Modeling the Property Behavior of a Nickel-based Superalloy via Machine Learning

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Abstract: HAYNES® 718 is a nickel-based superalloy important in aerospace applications, due to its high strength, corrosion resistance, and operating temperatures. To meet industry standards, time-dependent deformation, known as creep, is crucial to understand and effectively quantify. Specifically, AMS 5596 requires a minimum stress rupture life and elongation above 23 hours and 4%, respectively, at 1200 °F and 95-100 ksi. In this study, we investigate the addition of microstructural features to predict creep properties using machine learning.

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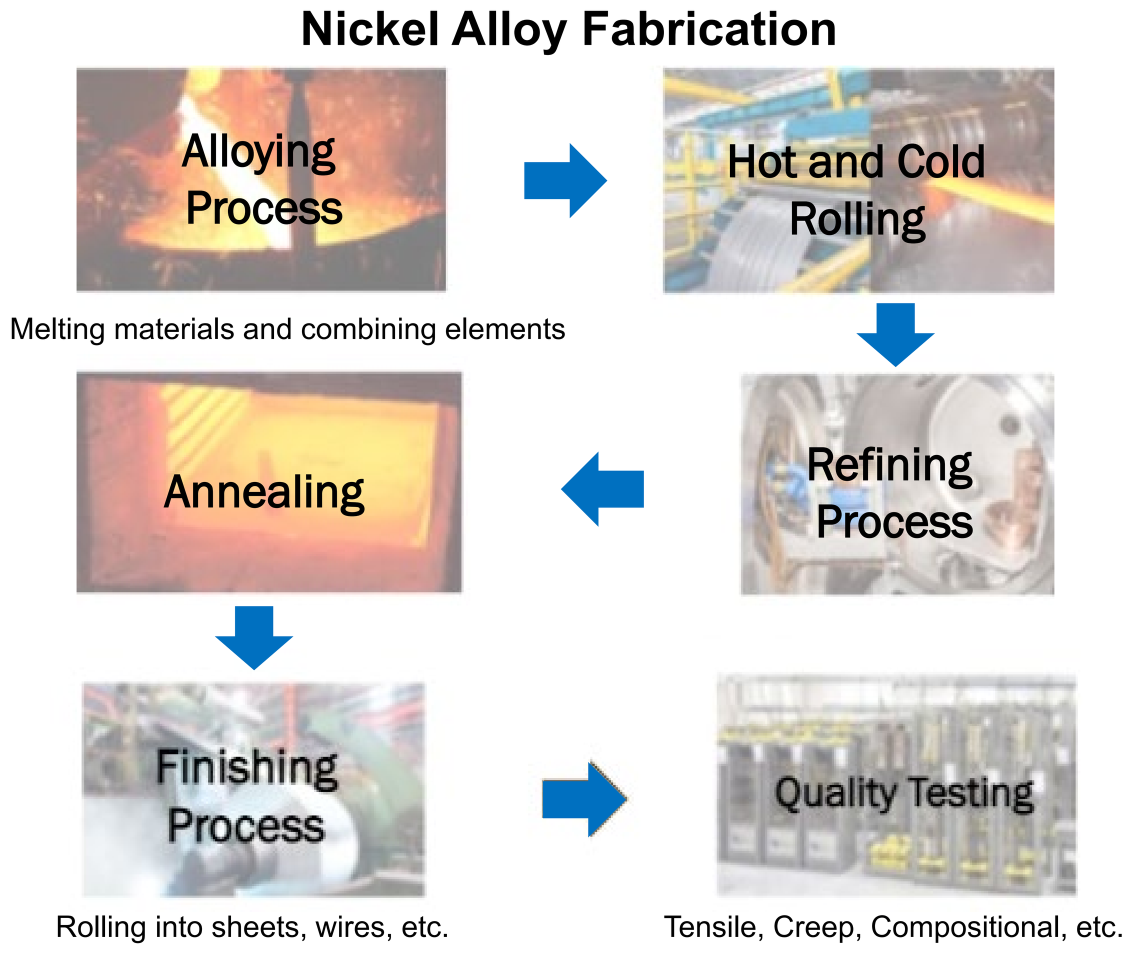
HAYNES International

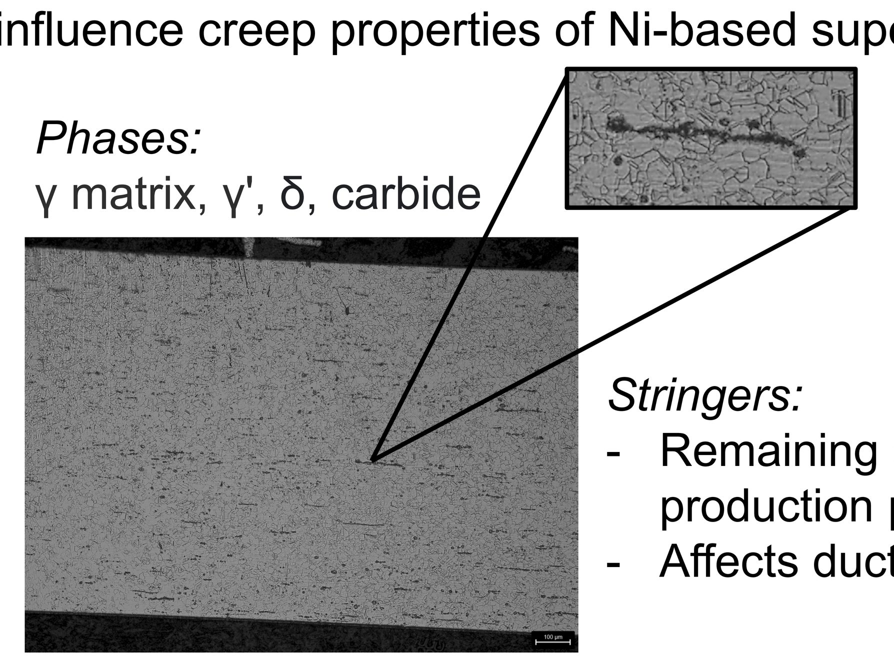
Background

Nickel Alloy Fabrication



Microstructure and thermo-mechanical processing influence creep properties of Ni-based superalloys.

Phases:
γ matrix, γ', δ, carbide



Stringers:
- Remaining slag after production processes
- Affects ductility

Objective: Based on experimental data, utilize machine learning to predict creep properties of HAYNES® 718.

Dataset

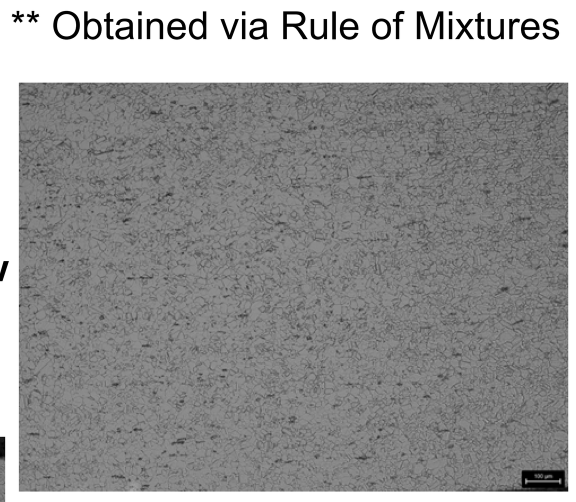
Dataset of 1350 samples obtained from Haynes.

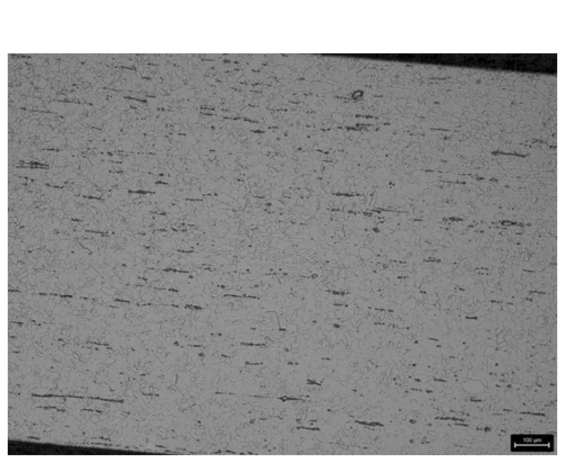
Compositional	Al	B	C	Nb	Ta
	Cr	Co	Cu	Fe	Mn
	Mo	Ni	P	Si	Ti
Processing	Finish Gauge	Ingot Gauge	Slab Cutback Weight		Final Anneal Furnace
	Total % Reduction		Final % Reduction		Melt Date
Microstructural	Average Grain Size		Phase Volume Fractions (δ, γ-matrix, γ')*		
Properties**	Bulk Modulus	Youngs Modulus	Shear Modulus	Density	Hardness
	Poisson's Ratio	Melting Point	EN	Resistivity	Elongation
	Coefficient of Thermal Expansion		Ultimate Tensile Strength		Yield Strength

* Obtained via ThermoCalc ** Obtained via Rule of Mixtures

112 optical micrographs at 100x magnification.

Low





High

Representative stringer content raw images.

Model Predictions

HAYNES® 718 Dataset
42 descriptors
2 target features:
SR Elongation
SR Life

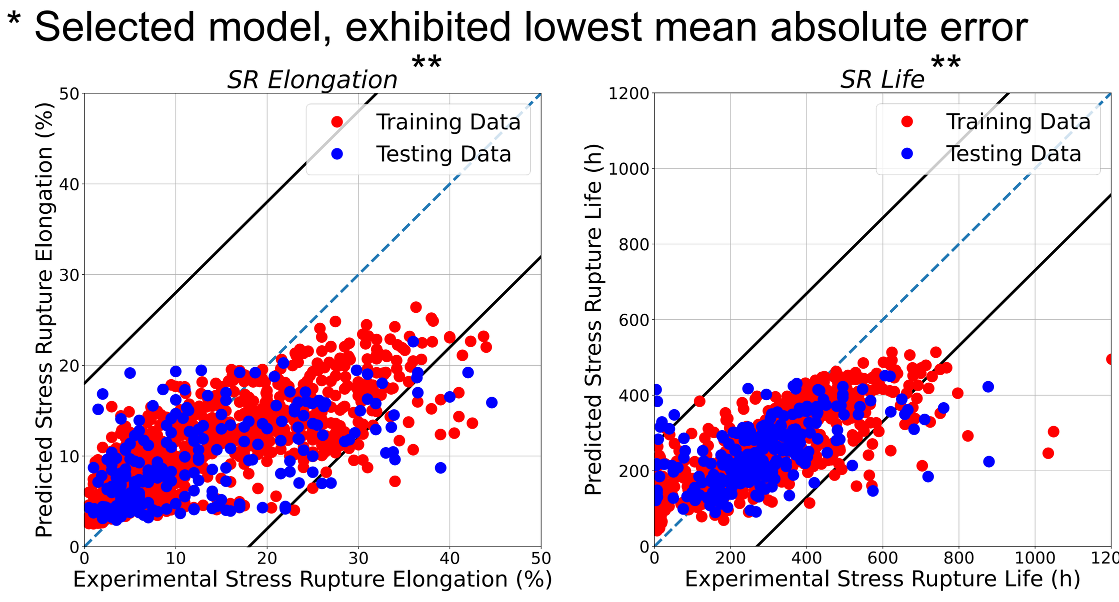
→

Regression Models
Random Forest*
Neural Network
Gradient Boosting
XG Boost
Gaussian Regression

→

Model Evaluation
Mean Absolute Error (MAE)
Mean Squared Error (MSE)
Root Mean Squared Error (RMSE)

* Selected model, exhibited lowest mean absolute error



**80-20 test-train split

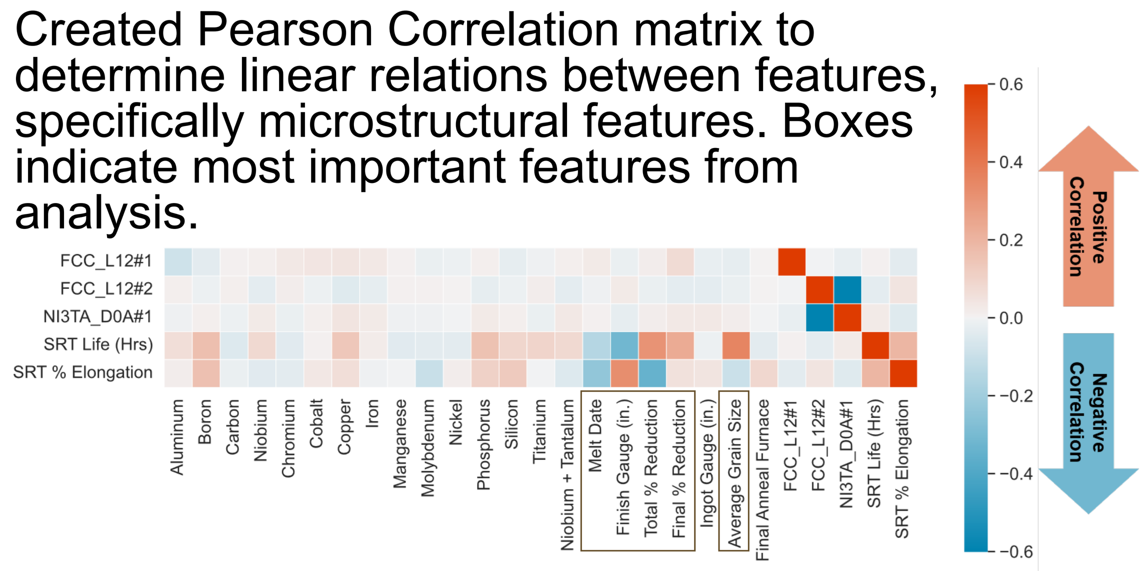
Dashed Line = Perfect Accuracy (slope = 1)
Solid Lines = Two Standard Deviations Away

Model exhibits reasonable predictions within the median ranges, but noticeable underpredictions for larger values.

Output	Mean Absolute Error
Stress Rupture Life (hrs)	98.6 ± 6.4
Stress Rupture Elongation (%)	6.64 ± 0.31

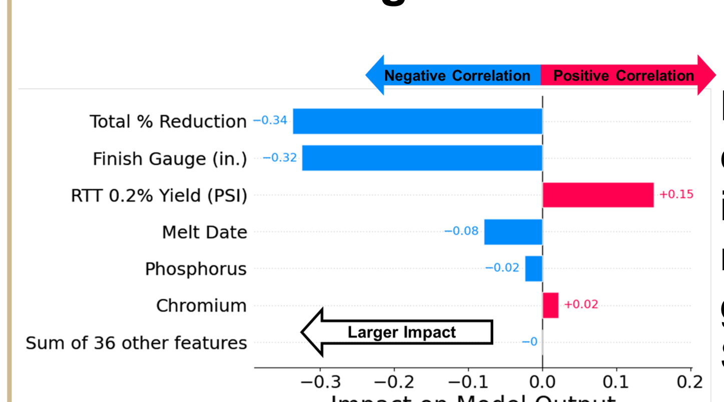
Feature Importance

Created Pearson Correlation matrix to determine linear relations between features, specifically microstructural features. Boxes indicate most important features from analysis.



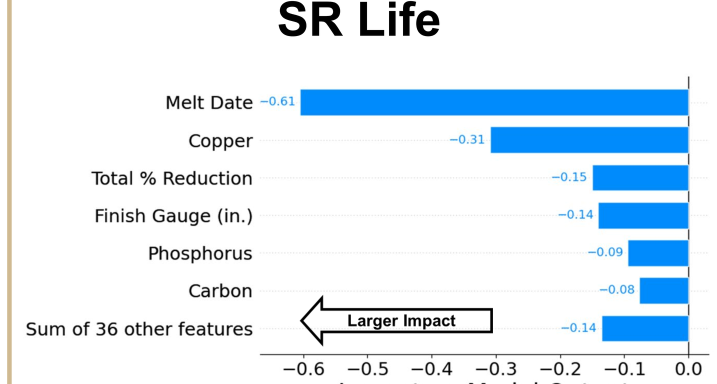
Conducted SHAP (SHapley Additive exPlanations) analysis to extract importance of features to the model.

SR Elongation



Processing descriptors exhibit the greatest impact. Total % reduction and finish gauge values decreased SR Elongation.

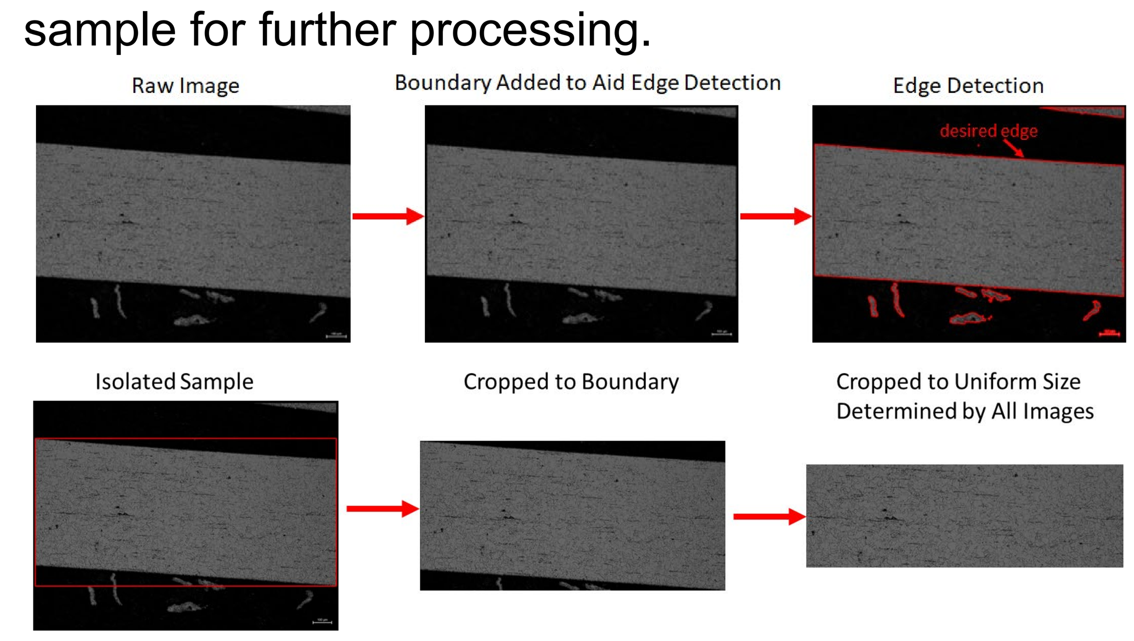
SR Life



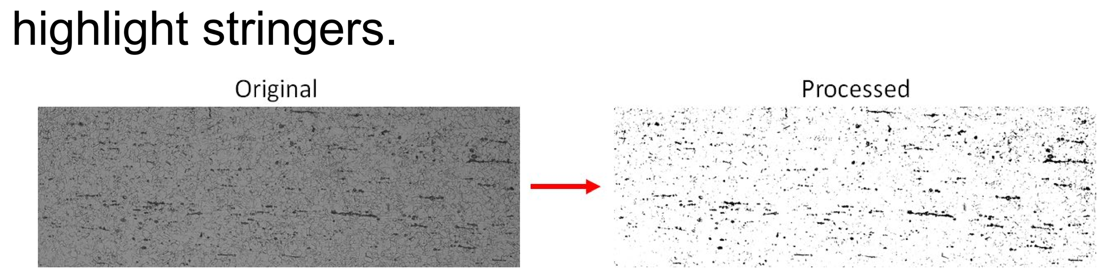
Melt date as an important feature indicates that the model prediction remains a stochastic process.

Image Analysis

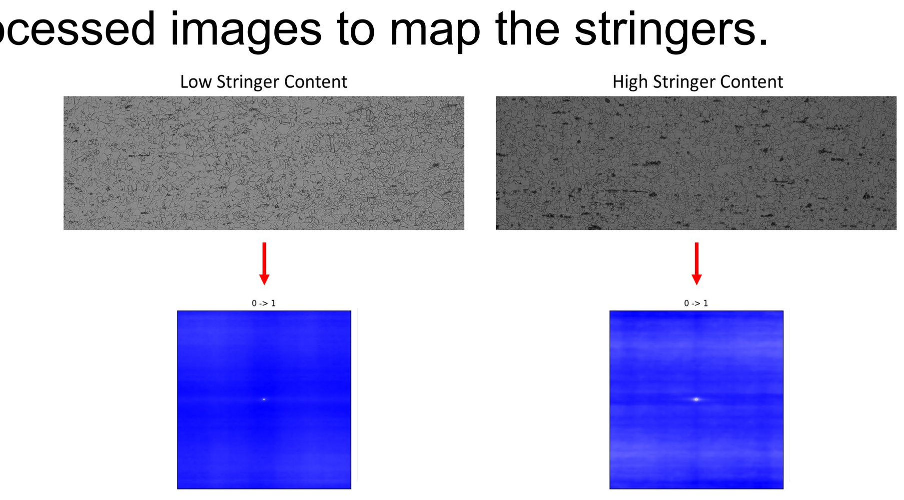
Images were cropped using OpenCV to isolate the sample for further processing.



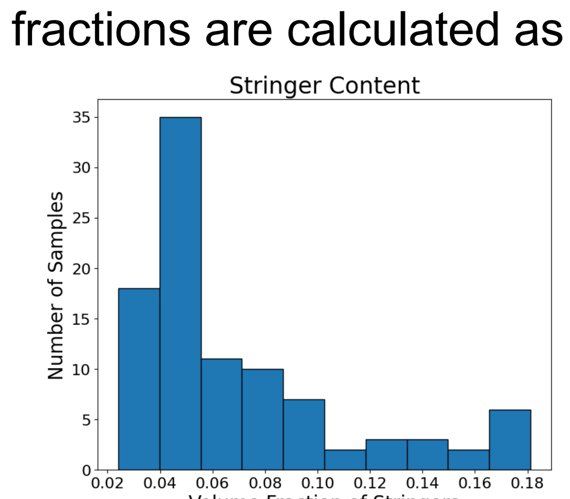
Cropped images were normalized and thresholded to highlight stringers.



Two Point Correlation was performed on the processed images to map the stringers.



The directional and shape trends are mapped with lighter/white areas representing stringers. Volume fractions are calculated as a numeric output.



Stringer content of 97 images. The volume fraction value can be used as an additional descriptor for future models.

Conclusions

1. The addition of phase volume fractions had no noticeable impact on model predictions.
2. The processing parameters remain the descriptors with highest correlation.
3. Data relating to stringer content can be extracted from micrographs for use in the model.
4. Obtaining more descriptors related to heat treatment and test conditions might help improve the model in the future.

References

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