OAK RIDGE National Laboratory

Project ID#194

Accelerated Design of Alumina-Forming, High-temperature Austenitic Alloys*

*Subtask 2B1 under the Powertrain Materials Core Program (PMCP)

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June 4th, 2020

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Overview: New exploratory effort from *subtask 2B1 in Powertrain Materials Core Program (PMCP)

Timeline

- Effort start: Mar 2020
- Effort end: Sept 2020 (may be extended depending on results)
- Percent complete: 20% (1month)

Barriers

- Changing internal combustion engine regimes requiring higher-temperature capable materials
- Development time/cost of new materials

Budget

- Total effort funding: $75k in FY20

Collaboration

- Thermo-Calc Software
- Internal ORNL Collaboration Among Computational Science and Materials Science Organizations

* Exploratory effort to demonstrate a novel machine learning alloy design approach in support of Subtask 2B1 Development of Cast, Higher Temperature Austenitic Alloys.

Increased temperatures and pressures to enable cleaner, more efficient engines with alumina-forming austenitic (AFA) alloys

- Current exhaust component alloys: lose oxidation resistance and strength ≥ ~800°C
- Ni-base alloys: meet these targets but are too costly (≥ 3 - 10x Fe-base)

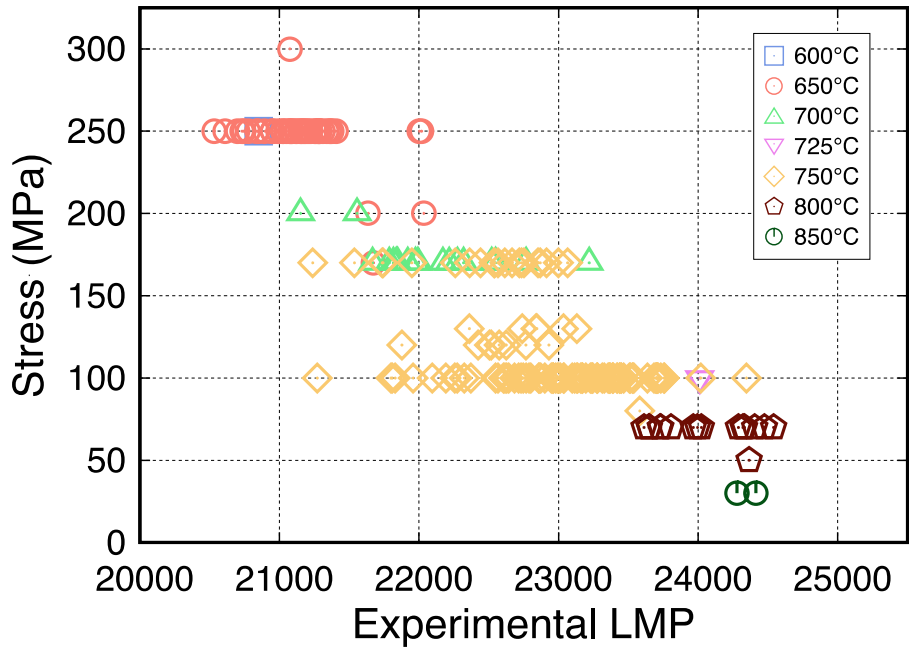
2B1 Objective: Develop low-cost "Fe-base alloys" for ">900-950°C"

- Improved oxidation resistance by forming protective Al_2O_3 scale formation (→ AFA) instead of Cr_2O_3
- Increased strength & creep by nano-precipitates

Objective: Demonstrate machine learning accelerated design of AFA-type alloys

- Leverage 10 years of creep data over multiple wrought AFA alloys previously developed at ORNL
- Couple high-throughput computational thermodynamics with machine learning in the AFA dataset to train for **prediction of creep resistance**
- Predict creep resistance of millions of systematically generated hypothetical AFA alloys

ORNL AFA alloys creep data



$LMP^*=(T(°C)+273)x(20+\log t_{rupture}[h])$

*Larson-Miller Parameter: time-temperature correlative approach based on the Arrhenius rate equation for creep rupture life prediction at a given stress

Rapidly exploring high-dimensional multi-component alloy space with high-throughput data analytics approaches

Composition ranges from ORNL AFA experts

→ **Design of Experiments (DOE)**

2,000,000 hypothetical AFA alloy compositions

→ input

High-throughput Computational Thermodynamics

Thermo-Calc Software

input

CADES

800-1,200 calculations/min. with ~1,000 cores

wt.%	Max	Min	wt.%	Max	Min
Fe	Bal	Bal	V	0.3	0
Cr	25	12	Ti	1	0
Mn	7	0	Mo	2	0
Ni	40	15	W	2	0
Cu	3	0	Zr	0.2	0
Al	6	2.5	C	0.2	0
Si	1	0	B	0.02	0
Nb	3.5	0.3			

15 elements, 5 variants
~ 5^{15}=30,517,578,125(!)

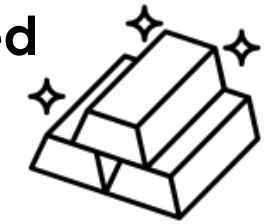
Impossible to search all these

Pre-trained Machine Learning (ML) Model

Processing Conditions + Degree of Supersaturation*

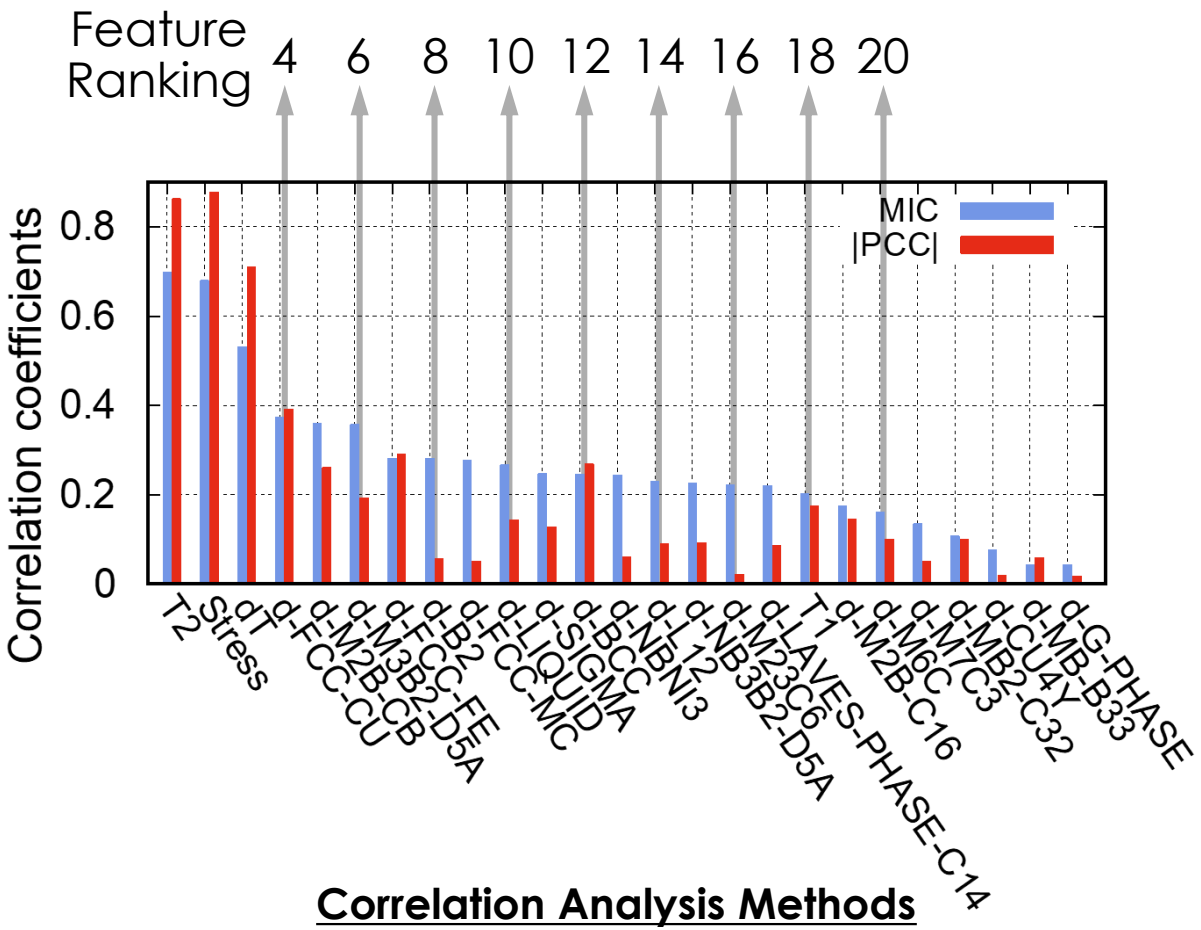
↓

Virtually validated new "recipes"



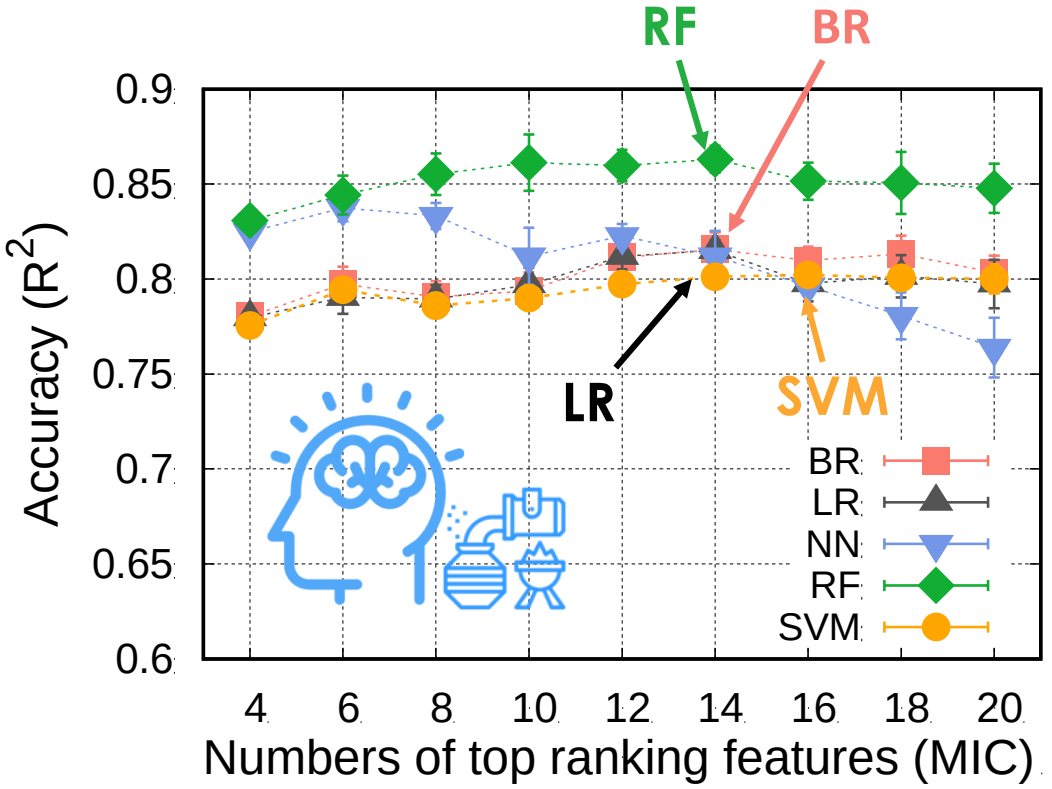
*D. Shin, et al., Acta Mater. 168 (2019) 321-330

Highly relevant features from computational thermodynamics have been used to train ML models



Correlation Analysis Methods

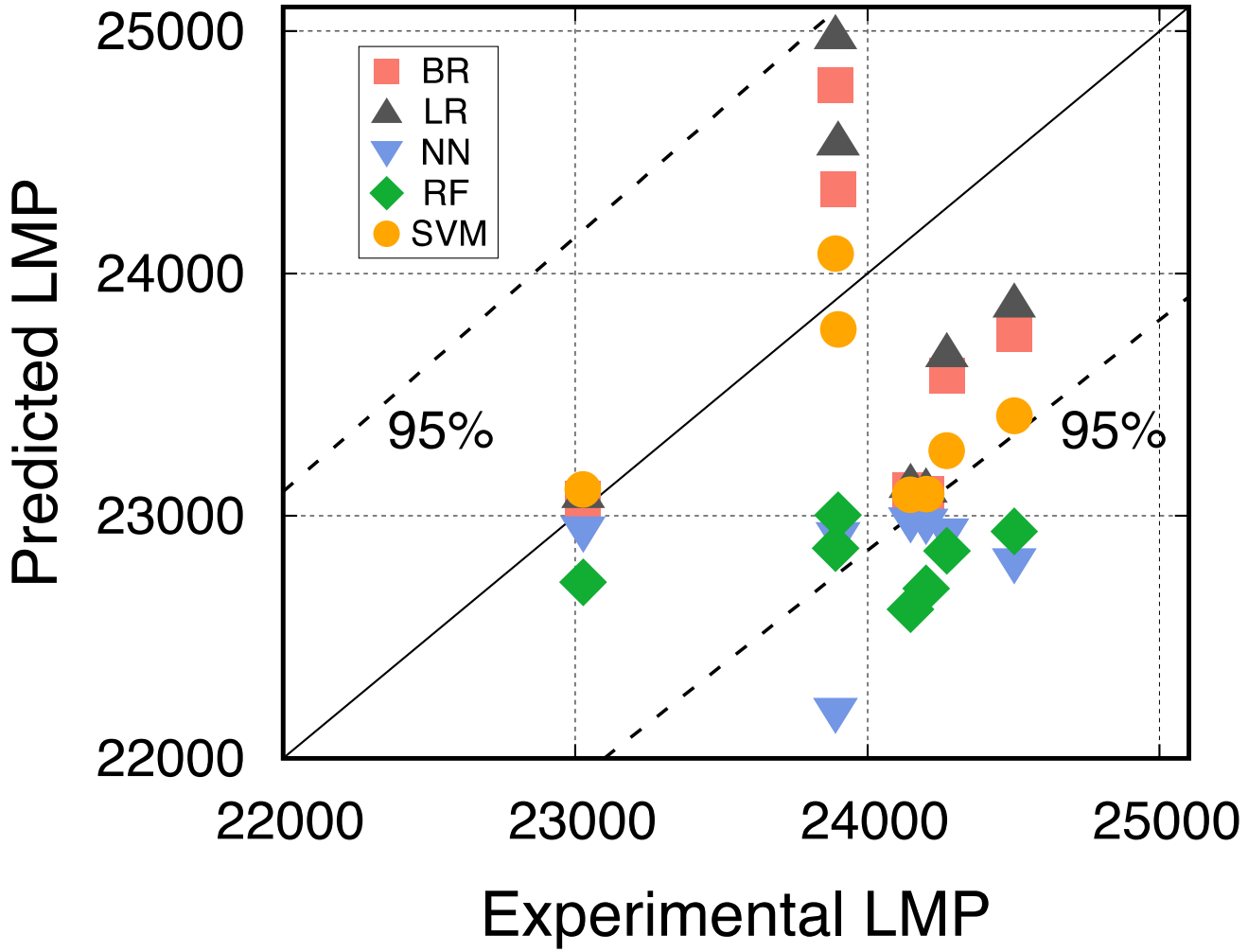
|PCC|: The absolute value of Pearson's Correlation Coefficient
MIC: Maximal Information Coefficient



Machine Learning (ML) Models

LR: linear regression, **BR**: Bayesian ridge, **NN**: *k*-nearest neighbor, **RF**: random forest and **SVM**: support vector machines regression

Linear regression-based models (BR and LR)outperform other ML models in predicting LMPs of new* AFA alloys

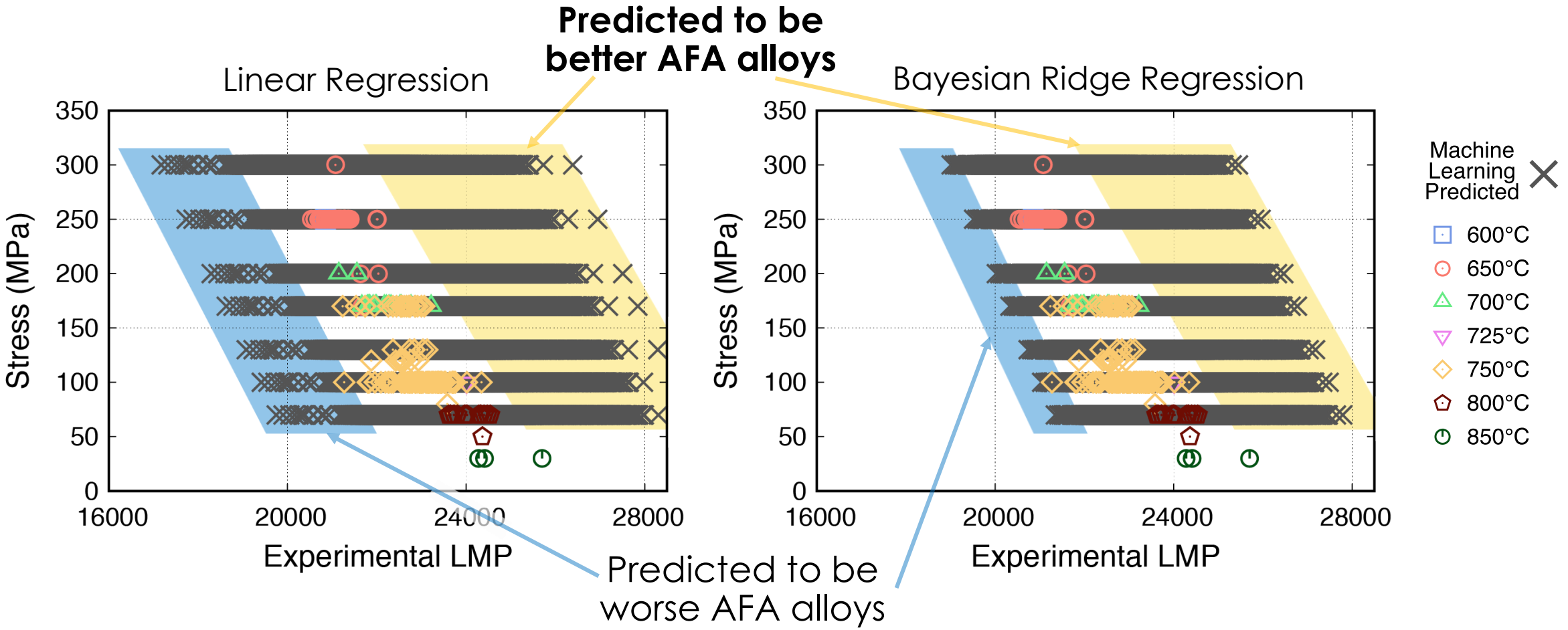


* Alloys that are not in the training dataset

- The accuracy of trained models for non-linear regression based MLs are better than BR and LR.
- It is possible that non-linear ML models have been over fitted.

LR and BR models to predict LMPs of 2M hypothetical AFA alloys

ML trained with key microstructure features identified a range of hypothetical AFA alloys with better & worse LMPs



Small subset of predicted hypothetical alloys will be experimentally validated to evaluate effectiveness of alloy design via ML methods

Collaboration and Coordination with Other Institutions

- **Thermo-Calc Software:** high throughput computational thermodynamic calculations of millions of hypothetical AFA alloys
- **ORNL CADES** (**C**ompute **A**nd **D**ata **E**nvironment for **S**cience)
  - AWS-like cloud computing
- **ORNL Computational Sciences Division:** for Data Analytics Expertise
- ORNL Materials Science for computational thermodynamics and alloy design, alloy manufacture, and creep evaluation expertise

Proposed Future Research

- Experimental validation of alloys with predicted good LMPs
  - Manufacture 0.5 kg lab heats of select predicted alloys and creep test under an accelerated test conditions of 750°C and 130 MPa.
  - Success is defined by extent to which the predicted alloys exceeds creep resistance of best previously developed AFA alloys to date

- Uncertainty quantification to assign error bars of ML predicted LMPs by considering different number of features for a given ML model

Any proposed future work is subject to change based on funding levels.

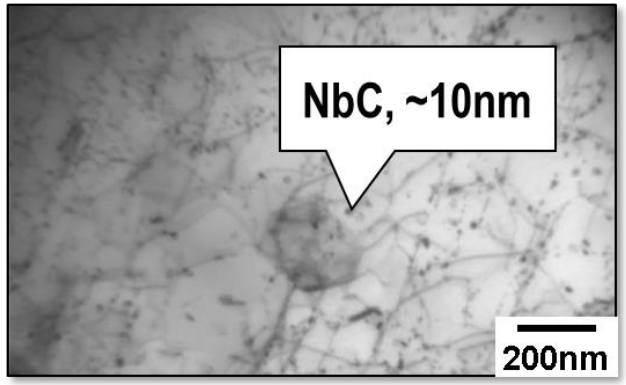
Summary

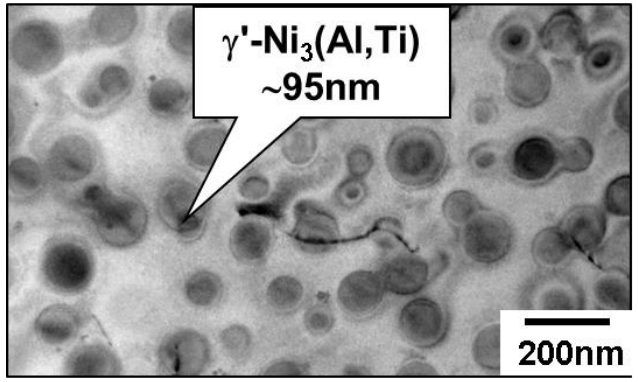
- New high-fidelity machine learning models have been trained with ORNL AFA creep data and key microstructure features.
- Creep properties (i.e., LMP) of 2 million hypothetical AFA alloys have been predicted.
- Small subset of identified AFA alloys with improved creep will be experimentally validated.

Technical Back-Up Slides

Alumina-Forming Austenitic (AFA) Alloy Family: a Lower Cost, Fe-Base Alloys with Improved Oxidation Resistance + Strength

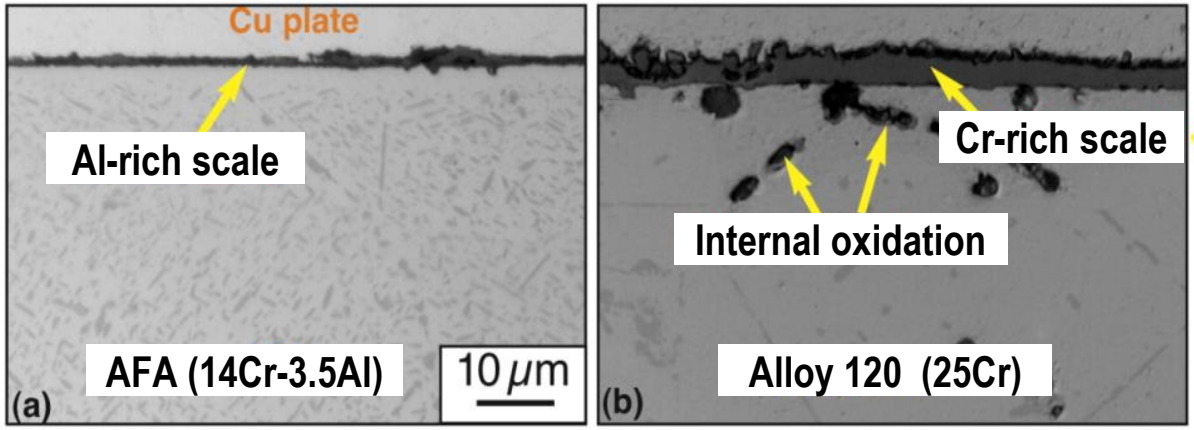
- **Wide composition range (wt.%) :**
  Fe-(10-25)Cr-(2-5)Al-(12-35)Ni-(0.6-3)Nb-(0.05-0.5)C+(B, Hf, Mn, Mo, Si, Ta, Ti, V, W, Y, Zr, …)
- **AFA Strengthening: nano-carbides ± intermetallics**
  while forming protective alumina





Design better AFA alloys by machine learning?

- **Good oxidation resistance**



800 °C, 10,000 h in air

Commercialization of 1st Generation AFA in progress

Yamamoto et al., Science 316 (80) (2007) 433, Brady et al., JOM 60 (2008) 12

Coupling physics into the machine learning predictions

Data Collection/Population

Composition

Creep (LMP)

input

ORNL Alumina-forming Austenitic (AFA) alloys ~ a decade work

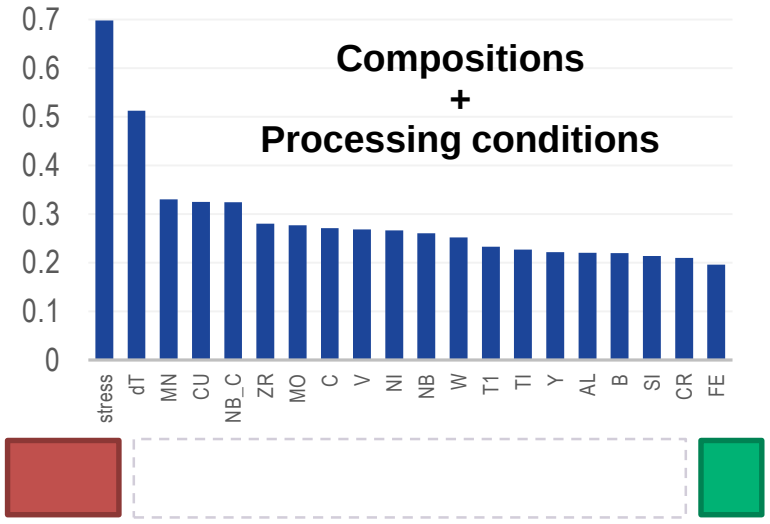
High-throughput data population

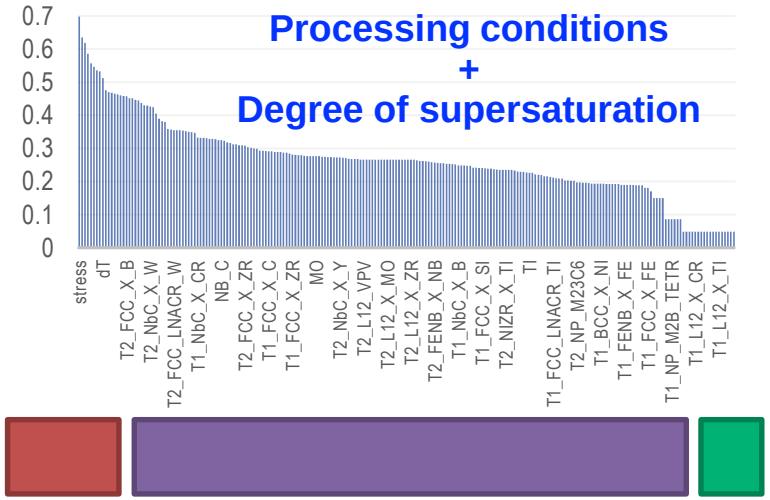
output

Microstructure related features
- Degree of supersaturation

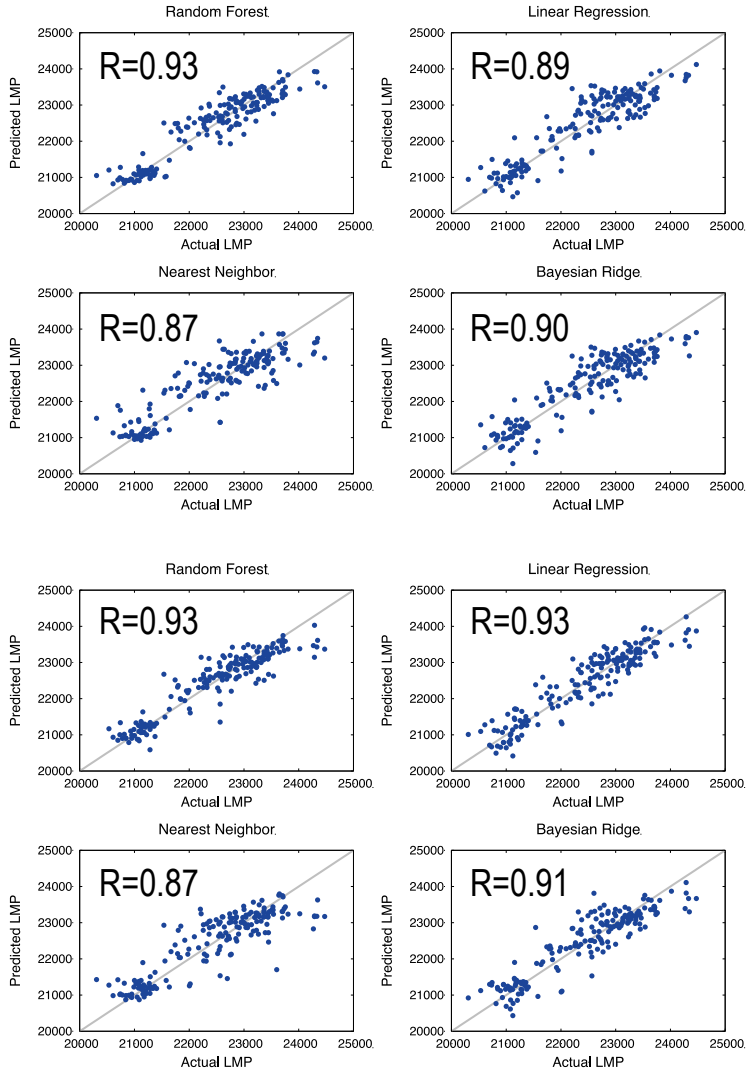
D. Shin, et al., Acta Mater. 168 (2019) 321-330

Correlation Analysis





Machine Learning



Augment experimental data with scientific features

Elements		Fe, Cr, Mn, Ni, Cu, Al, Si, Nb, V, Ti, Mo, W, Y, Zr, Hf, C, B
T1 (solutionizing, °C)		1100, 1150, 1200, 1250
T2 (creep test, °C)		650, 700, 750, 800
Stress (MPa)		70, 100, 130, 170, 200, 250, 300
Phases	FCC	Austenite (FCC matrix), NbC, L12
	BCC (B2, A2)	NiAl, FeCr
	C14 Laves	NiZr, FeNb
	others	M23C6, M7C3, M2B, M3B2, MB2_C32, Ni3Ta_D0A, Sigma

Experimental details

Phases determined by thermodynamic calculations

w{Elements}	Elemental composition in weight percent
T1, T2, dT	Solutionizing, creep test temperatures, dT=T1-T2
NB_C	Ratio between Nb and C
Creep stress	Stress
LMP ← **Target**	Larson–Miller parameter
{Temperature}_VPV_{Phases}	Volume fractions of phases at T1 and T2
{Temperature}_X_{Phases}_{Elements}	Concentrations of elements in phases at T1 and T2
d{Phases}	Degree of supersaturation (volume fraction difference between T1 and T2)

Composition only

Scientific features

Features in the dataset