Linking Stress Rupture Properties and Processing Parameters of HAYNES 718 Nickel Superalloy via Machine Learning

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Abstract: The wrought Ni-based superalloy HAYNES® 718 is utilized at high operating temperatures, in corrosive atmospheres, and under high mechanical loads–applications in which time-dependent deformation, known as creep, often occurs. Industry specifications such as AMS 5596 require that the material fails after a minimum of 23 hours with at least 4% elongation at 1200 ºF and 105 ksi. In this study, we seek to link high-dimensional processing parameters to creep properties via machine learning to improve material performance and accelerate specification testing.

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HAYNES International

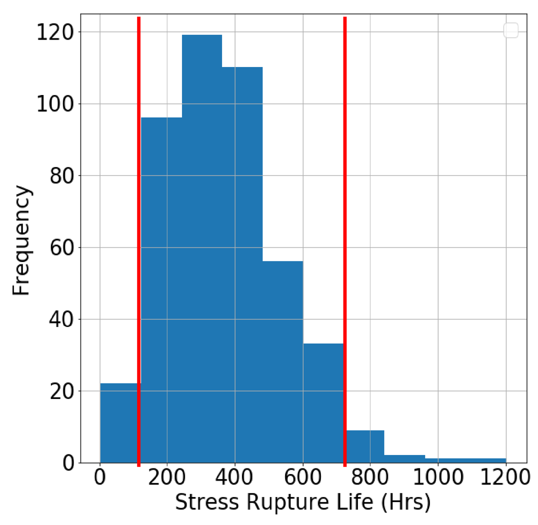
Project Background

HAYNES®718 is an age-hardenable nickel-based superalloy with high mechanical properties in extreme environments.

Element	Ni	Co	Fe	Cr	Nb+Ta	Mo	Mn	Si	Ti	Al	C	B
wt.%	52	1	19	18	5	3	0.35	0.35	0.9	0.5	0.05	0.004

Objective is utilizing Machine Learning (ML) to link compositional, processing, and mechanical input parameters with manufacturer specifications such as Room Temperature Tensile (RTT) and Stress Rupture (SR). Focus of our study is SR Life (Hrs), a measurement describing time taken for alloy to failure at elevated stress and temperature.

Quality of ML regressors is reliant on input data. A lack of data at extreme ends of the distribution results in biasing toward the median. A classifier is implemented to help deal with ends of distribution.

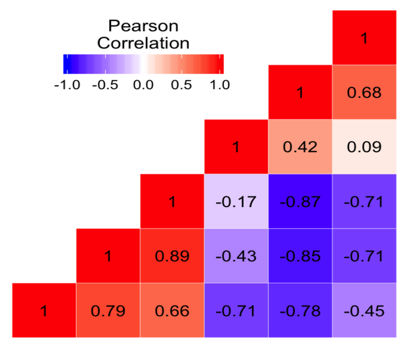


Computational Methods

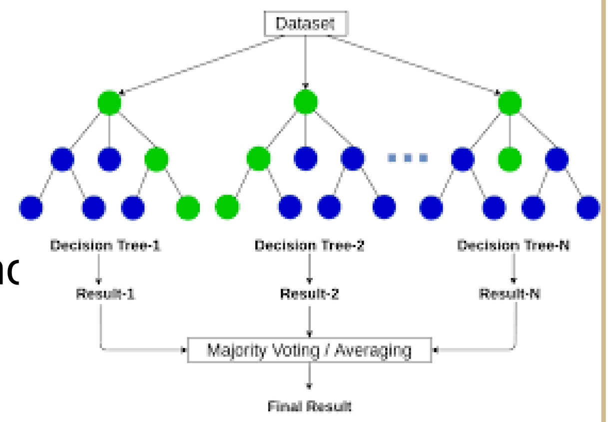
1. Utilize rule of mixtures and available environmental data to expand dataset.

Input Parameters					
	Compositional	Al	B	Co	Cr
		Mo	Ni	P	Si
		Ti	W	Nb	Fe
		Cu	Mn		
	Processing	Finish Gauge	Total Reduction	Final Reduction	ESR Furnace
	Thermochemical	Electronegativity	Electrical Resistivity	Melting Point	
	Mechanical	Bulk Modulus	Young's Modulus	Density	
	Environmental	Daily temperature maximum	Daily temperature minimum	Humidity	Barometric Pressure

2. Create Pearson Correlation map to determine linear correlation coefficients between features.

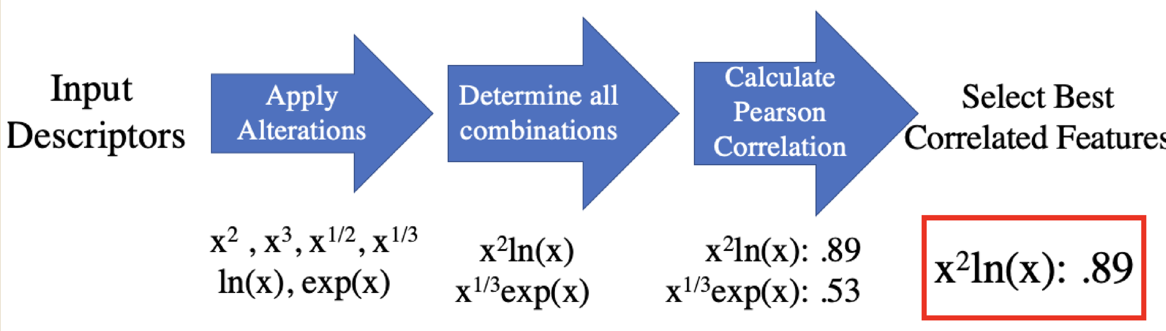


3. Create Random Forest (RF) model linking processing and new features to SR Life



4. Extract feature importance using Gini Coefficient, Mean Accuracy, and SHAP analysis.

5. Generate complex, higher-order features by implementing the SISSO algorithm.



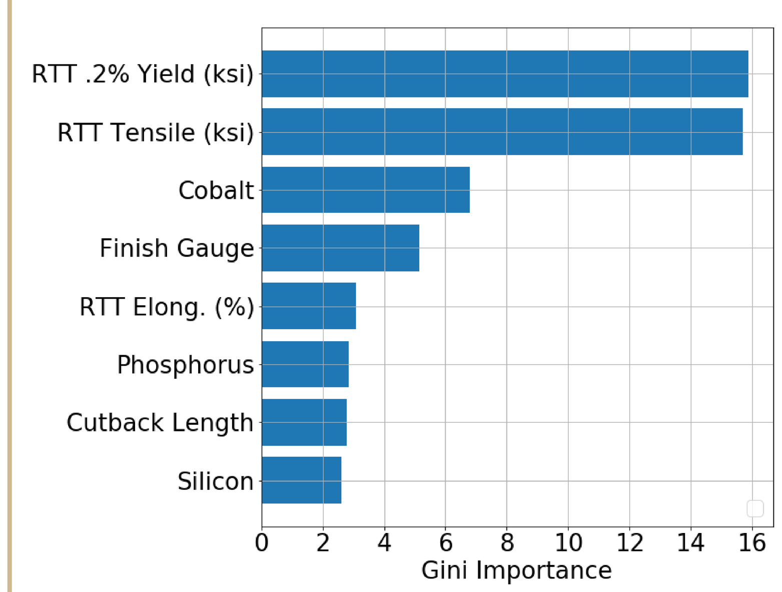
6. Train RF Regressor and Classifier with 80/20 split training/testing data, validate with Mean Absolute Error (MAE)

Feature Analysis

The Pearson Correlation Map provided no useful information, therefore proceeded with RF methods.

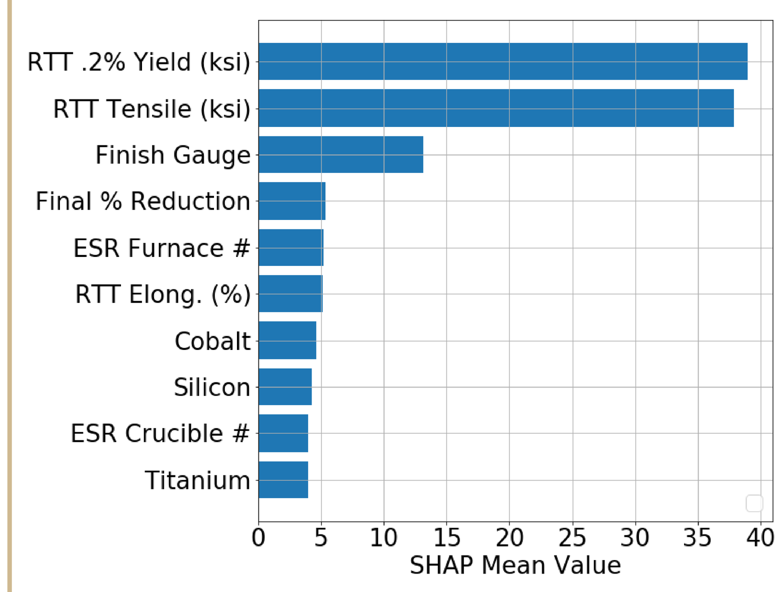
RF importance is expressed as the percentage of a feature's contribution to SR Life (totaling 100%)

Adding impactful features from these RF methods and SISSO continually decreases the RF regressor error.



Using features from the Gini Coefficient, error from the RF regressor MAE was 109±**10.3** hrs.

Elements Co, P, and Si were found to be impactful.



Implementation of SHAP and Mean Accuracy features reduced error to 104±**9.5** hrs.

Finds ESR Furnace and Crucible # indicating process inconsistency.

Implementation of the SISSO algorithm elucidated higher order compound features improving accuracy to 102±**8.5** hrs.

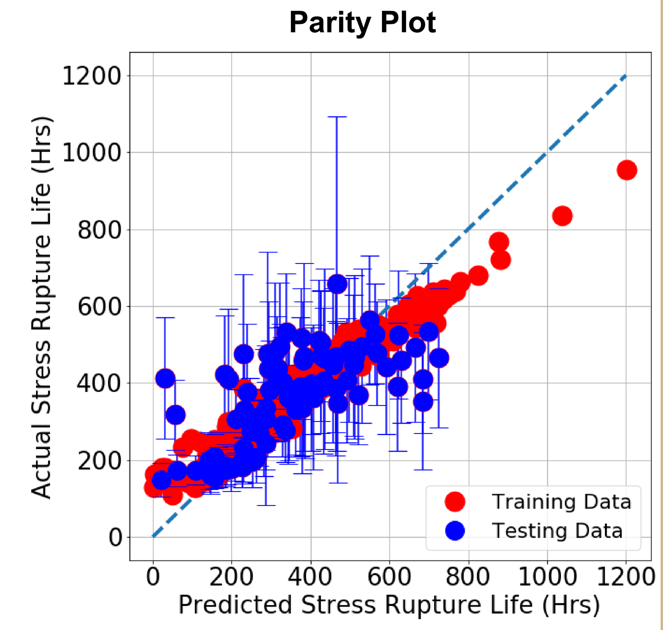
SR Life Cmpd. Features via SISSO	Pearson Corr.
Original Highest Correlating Feature: Yield	-0.5201
(Finish Gauge - $[Ni]^{1/3}$) + ($Yield^{1/3}$ × $[Ti]^{1/3}$)	-0.5815
($[P]^4$ × $Reduction^4$) + ($Yield^{1/4}$ + $[Ti]^4$)	0.5933

>1.5x improvements in Pearson correlation were achieved in prediction of other features such as RTT strength.

RT Tensile Cmpd. Features via SISSO	Pearson Corr.
Original Best Correlating Feature: Finish Gauge	0.5232
($[Cr]^{1/4}$ - $Reduction^{1/4}$) × (Finish $Gauge^{1/4}$ × Reduction)	-0.8792
($[B]^{1/4}$ × Reduction) × (Finish $Gauge^{1/4}$ × Reduction)	0.8817

Regressor Model

- Regressor was trained using lolopy library.
- If slope = 1 (dashed line), perfect accuracy.
- Regressor trained from all features in feature analysis.

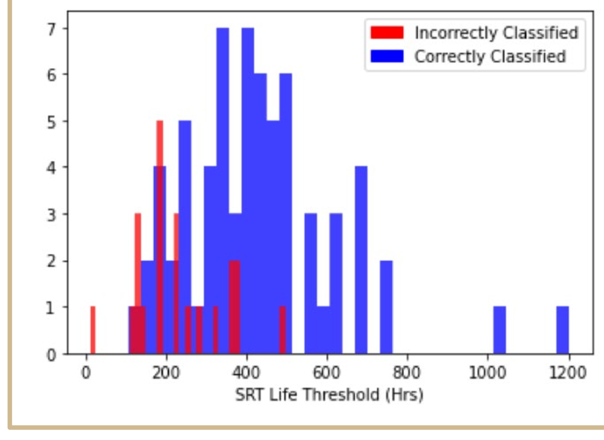


Classification Model

- The classifier model groups inputs instead of predicting precise values.
- Ability to choose specification threshold and predict if SR life will exceed

		Predicted Condition	
	Total Population = P + N	Positive (PP)	Negative (PN)
Actual Condition	Positive (P)	14	9
	Negative (N)	4	85

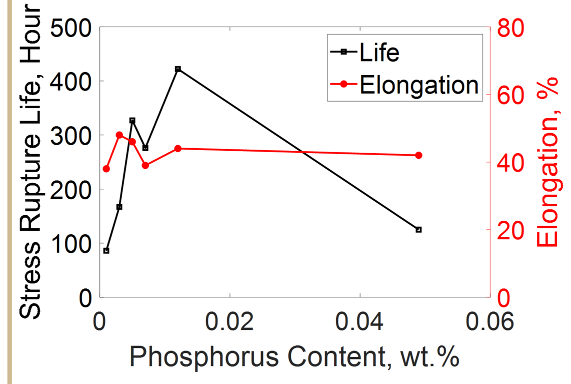
Classification Accuracy Distribution @ 200 hrs.



- RF classifier makes accurate predictions at the extremes of the dataset.

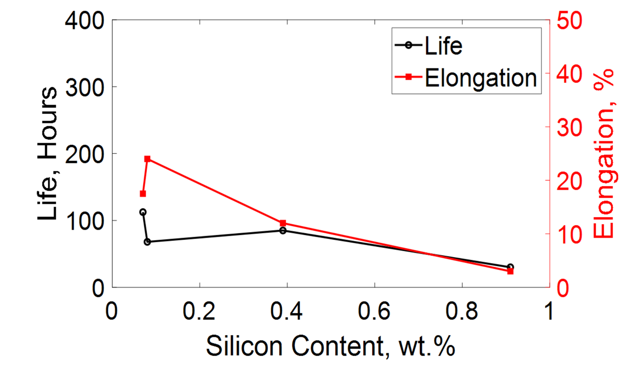
Discussion

Compositional: Excess amounts of P (>0.009 wt.%), Si (>0.07 wt.%) and Co (>0.45 wt.%) result in extreme SR life values as supported by the literature.



Nucleation of δ-phase particles influences SR properties. SR life maximized at 0.017 wt.% P. SR life is minimized at the extreme P concentrations [1].

Large concentrations of elements such as Si and S reduce SR performance. Si and S maximize SR life at 0.06 and 0.1 wt.%, respectively [2].



Processing: The high feature importance of Furnace and Crucible #'s suggests that residual elements may be leading to difficulties.

Mechanical: The data indicates that as finish gauge increases the likelihood of an extreme SR Life (Hrs) value reduces. RTT tests have strong correlation to SR life but do not physically explain the behavior.

Conclusions

- Haynes Intl. should further analyze how Cobalt, Phosphorus, and Silicon affect secondary phase formation.
- The provided Furnaces and crucibles may have large residual quantities of P, Co, and Si.
- models have displayed quantifiable accuracy in predicting trends of the dataset.

References

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