Data-Driven Study of Shape Memory Behavior of Multi-component Ni-Ti Alloys

Shreyas J. Honrao, Othmane Benafan, John W. Lawson

Computational Materials Group

NASA Ames Research Center, Moffett Field, CA

shreyas.j.honrao@nasa.gov

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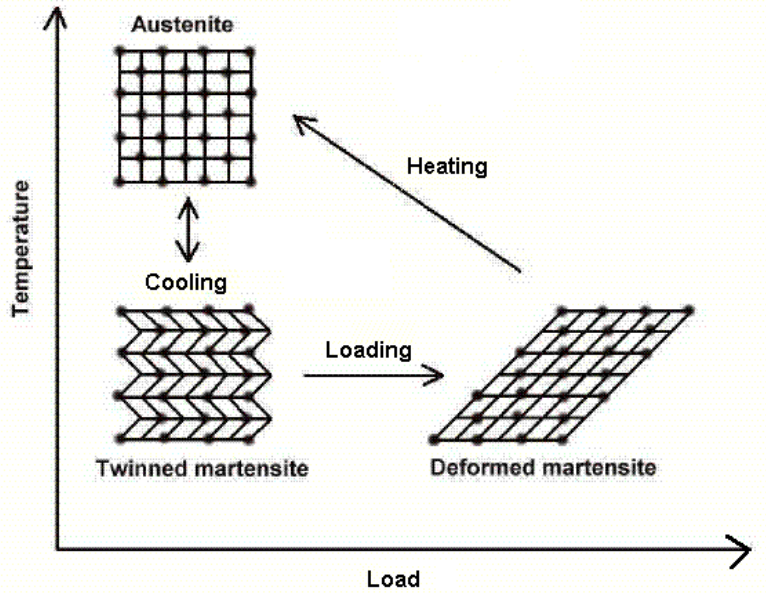
Shape Memory Alloys

NiTi based alloys

- favorable shape memory properties, mechanical strength, ductility, corrosion resistance, biocompatibility
- used as sensors, actuators, dampers
- excellent choice for aerospace, automotive, commercial, biomedical applications



Specific NASA applications

- Vortex generators
- Morphable aircraft wings

https://www.nasa.gov/feature/glenn/2019/memory-metals-are-shaping-the-evolution-of-aviation

Motivations for study

- High accuracy, rapid predictions of SMA properties enables full computational exploration of SMA design space and discovery of novel materials with targeted properties

- **Current approaches:** trial-and-error based, result in expensive and time-consuming synthesis-characterization loops with slow progress, difficult to extend past ternary compositions

- **Data-driven methods:** can offer rapid predictions but require extensive, high quality datasets, can model multiple parameters simultaneously at little additional cost

"Develop machine learning models for rapid prediction of SMA properties in multi-component NiTi alloys"

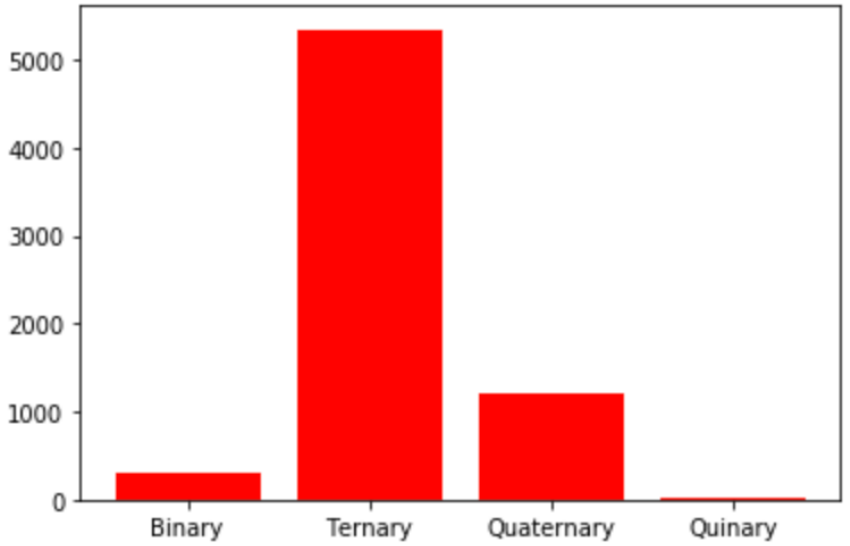
ML for materials: Unique challenges

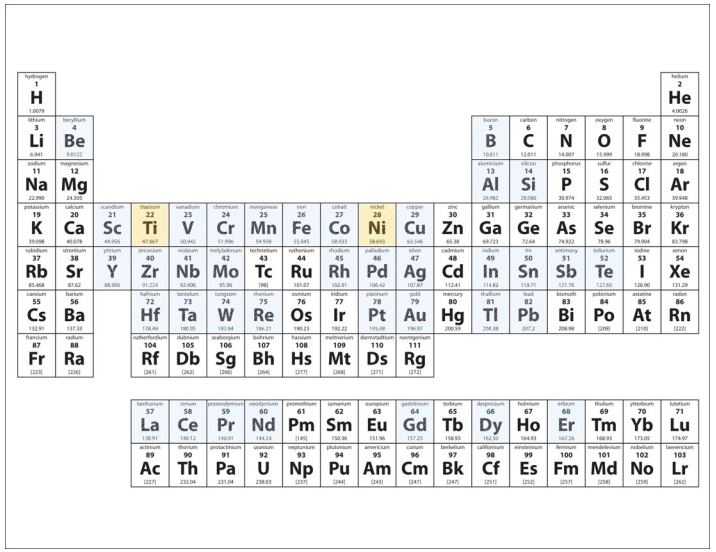
	Traditional MI Applications	Materials MI Applications
DATA TYPE	Often standardized	Rarely standardized
DATA VOLUME	Big, dense (up to ~10^8 examples)	Small, sparse (~10^2 examples)
ESTABLISHED DOMAIN KNOWLEDGE	Not applicable—rely on data to learn patterns	Must be physics-aware
DATA REPRESENTATION	Can often be optimized by algorithms	Requires deep domain knowledge
PREDICTION TASK	Accurately pattern-match common cases	Predict unusual or "extreme" materials
SAMPLE BIAS	Often present	Experiments correlated; negatives stigmatized
UNCERTAINTY IN DATA AND MODELS	Usually unimportant	Always important
INTERPRETABILITY	Usually unimportant	Often required by scientists & engineers

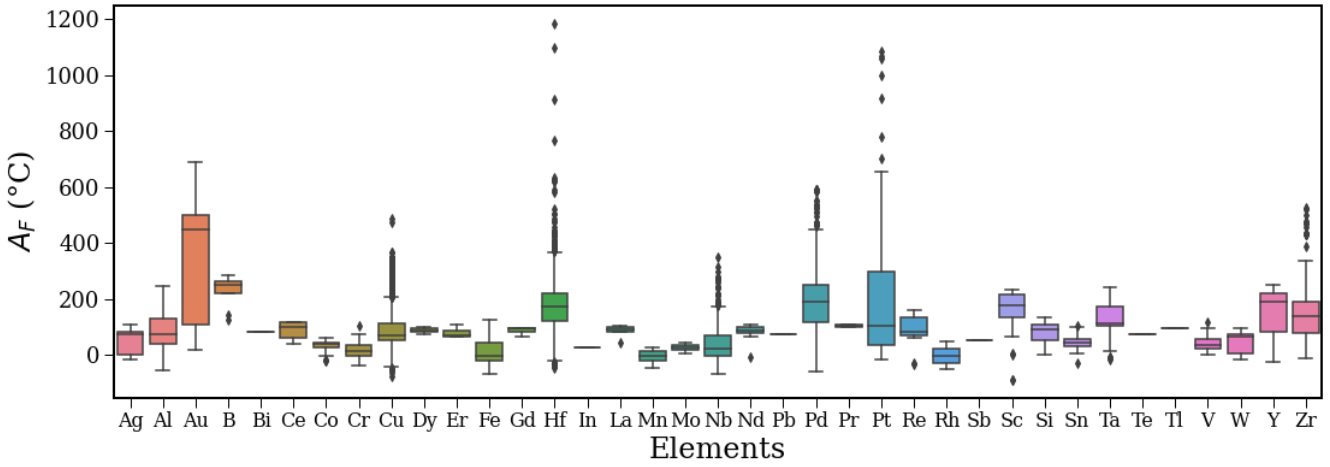
https://citrine.io/

Dataset

Compounds by number of elements:





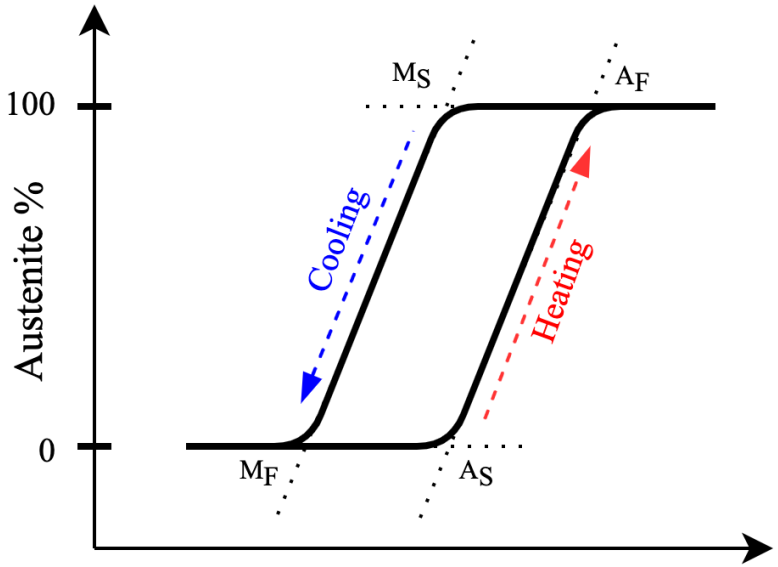


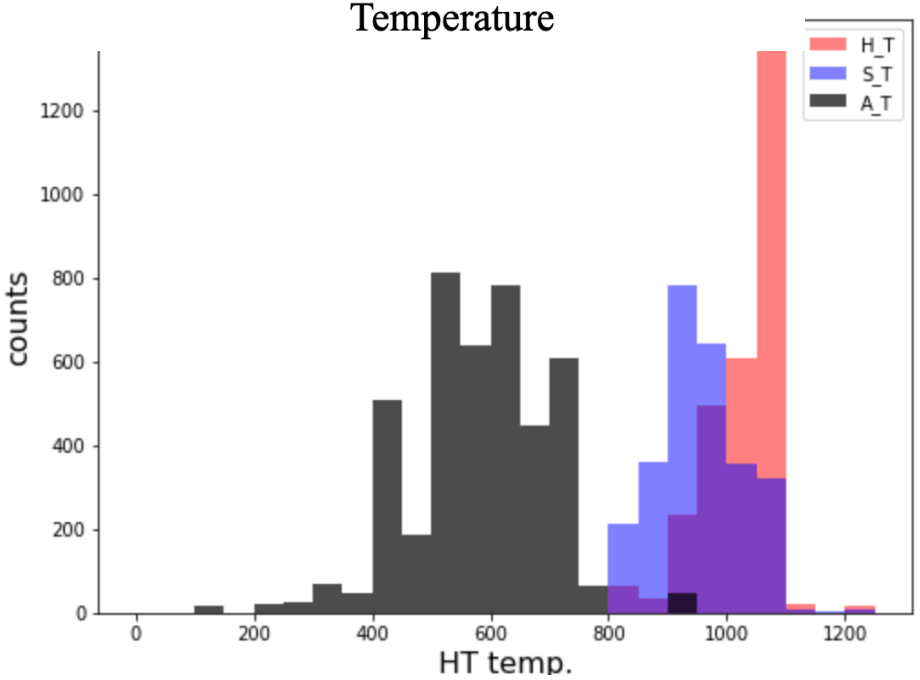
Properties

- Martensite transition temps: M_S, A_S, M_F, A_F
- Hysteresis: $A_F - M_S$
- Transformation strain

Feature representation

Compositions	Processing Conditions	Test Parameters
Ni atomic %	Preparation Technique [**x 6**]	Applied Stress (MPa)
Ti atomic %	Homogenization Temp. (°C)	
Alloy elem. atomic % [**x 37**]	Homogenization Time (hrs)	
	Solutionizing Temp. (°C)	
	Solutionizing Time (hrs)	
	Aging Temp. (°C)	
	Aging Time (hrs)	





Additional data available, but not used

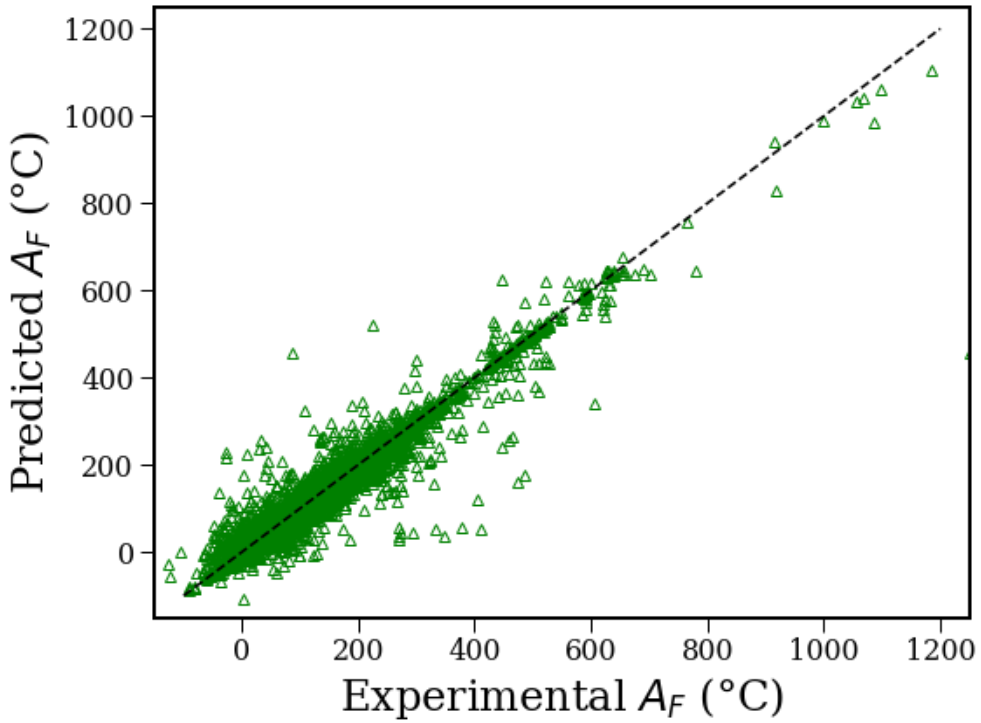
- Cycle number
- Heating, cooling rate
- Cycling Temperature Range (upper, lower temp)

Machine Learning results

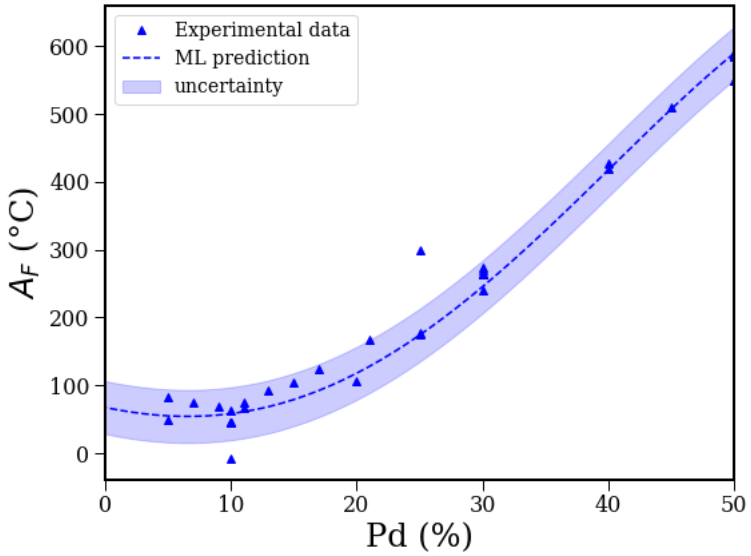
Algorithms: Ensemble learning (Random Forest, EXTremely RAndom Trees, XGBoost)

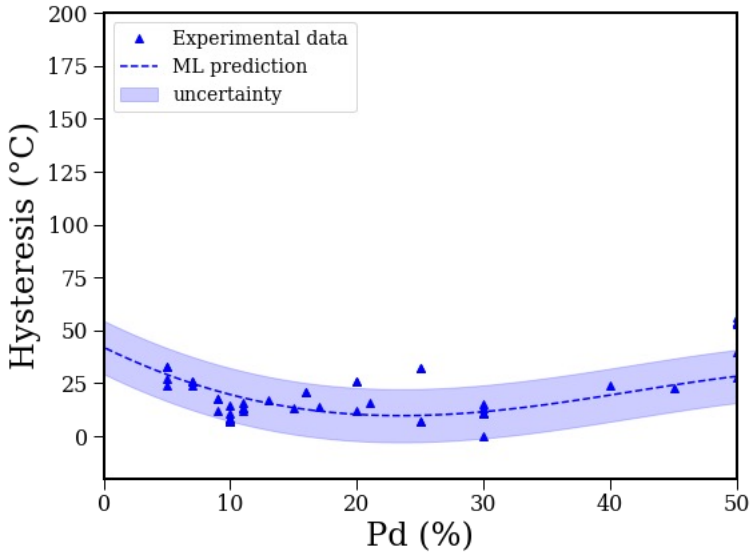
Property	**Training Set**	**MAE**	**R^2**
Martensite Start Temperature (M_S)	7305	13.6 °C	0.95
Martensite Finish Temperature (M_F)	5390	15.9 °C	0.92
Austenite Start Temperature (A_S)	6032	15.6 °C	0.94
Austenite Finish Temperature (A_F)	6513	14.8 °C	0.94
Hysteresis ($A_F - M_S$) [a]	5961	7.2 °C	0.65
Transformation strain	2350	0.36 %	0.81

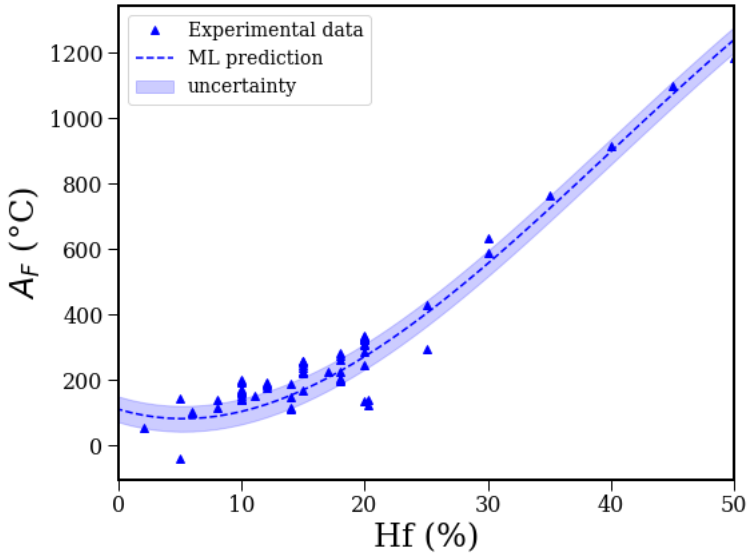
[a] MAE for the hysteresis model is computed using the predictions from the A_F and M_S models.

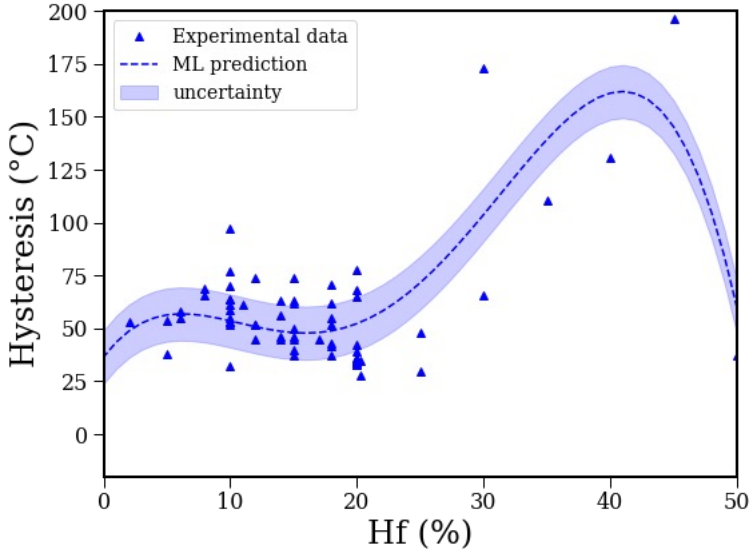


Effects of ternary additions (Pd, Hf)

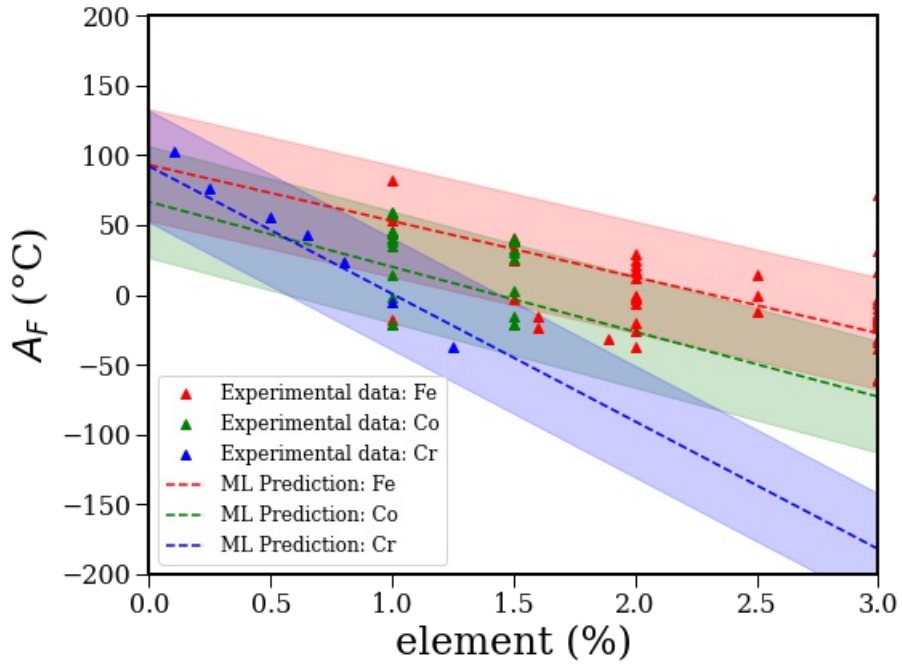


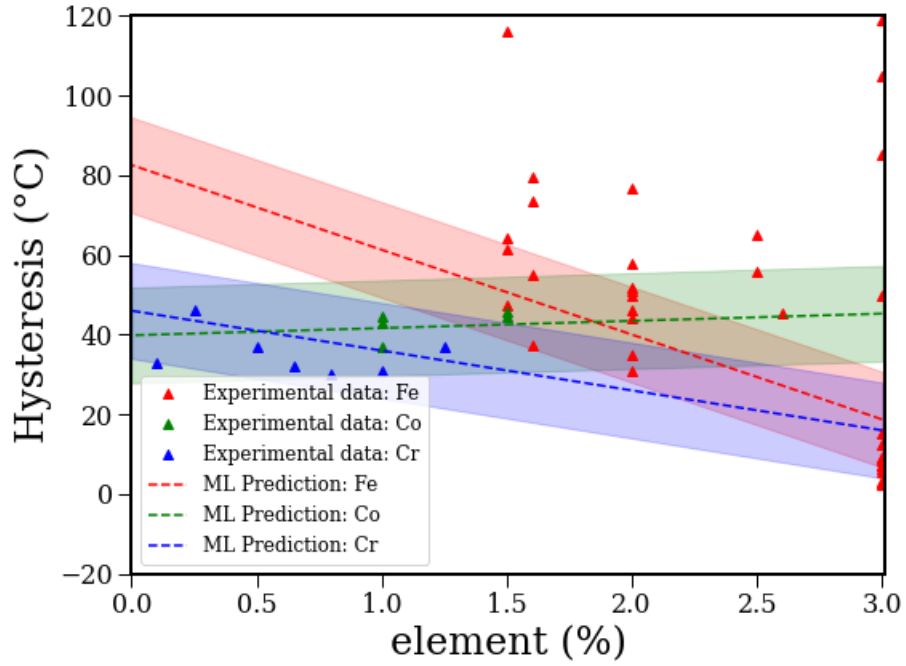




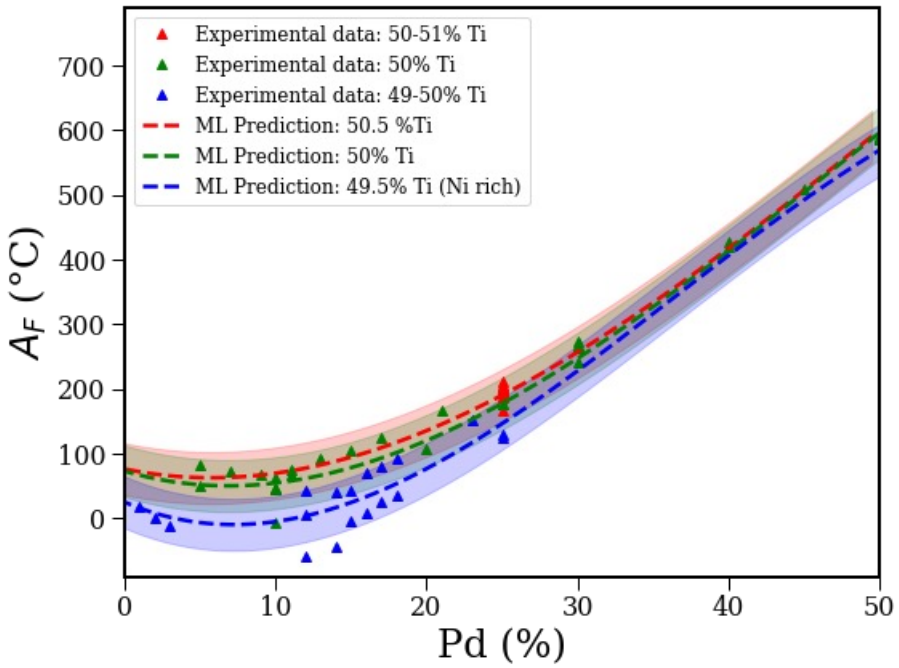


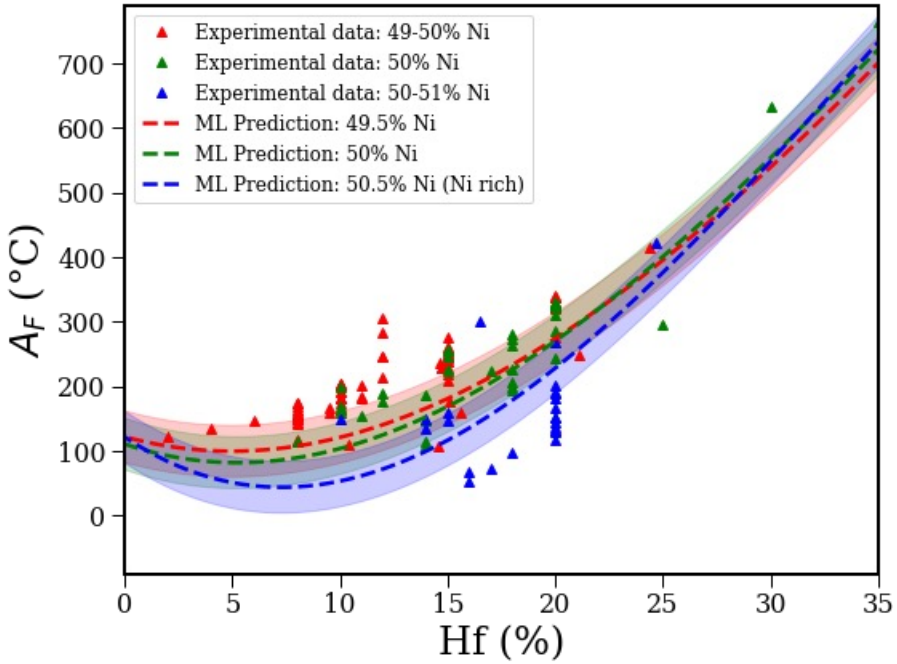
Effects of ternary additions (Fe, Co, Cr)



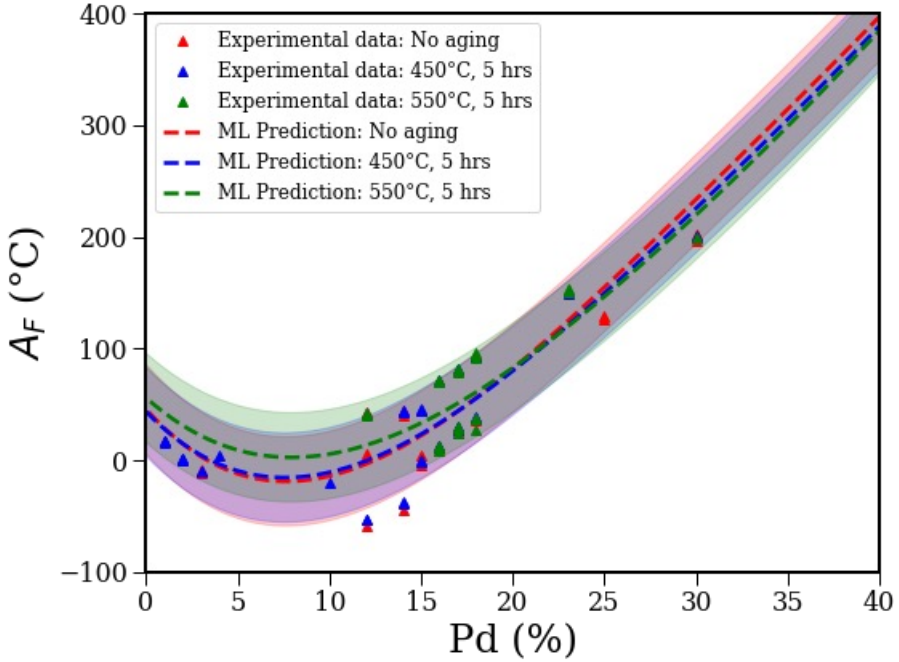


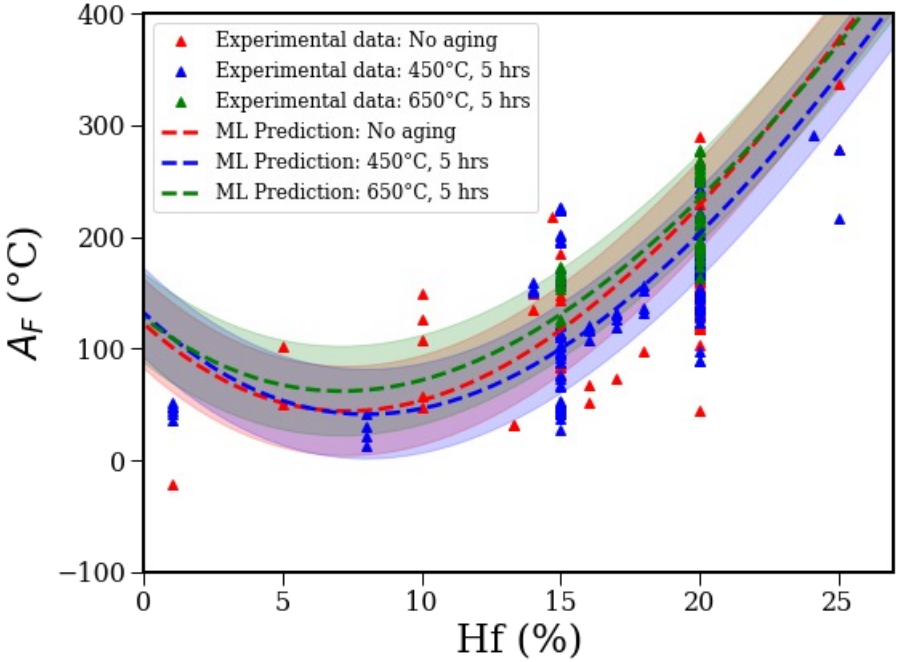
Effects of small Ni/Ti variation



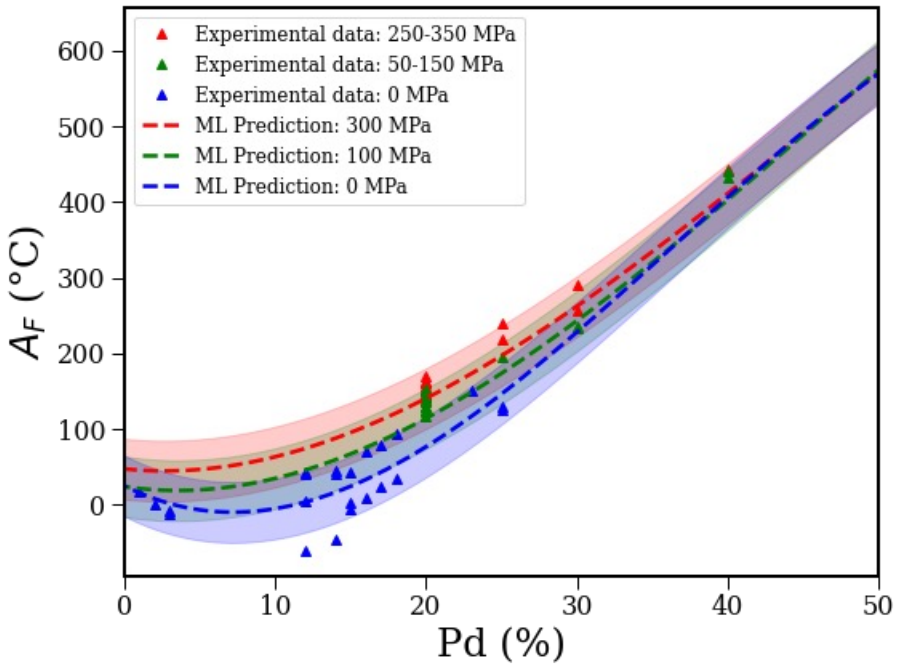


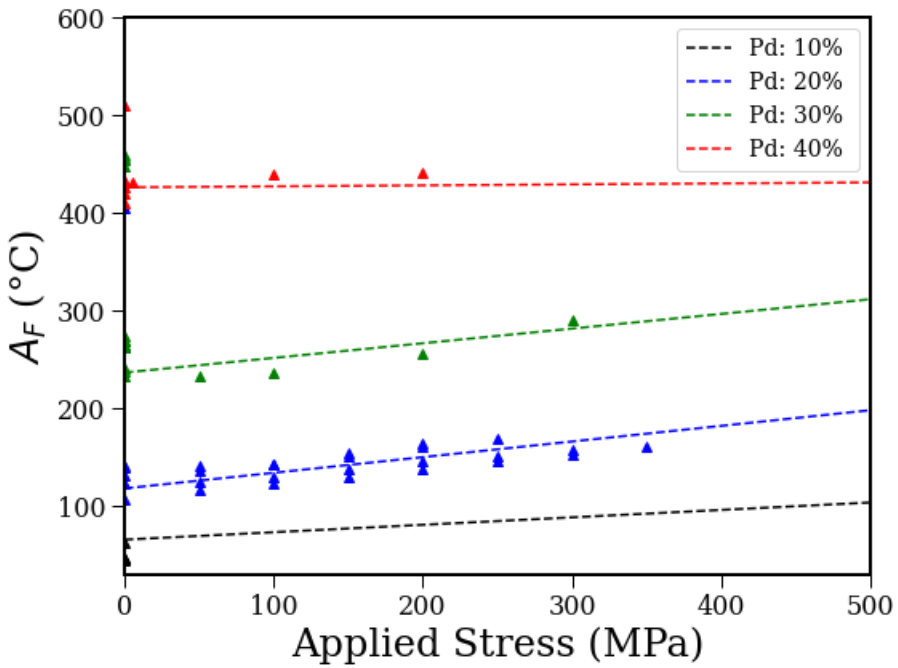
Effects of aging heat treatment





Effects of external applied stress





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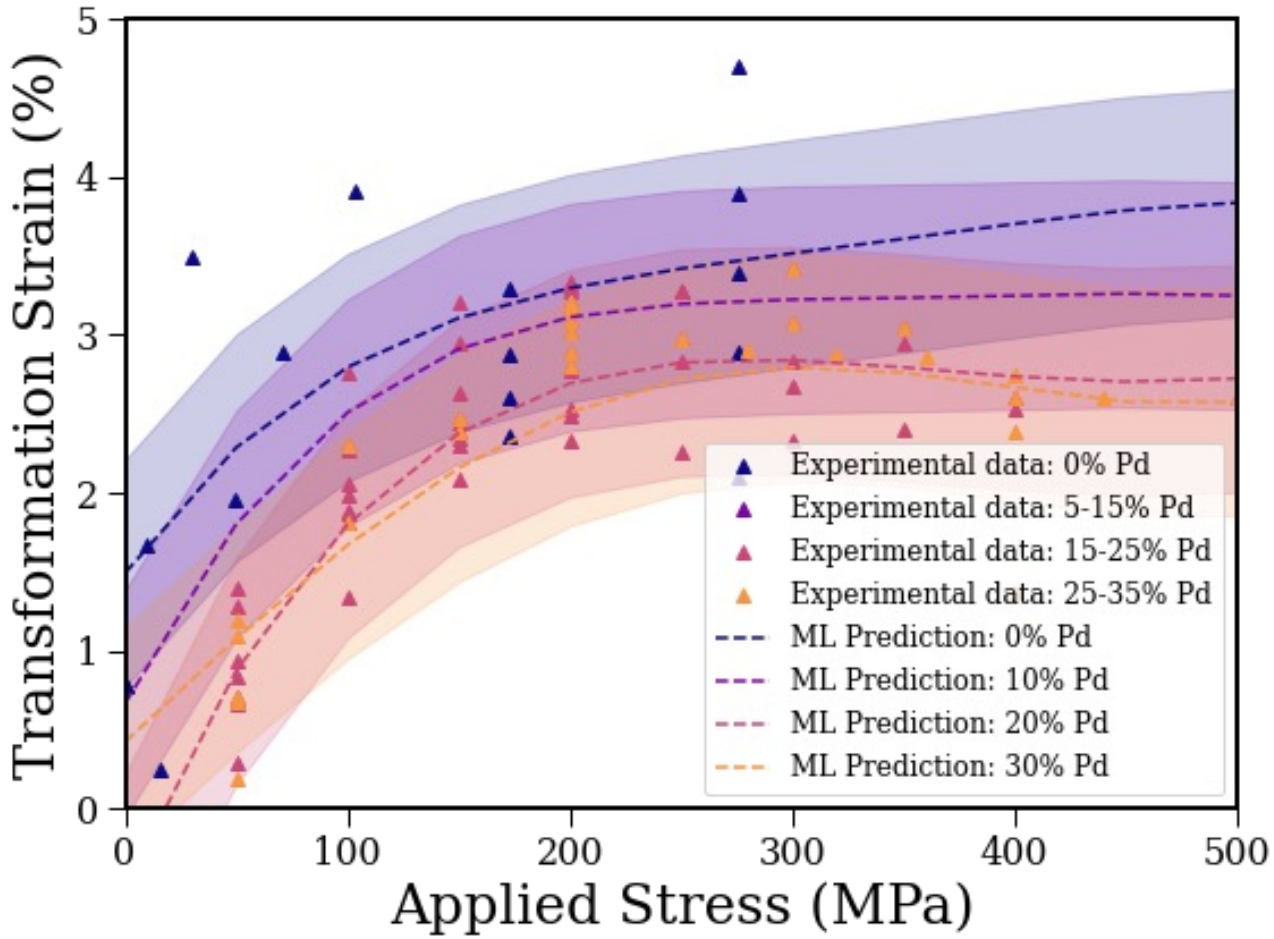
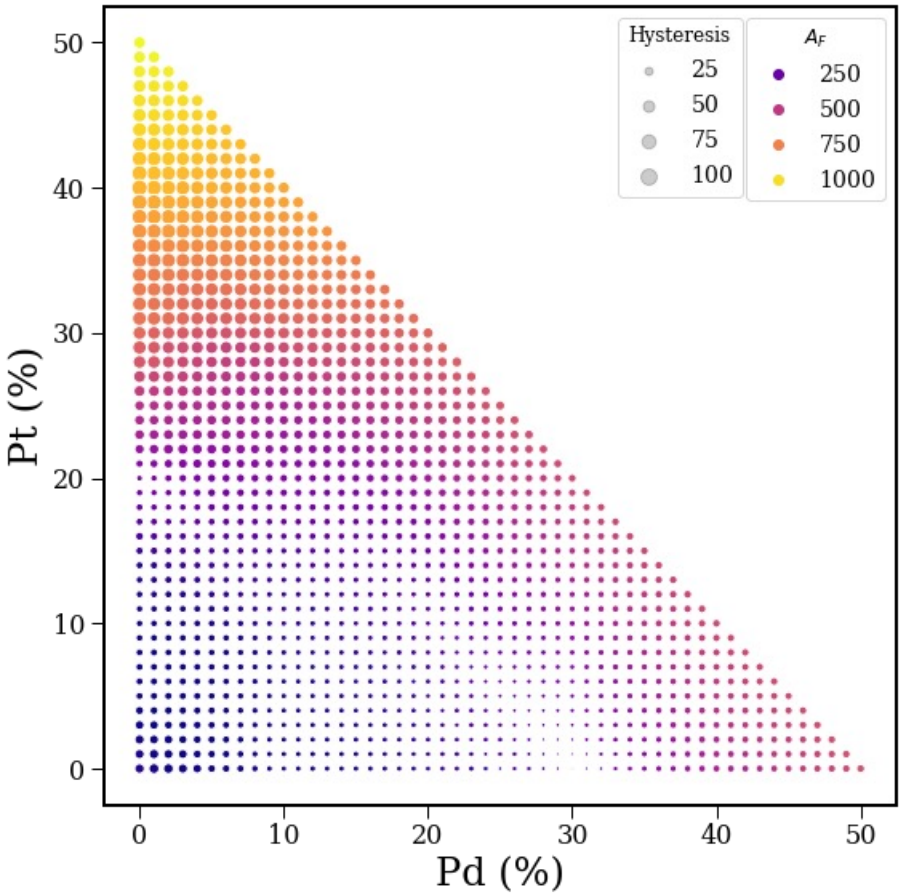
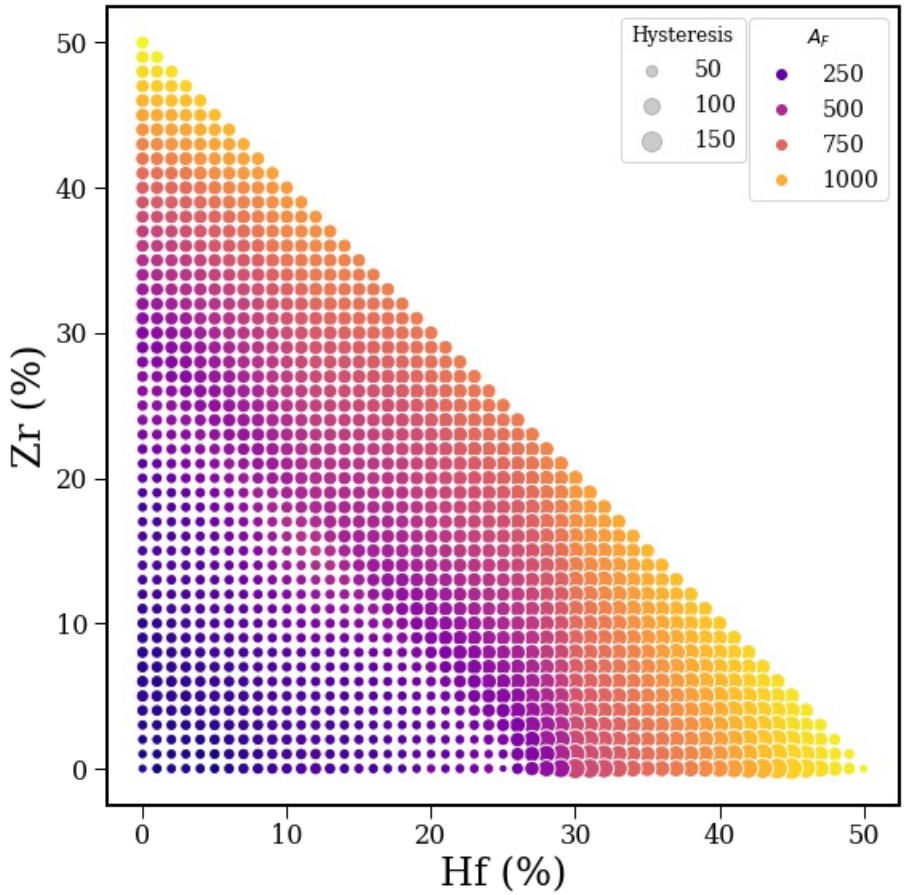
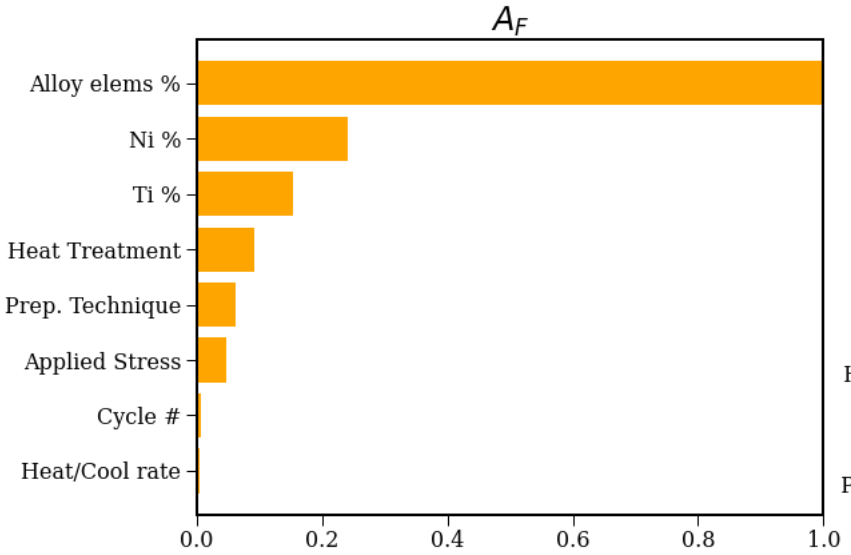


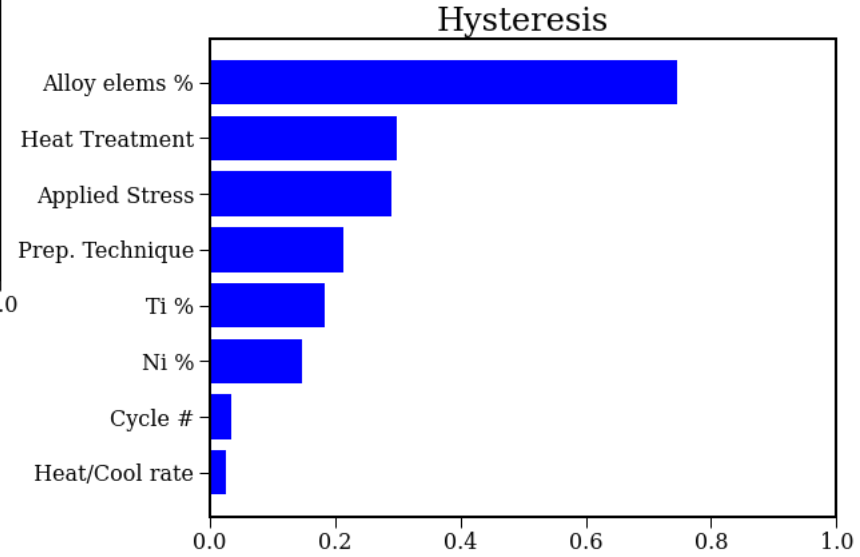
Predictions of quaternary systems

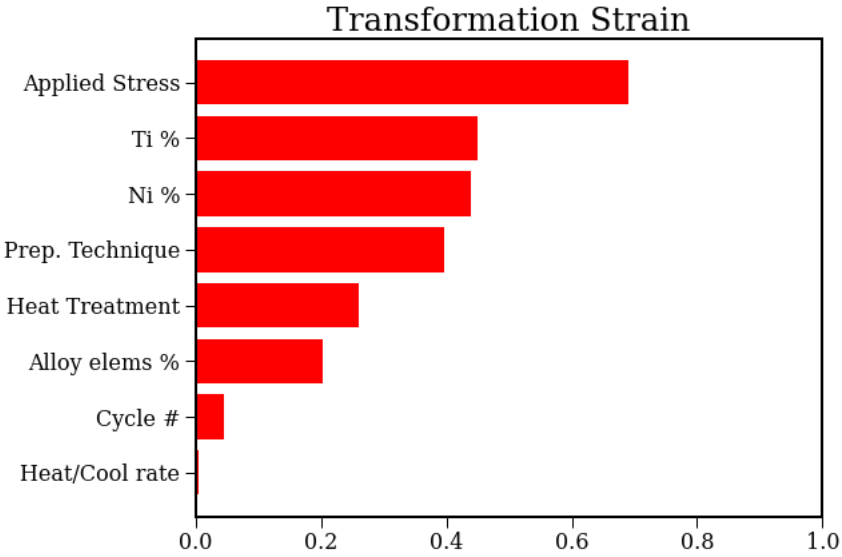




Permutation Feature Importances







Summary

We developed a a data-driven approach to study transformation behavior in multi component Ni-Ti SMAs.

- Using a dataset of about 8,000 Ni-Ti alloys containing 37 different alloying elements, ML models were trained to predict transformation temperatures (M_S, M_F, A_S, A_F), hysteresis (A_F - M_S), and transformation strain
- 52 composition, thermo-mechanical processing, and test parameter related inputs were identified, which helped achieve low MAE on all learning tasks
- Trained models were employed to study trends, learn correlations, and make predictions for new higher order alloy systems
- Current approach makes it possible to explore vast compositional and processing spaces using the same models, making it ideal for rapid discovery of new SMAs

Thank you

Back-up

Typical methods to study SMAs

- Experimental measurements
- Classical molecular dynamics (MD) simulations – require development of interatomic potentials
- *Ab-initio* approaches (eg. thermodynamic integration, P_4 method)
  - more accurate, but limited in their present capabilities, computationally expensive
  - still cannot estimate hysteresis or transformation strain accurately
  - do not account for processing history

Unconducive to large systematic studies over wide compositional and processing spaces

Machine Learning results

Algorithms: Ensemble learning (Random Forest, EXTremely RAndomized Trees, XGBoost)

Property	Training Set	MAE	R^2
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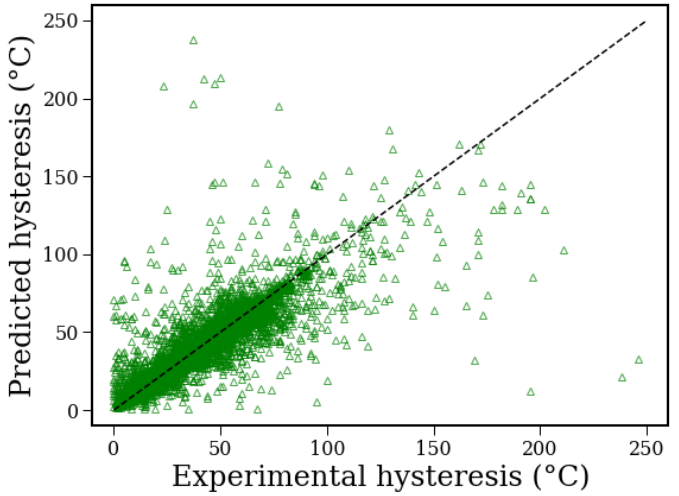
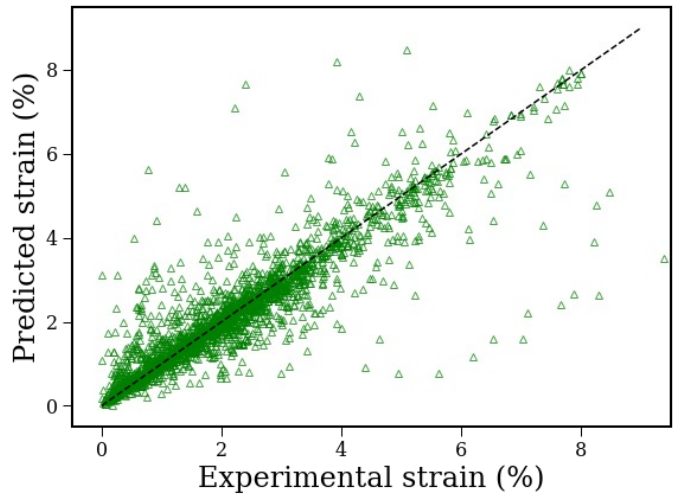
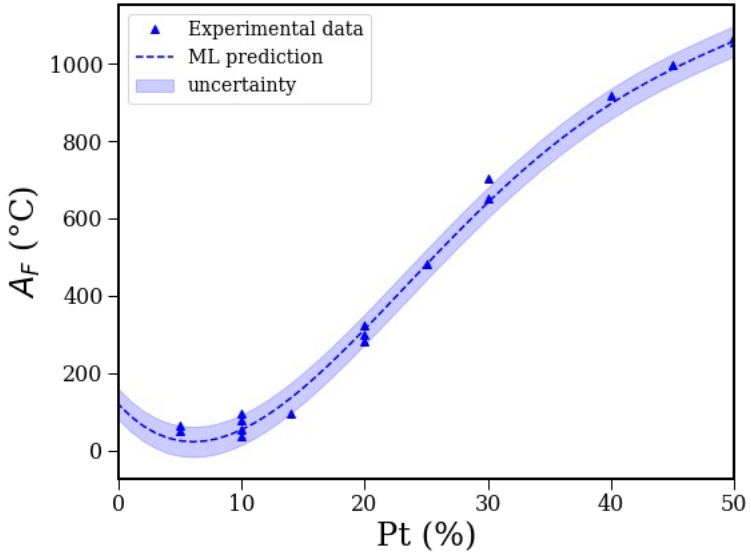
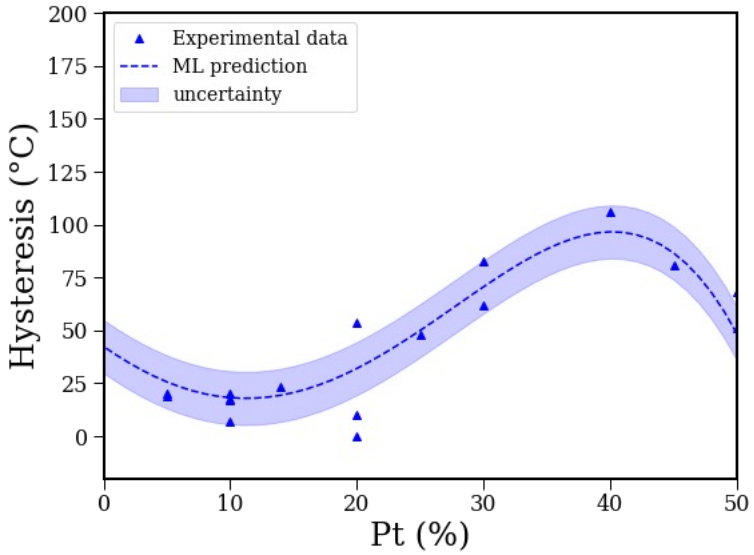
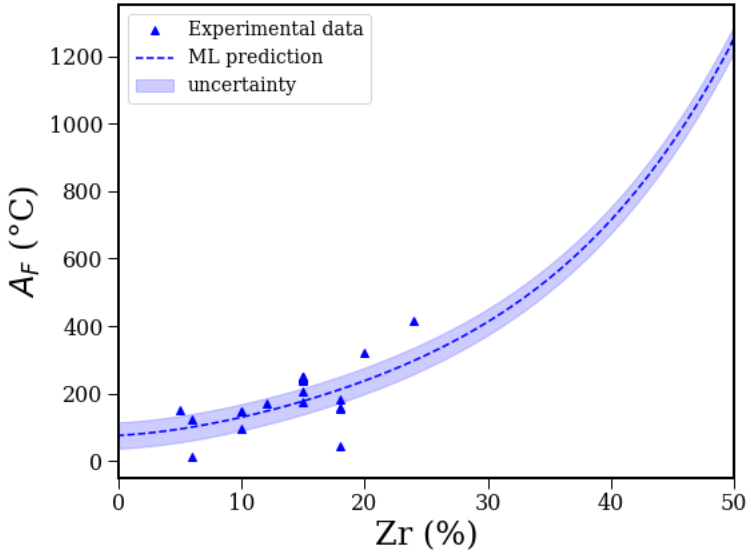


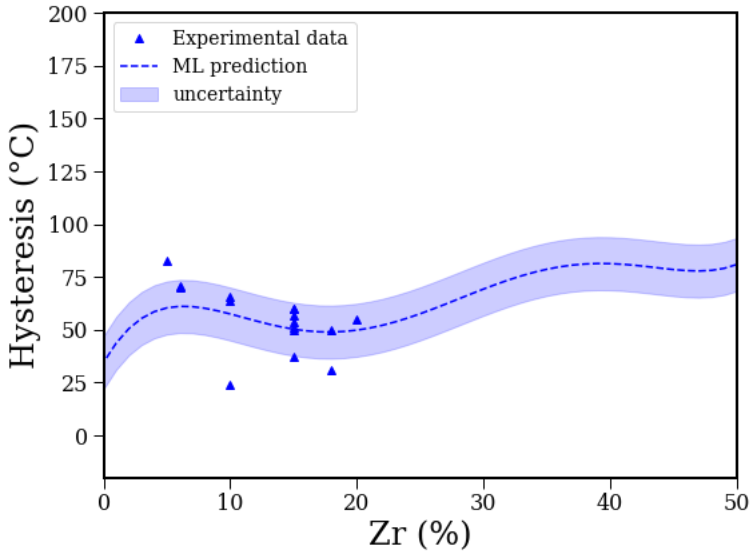


Effects of ternary additions (Pt, Zr)

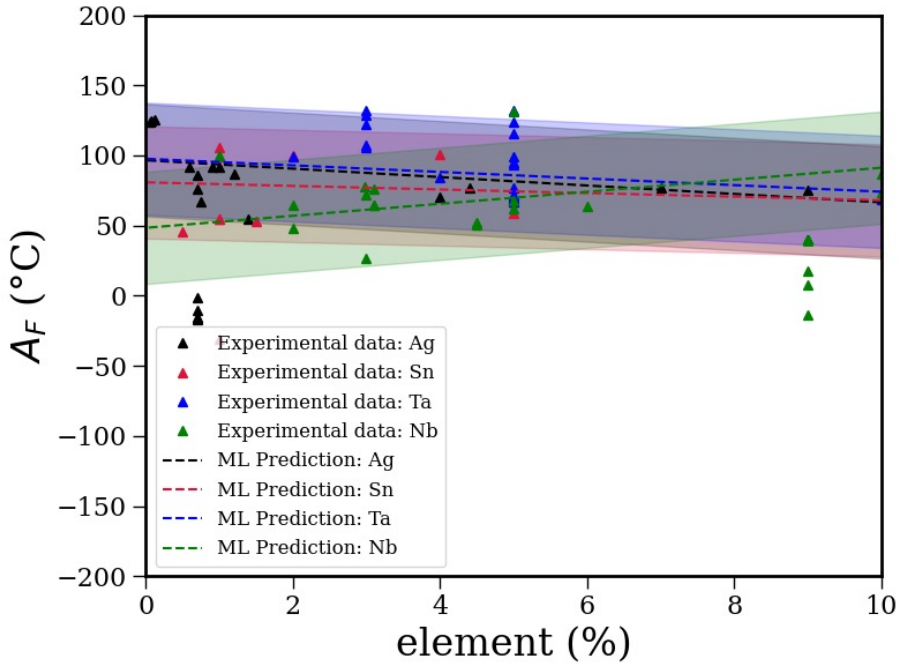


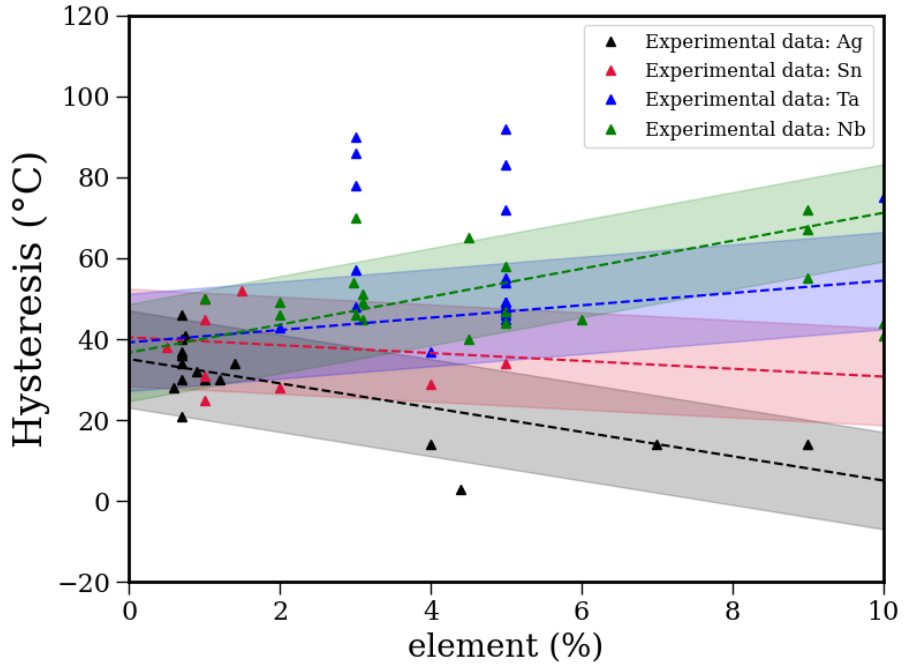






Effects of ternary additions (Ag, Sn, Ta, Nb)





Effects of external applied stress