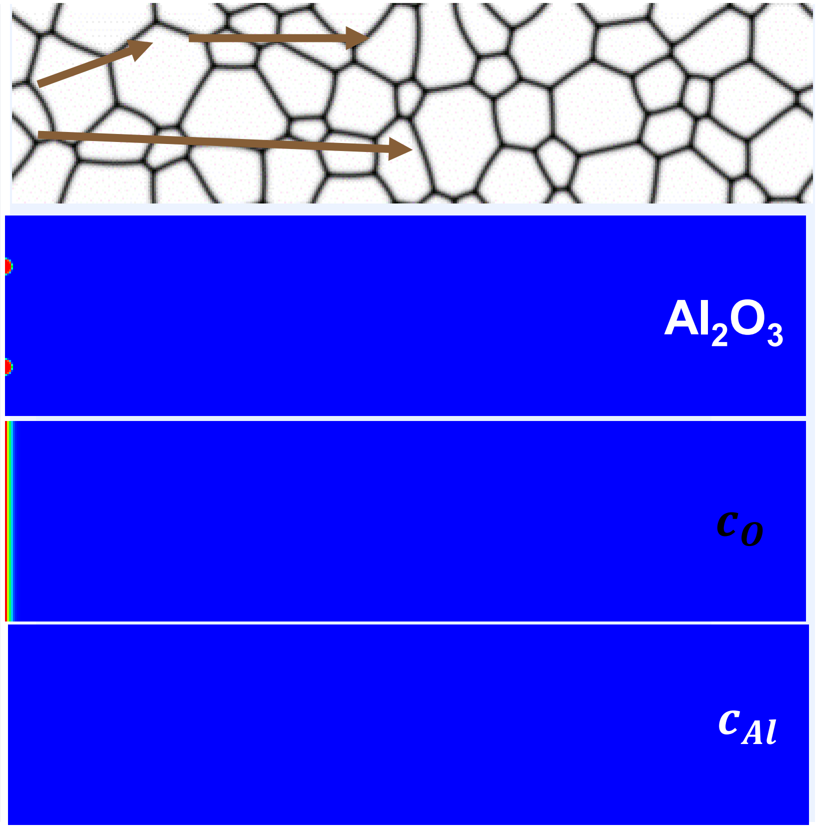
Output

- Support concurrent nucleation and growth governed by driving force



- Support coupling with polycrystalline structure





Shown for Ni-Al based on existing data, working to expansion to FCC Fe(Ni)-Al

Courtesy: Youhai Wen (NETL)

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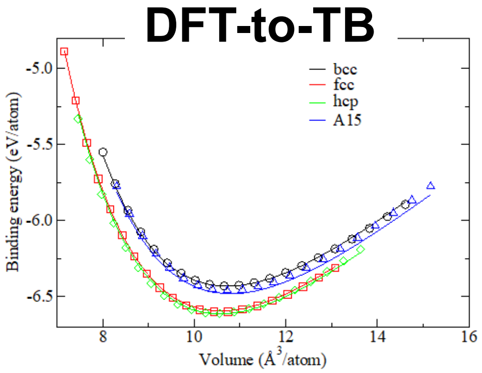
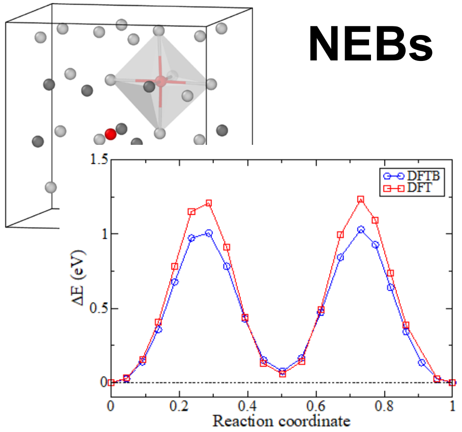
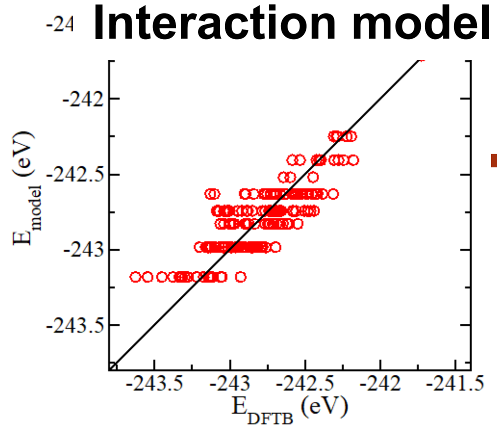
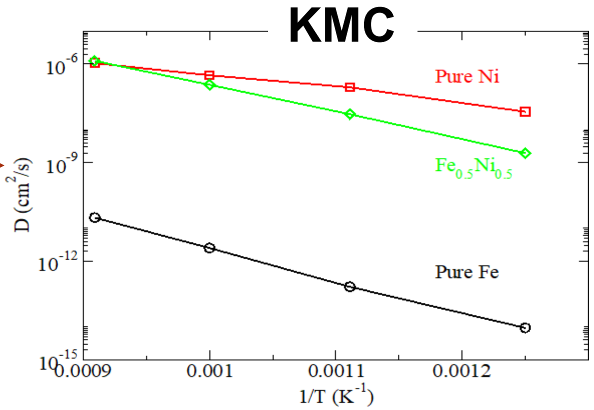
Simulating O transport in Fe/Ni ± Cr or Al









- O diffusivity in fcc Fe/Ni/Cr alloys as a function of composition has been computed using a new multi-scale framework
  - DFT data is used to parameterize a fast TB model for Fe-Cr-Ni-O bonding
  - Nudged elastic band calculations using our TB model give barriers to O diffusion
  - An interaction model gives an analytic model for barriers as a function of local chemistry
  - KMC simulations using interaction model give O transport rates
- Fe/Ni alloys have been used to develop our computational methods – other binaries come next followed by ternary Fe/Cr/Ni ; Fe/Ni/Al alloys

Courtesy: Marc Cawkwell/Romain Perriot (LANL)

Oxygen Permeation Study in Model Lean AFA FCC Austenitic Matrix Phase Alloys ~800-1000°C

- Coarse Poly- and Single- Crystal Alloys Grown at Ames Lab to Minimize Alloy Grain Boundary Transport Effects During Oxidation Exposures

Ni ± Cr effects ➔ impacts oxidation and alloy cost; Nb, Ti, V effects ➔ impacts oxidation and strengthening

Variables	Composition, wt.%								Remarks
	Fe	Cr	Al	C	**Ni**	**Nb**	**Ti**	**V**	
Ni in FeNiAl	Bal.		2.3		**15**				
	Bal.		2.3		**20**				
	Bal.		2.3		**25**				
Ni in FeNiAlCrC	Bal.	14	2.3	0.1	**15**				
	Bal.	14	2.3	0.1	**20**				
	Bal.	14	2.3	0.1	**25**				
20Ni + Nb, Ti+V	Bal.	14	2.3	0.1	20	**1.5**			0.88 at.% Nb
	Bal.	14	2.3	0.1	20		**0.5**	**0.3**	0.88 at.% Ti+V

- Findings feed into phase field modeling of internal/external oxidation and establishment of continuous Al_2O_3
- Findings complement simulation efforts for diffusivity of oxygen in FCC Fe(Ni,Cr) and Fe(Ni,Al)