Hybrid Structured Nickel Superalloys to Address Price Volatility and Weld/Weld Repair Based Supply Chain Issues

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Tanner Olson, Sophie Mehl, Yunsheng Su, Zequn Wang, Paul Sanders – Michigan Technological University

John Shingledecker – Electric Power Research Institute

Michigan Technological University Materials Science and Engineering

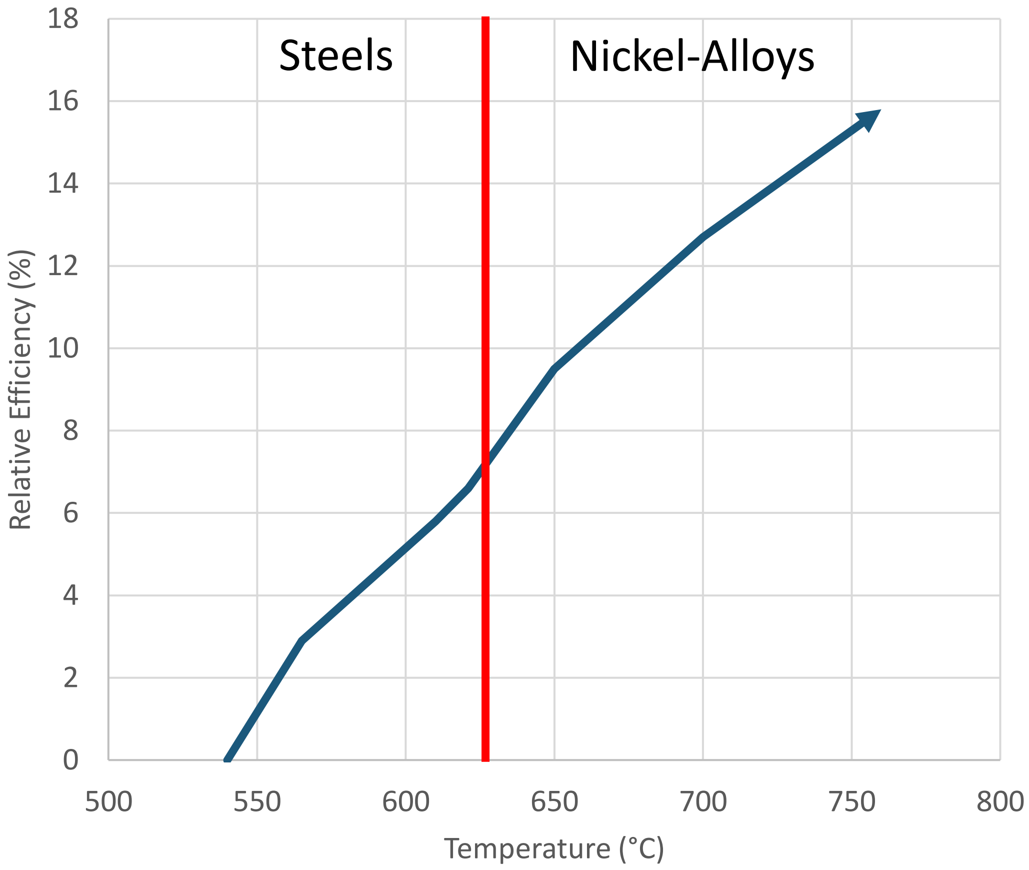
NATIONAL ENERGY TECHNOLOGY LABORATORY

EPRI ELECTRIC POWER RESEARCH INSTITUTE

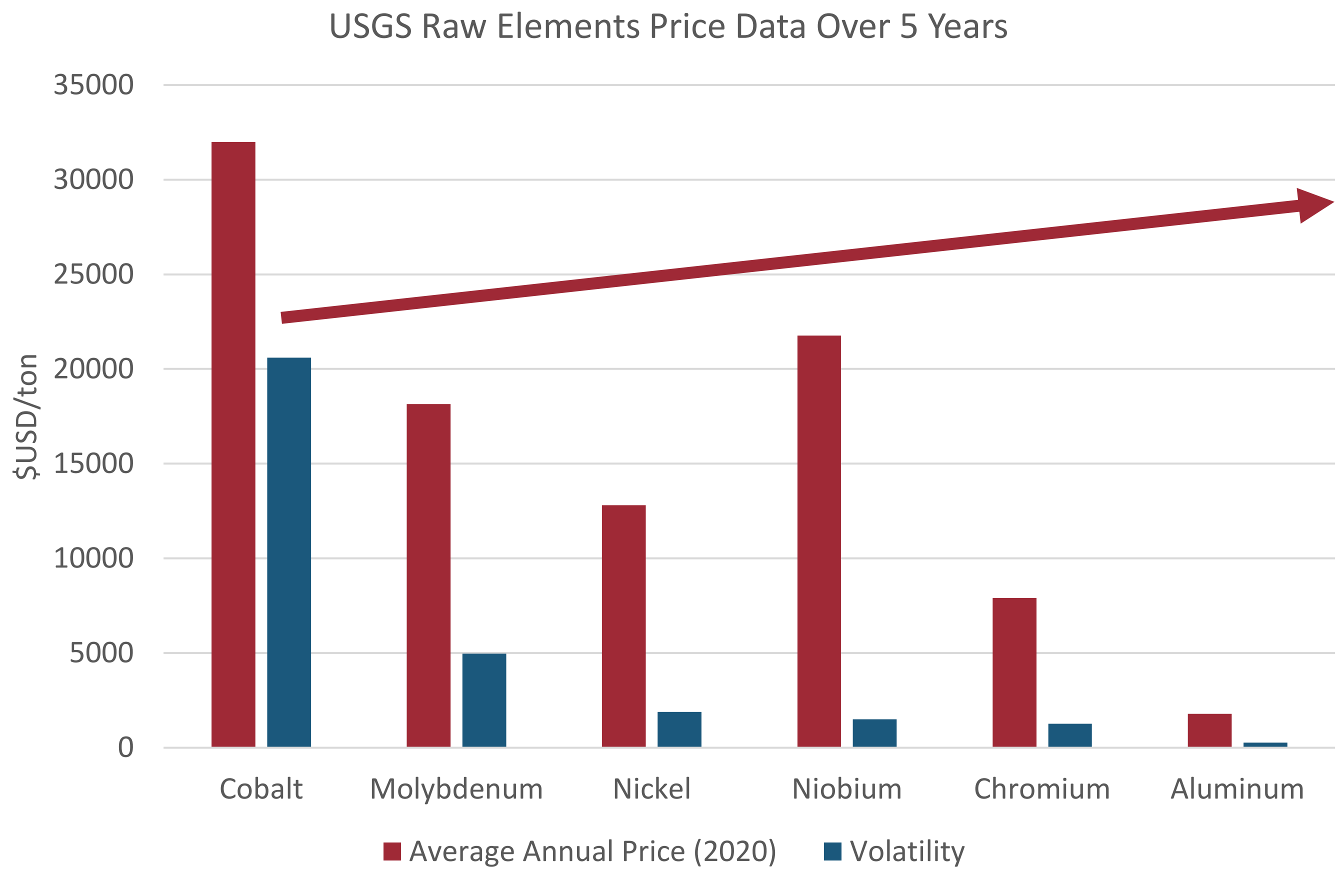
Outline

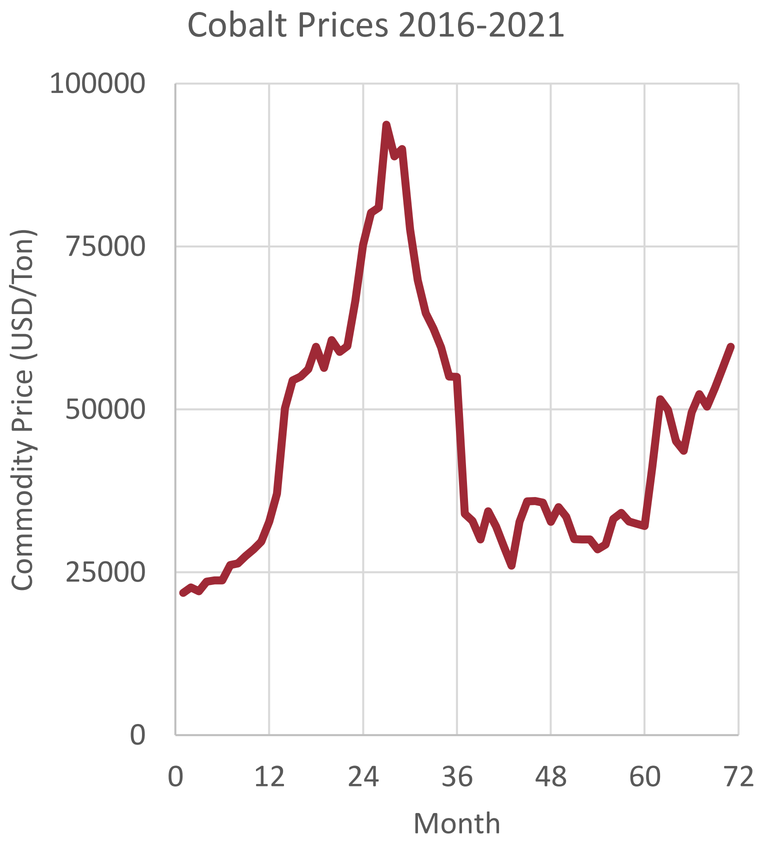
1. Background & Project Goals
2. Computational Material Design
   a. Design Space
   b. Parameter Modelling
   c. Multi-Objective Optimization
   d. Results
3. Experimental Material Design
   a. Sample Casting & Processing
   b. Property Analysis
4. Next Steps

Steels unable to perform at higher temperatures which limits efficiency growth



Cost and volatility concerns with common superalloy elements

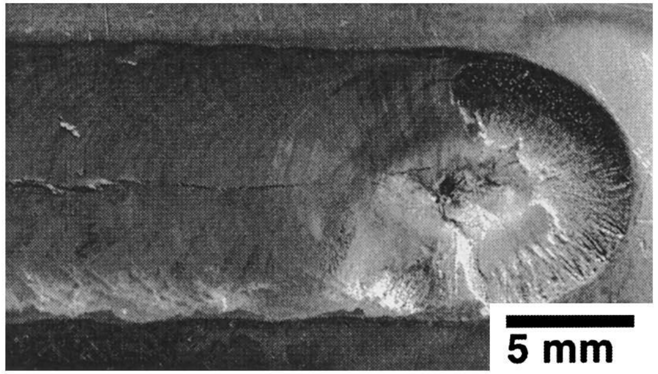




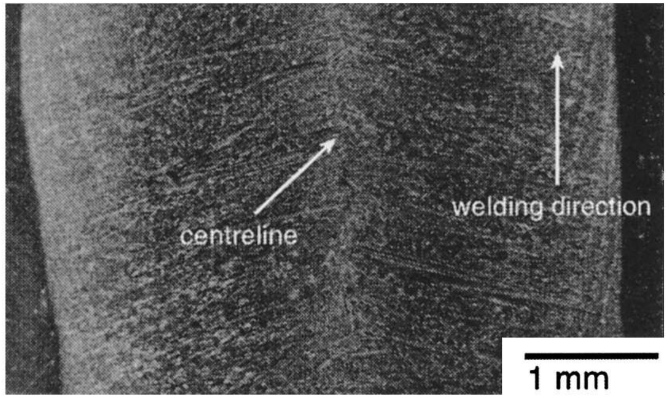
“Commodity Statistics and Information: Mineral Commodity Summaries for Co, Mo, Ni, Nb, Cr, and Al.” US DOI https://www.usgs.gov/centers/nmic/commodity-statistics-and-information

Weldability concerns in complex structures needed in power plants

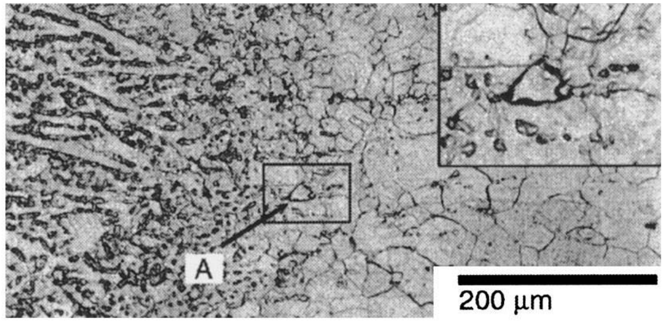
- Various types of weld cracking
  - Solidification cracking
  - Centerline boundary
  - Liquation cracking
  - Heat affected zone cracking
  - Strain age cracking (SAC)



(a) Solidification cracking

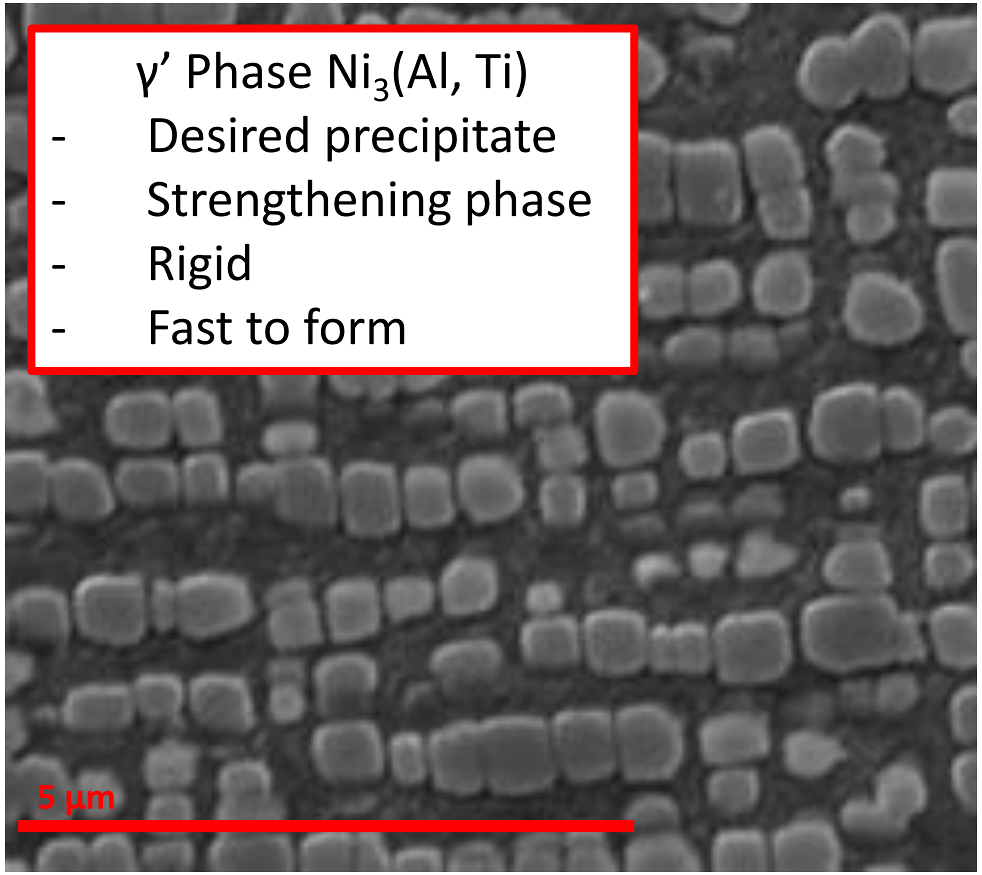


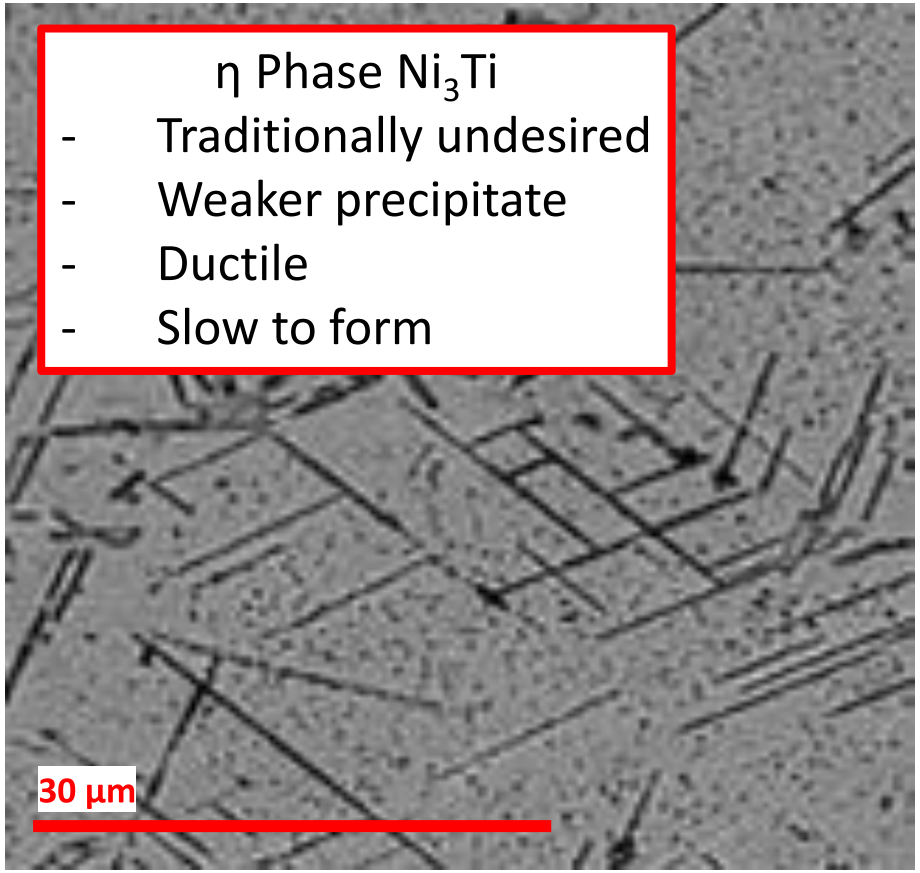
(b) Centreline Grain Boundary



(c) Heat-affected zone liquation

Potential improvement to weldability & other material properties with inclusion of η precipitates





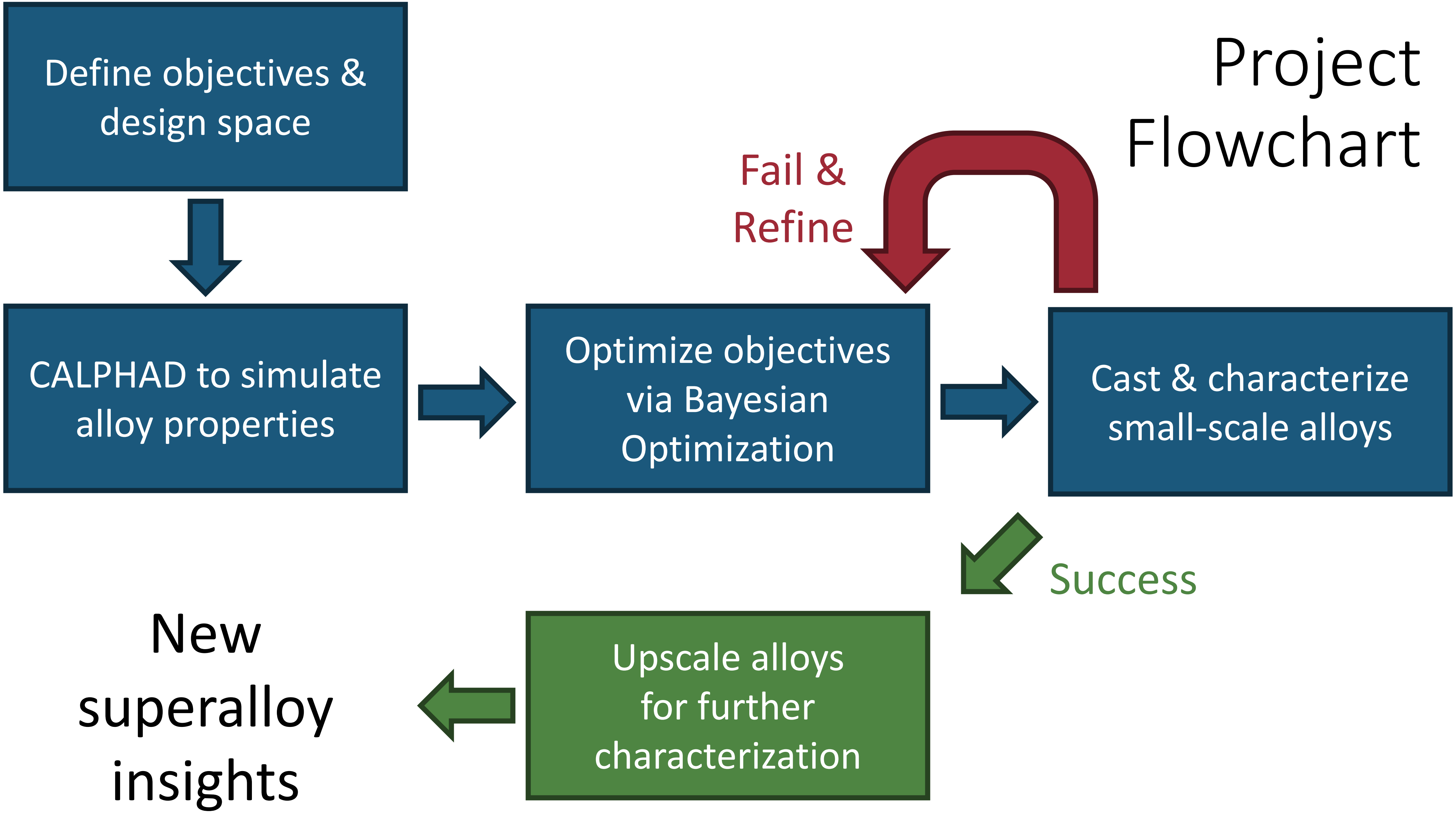
“Gamma prime,” ***Gamma Prime - an overview | ScienceDirect Topics*****.**
Wong, Sanders, Shingledecker, White – Design of an ETA-phase-precipitation-hardenable nickel-based alloy …

Threefold Project Goals:

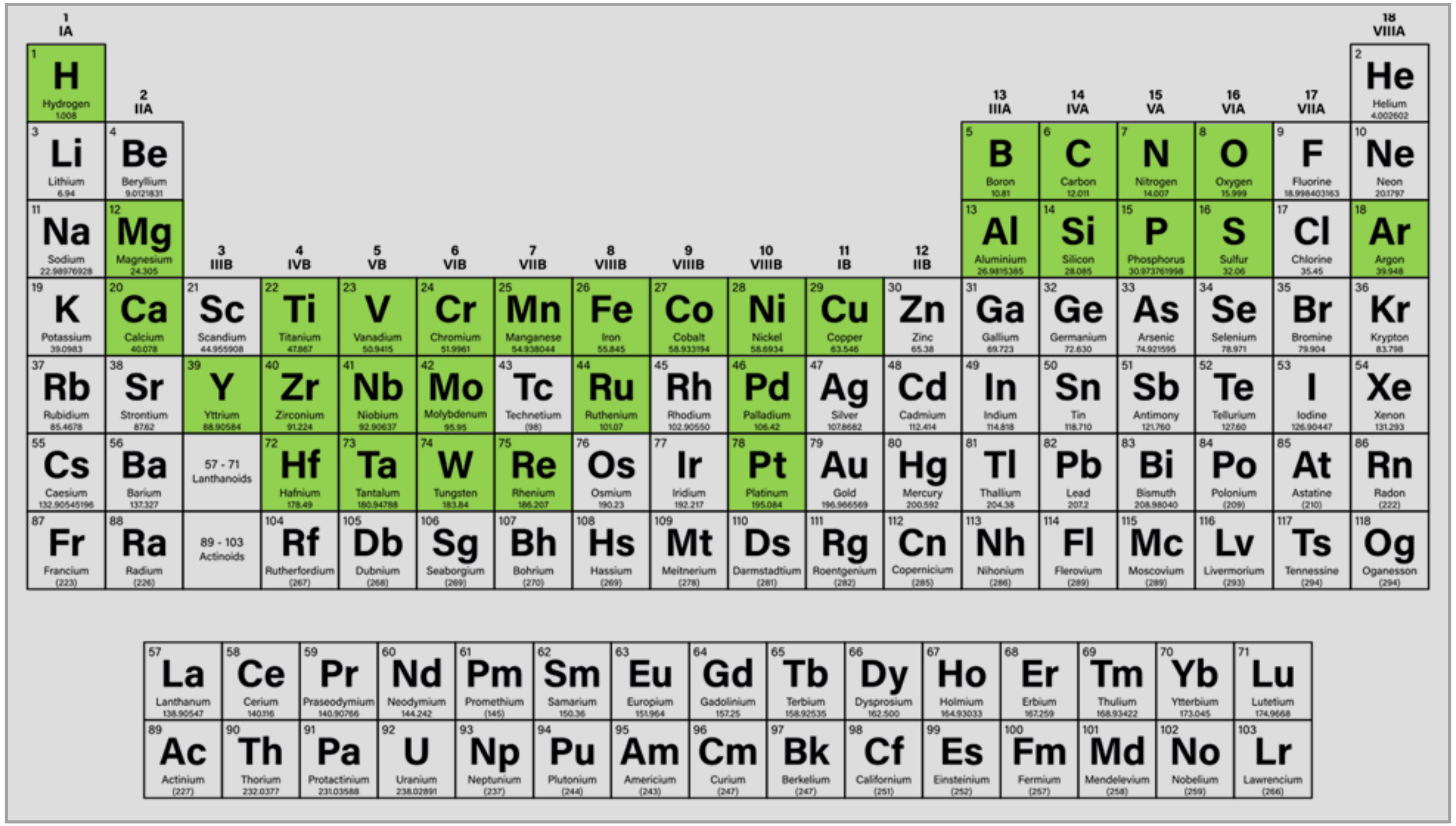
Create a nickel-base superalloy with the following considerations:

1. Reduce cobalt content to less than 5wt% and minimize overall cost
2. Meet weldability indices as measured by solidification and strain-age cracking resistance
3. Maintain material properties within 10% nano-indentation and hot-hardness values of a comparable superalloy (Nimonic 263)

Project Flowchart

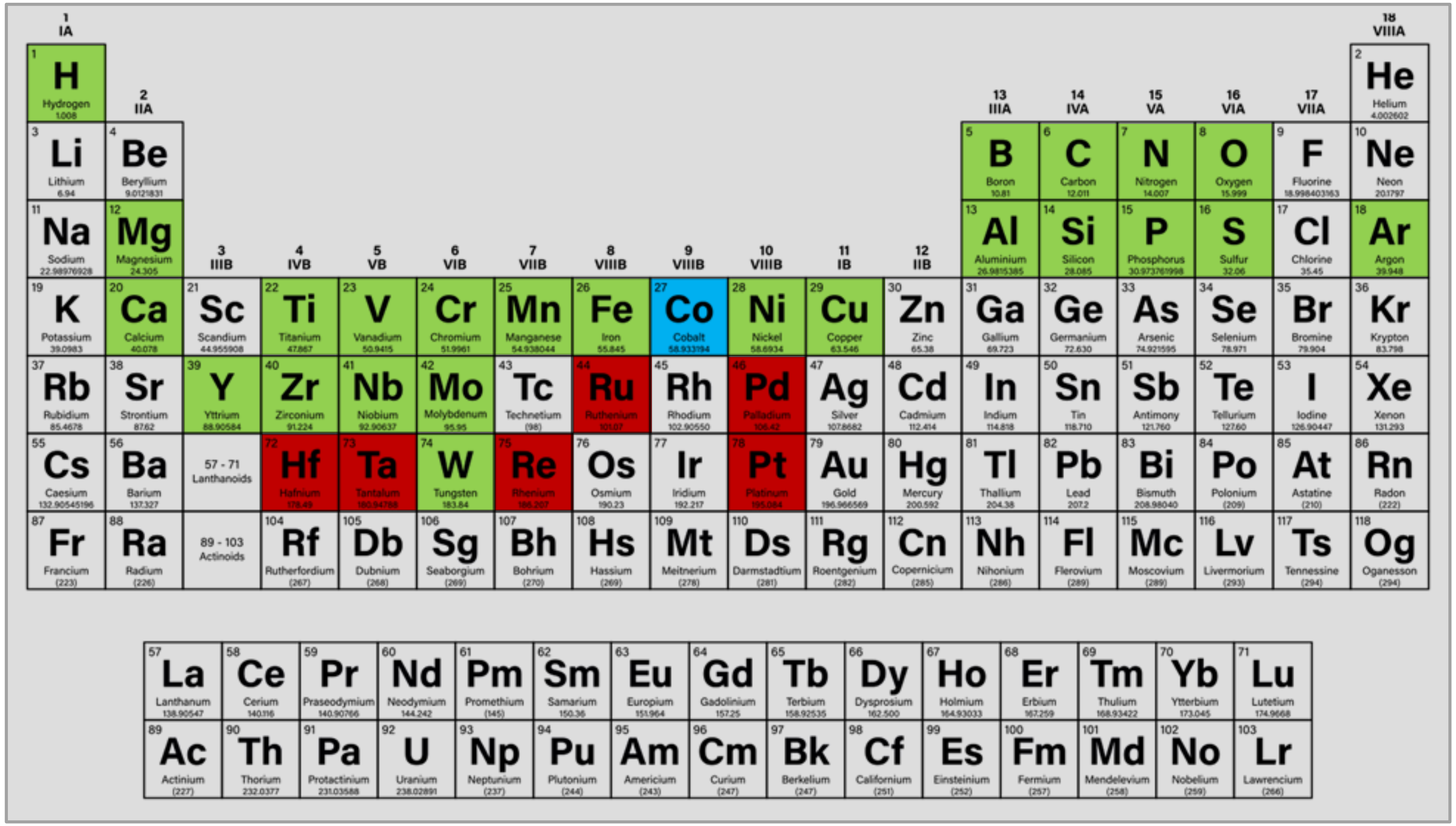


Design space limited by Thermo-Calc TCNI12 database



ThermoCalc TCNI12 databases, accessed via website

Elements more expensive than cobalt removed from consideration

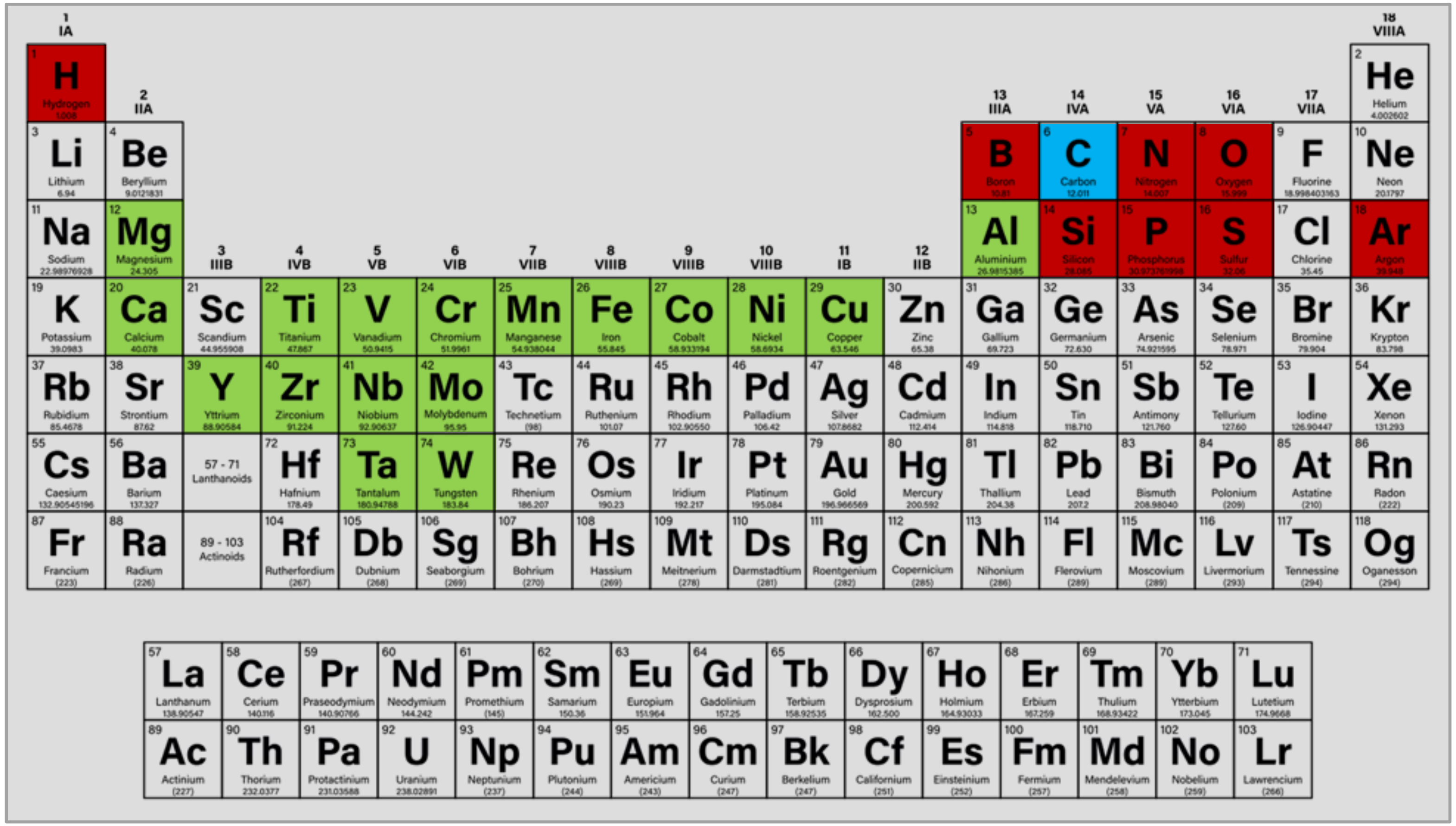


- Pd - \$66,000/kg
- Ru - \$37,500/kg
- Pt - \$27,000/kg
- Hf - \$1,800/kg
- Re - \$1,600/kg
- Ta - \$325/kg
- Co - \$54/kg

Michigan Technological University

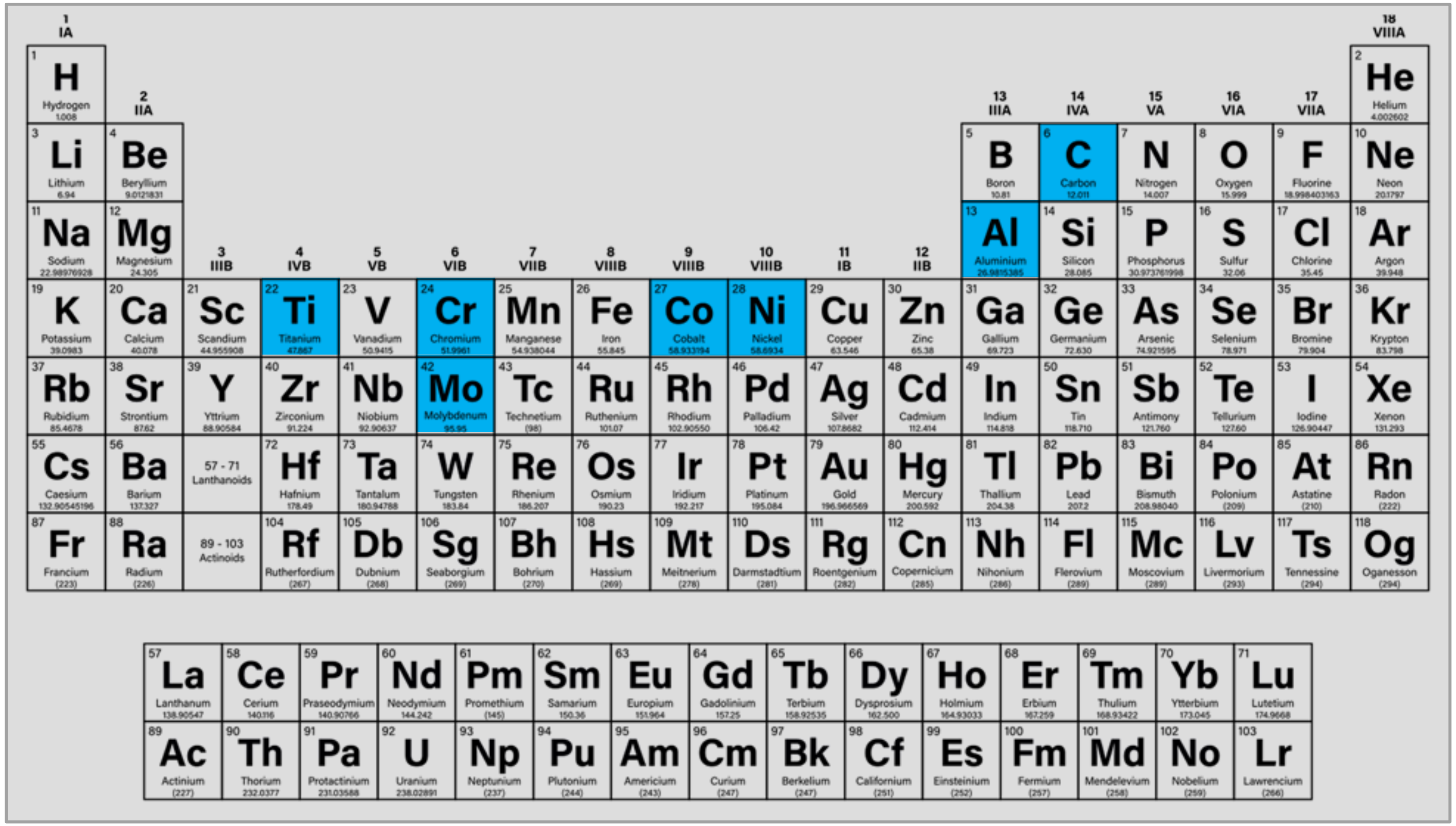
Approximate prices found via 2021 commodity prices throughout the total year (various sources)

Most nonmetals are not optimized, carbon cannot be ignored



- Carbides aid in creep resistance & high temperature strength
- C kept @ 0.06 wt%

Elements selected for experimentation



- Chromium
  - Matrix strength
  - Oxidation resistance
- Cobalt
  - High temperature performance
  - Creep resistance
- Molybdenum
  - Matrix strength
- Aluminum, titanium
  - Precipitates (γ' + η)

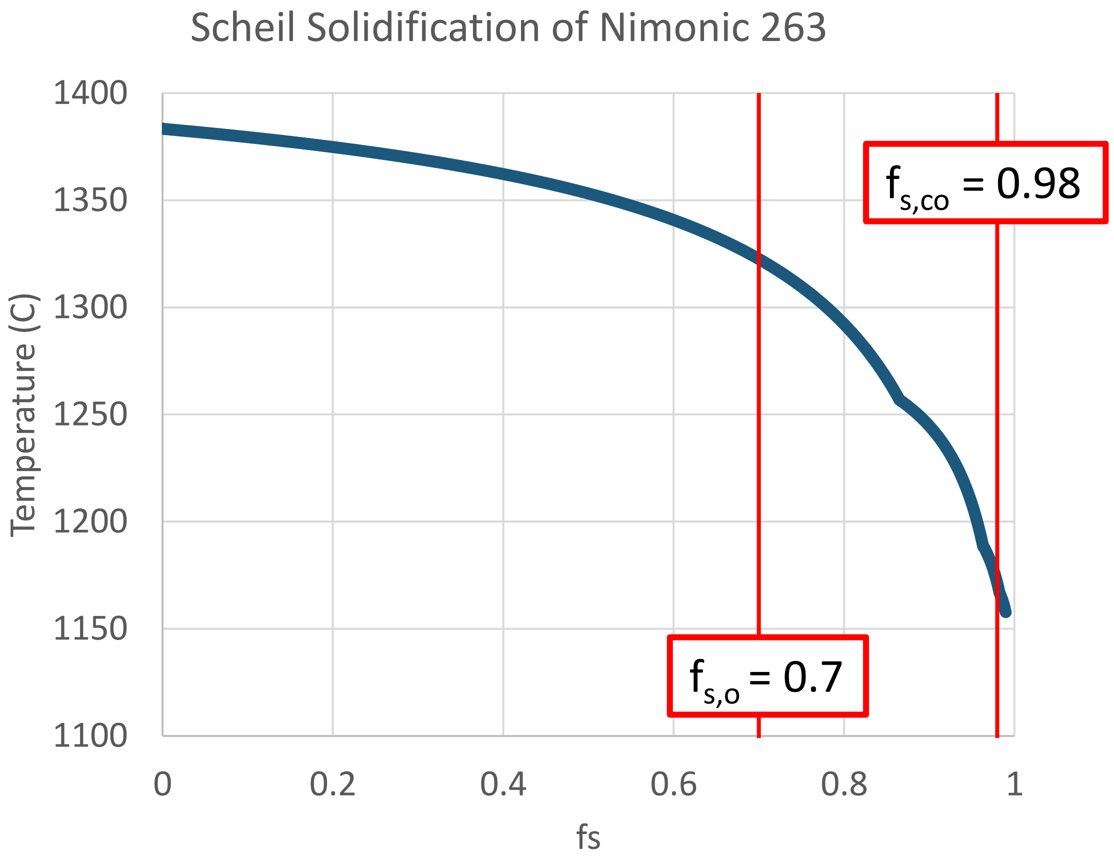
Objectives from project goals:

- Reduce cobalt content to less than 5wt% and minimize overall cost
  1. Alloy cost
- Meet weldability indices as measured by solidification and strain-age cracking resistance
  2. Solidification cracking resistance
  3. Strain age cracking resistance
- Maintain nano-indentation & hot-hardness values within 10% of a comparable superalloy (Nimonic 263)
  4. Material strength
  5. Creep resistance

Solidification cracking resistance assessed with Scheil calculation

- Numerical assessment of "mushy zone" during solidification
- Assess hot tearing conditions
  - T_{co} = coalescence @ $f_{s,o}$ = 0.7
  - T_o = coherency @ $f_{s,co}$ = 0.98
  - $f_s(T)$ = fraction of solid

$$Score_{Easton.Solid} = \int_{To}^{Tco} f_s(T)dT$$



Better performance as compared to Kou solidification model

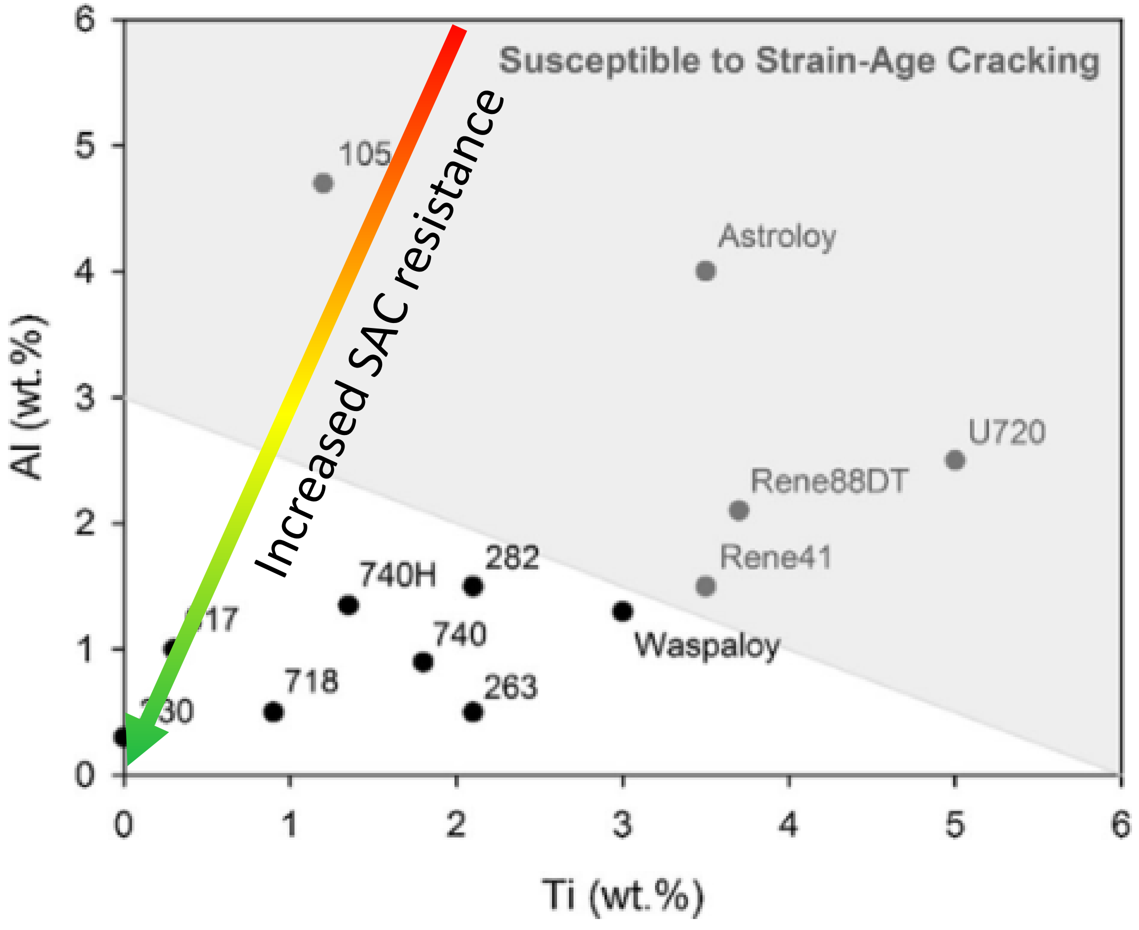
- Consistent extreme outliers from Kou calculations
- Easton scores more reliable

$$Score_{Kou.Solid} = max\left(\left|dT/d(f_s)^{1/2}\right|\right)$$

$$Score_{Easton.Solid} = \int_{To}^{Tco} f_s(T)dT$$

Strain-age cracking (SAC) traditionally measured as function of γ’ formers

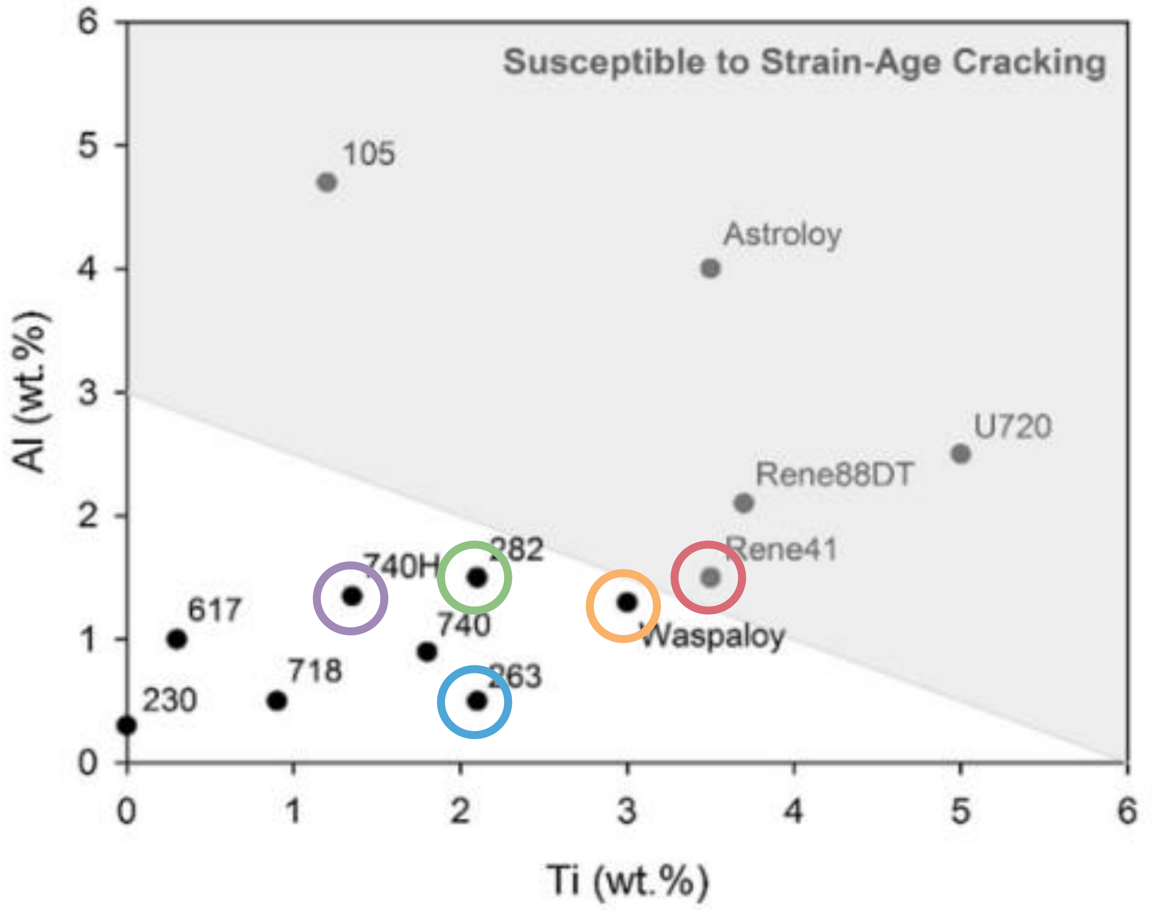
- Alloys with higher Al and Ti more susceptible to SAC (gray)
- Reduce γ’ volume fraction = less strength & more cracking resistance

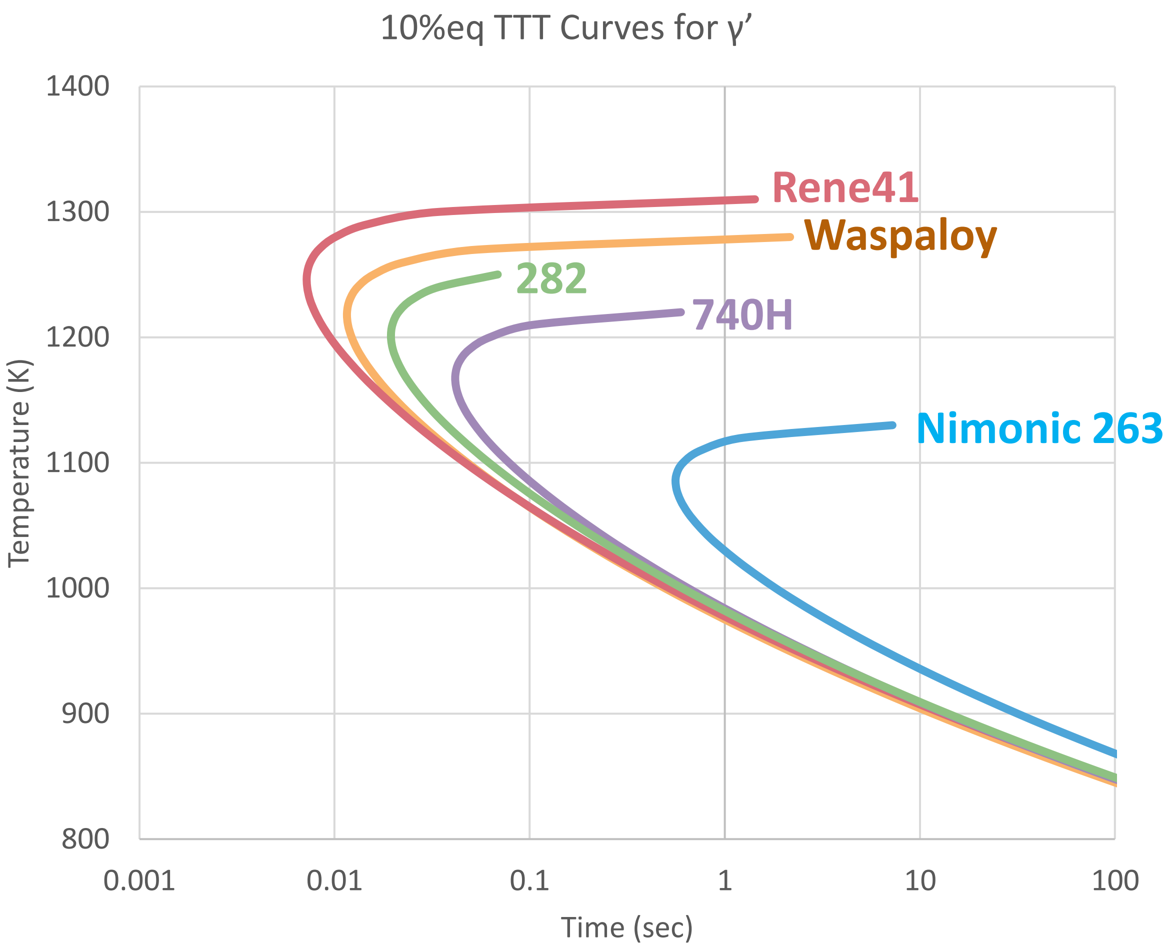


$$Merit_{SAC} = [Al] + [Ti] + [Nb] + [Ta]$$

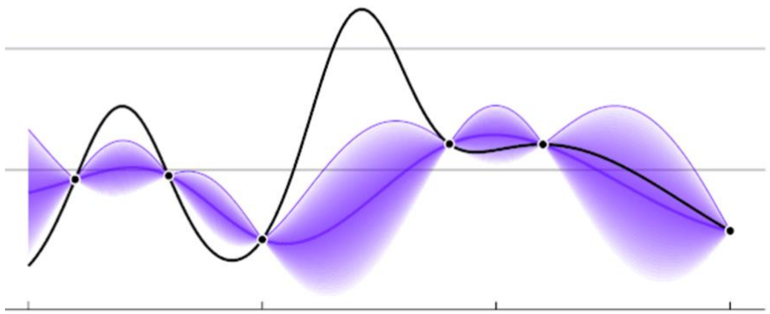
Compositions in at%

Strain-age cracking resistance correlates with slower γ’ kinetics

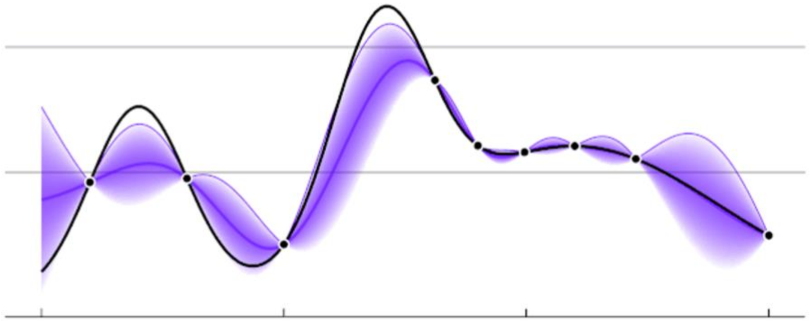




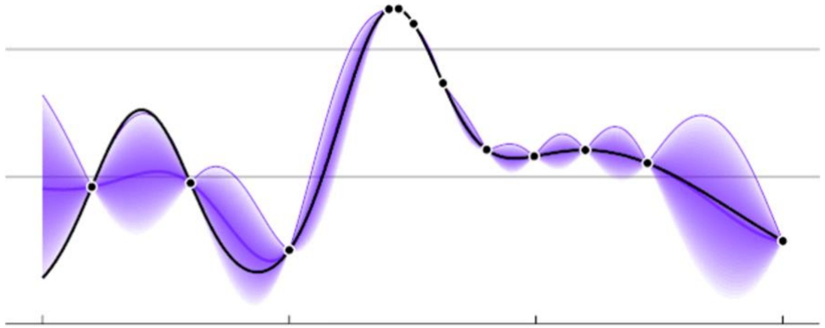
Utilize Bayesian Optimization to efficiently optimize utility functions



Initial BO does not find maxima



More calculations (dots) reduce uncertainty



Efficiently locate maxima

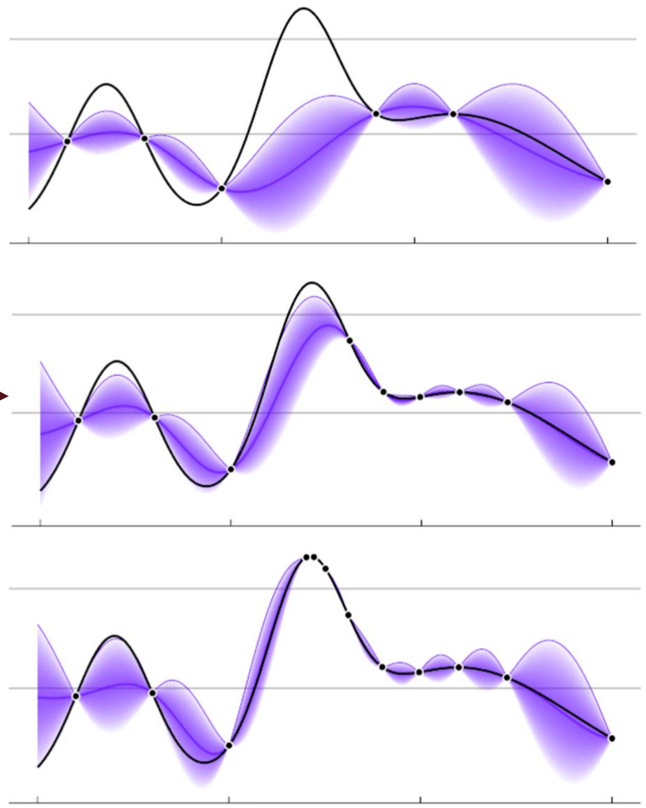
Explore high variance regions
Exploit high reward regions

Images taken from gif at: https://en.wikipedia.org/wiki/Bayesian_optimization

Bayesian Optimization can only be used for single target optimization

- Cost
- Solidification Cracking
- Strain-Age Cracking
- Yield Strength
- Creep

→ **Multi-Objective Score** →



Modified achievement function enables Multi-Objective Bayesian Optimization (MOBO)

$$Score_{MOBO}(y_m) = \sum_{m=1}^{M} y_m w_m 0.05 + \min_{m=1...M}[(y_m - g_m)w_m]$$

Normalization Term

Objectives

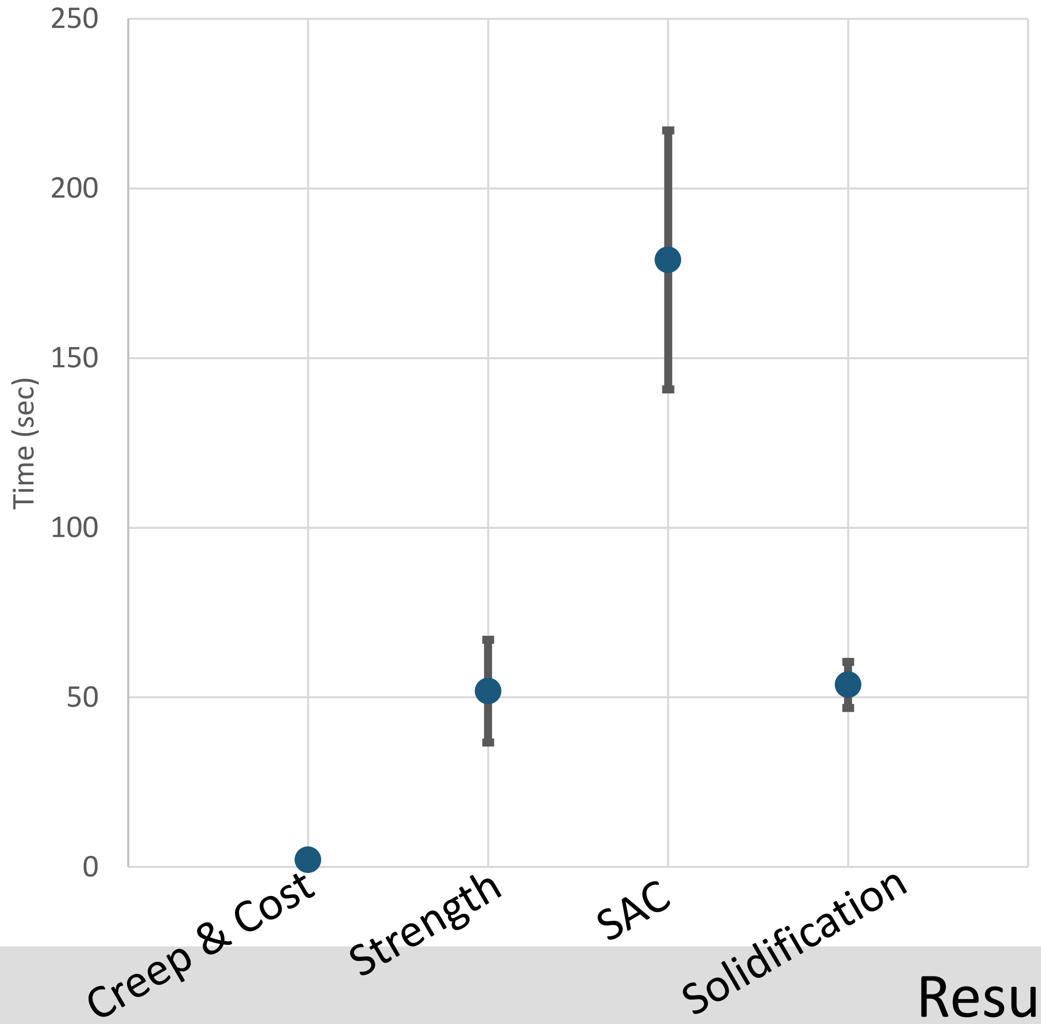
Parameter Goal

w_m: scaling/normalization term calculated from the inverse of the parameter range

Can calculate the normalized difference between parameters and pre-determined goal values and use these differences to optimize each parameter

Script can rapidly assess compositions' material properties

- Experiment has assessed 4000+ unique compositions
  - Approximately 1 month of computational time
  - Current script can run a composition every 5 minutes
- Timing limited by Python + CALPHAD



Error bars represent 95% CI

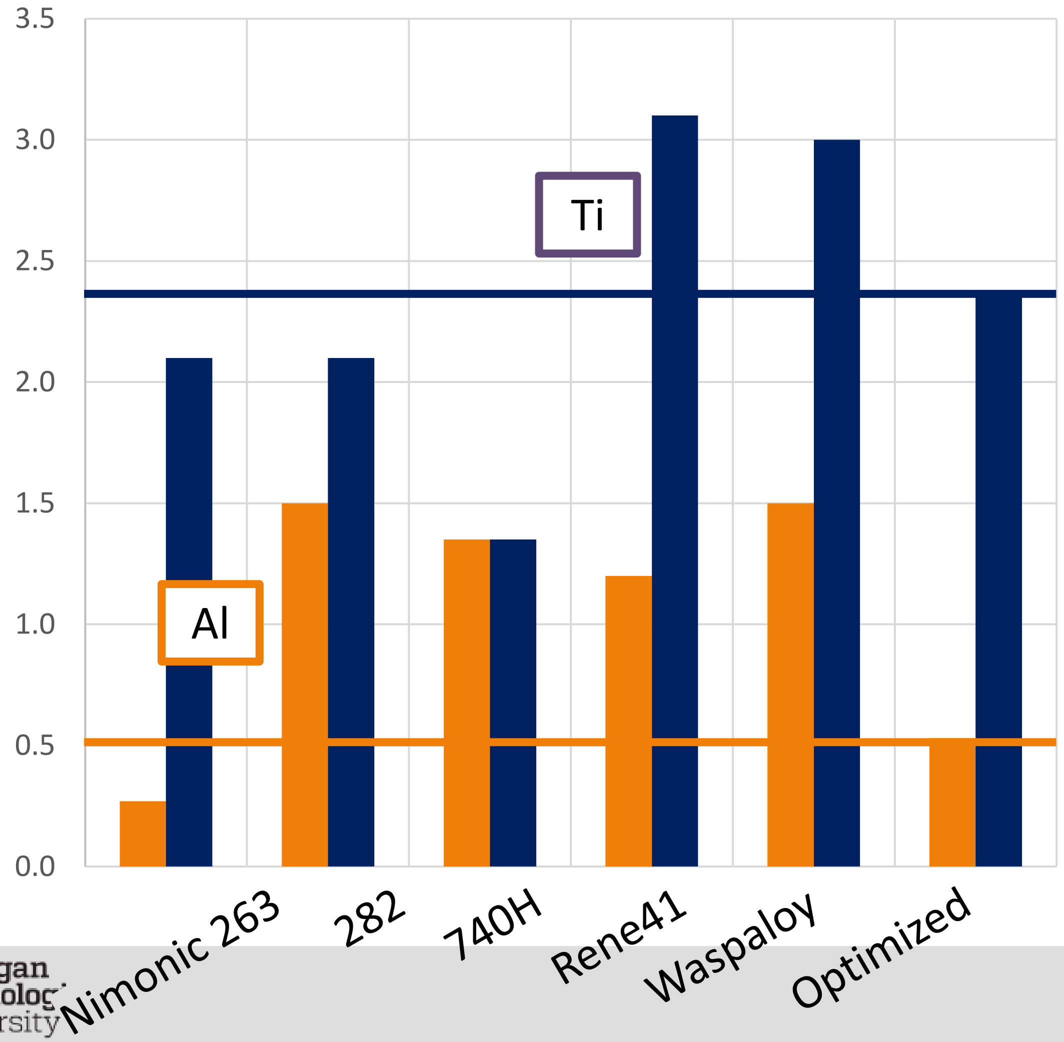
Best compositions from optimizations

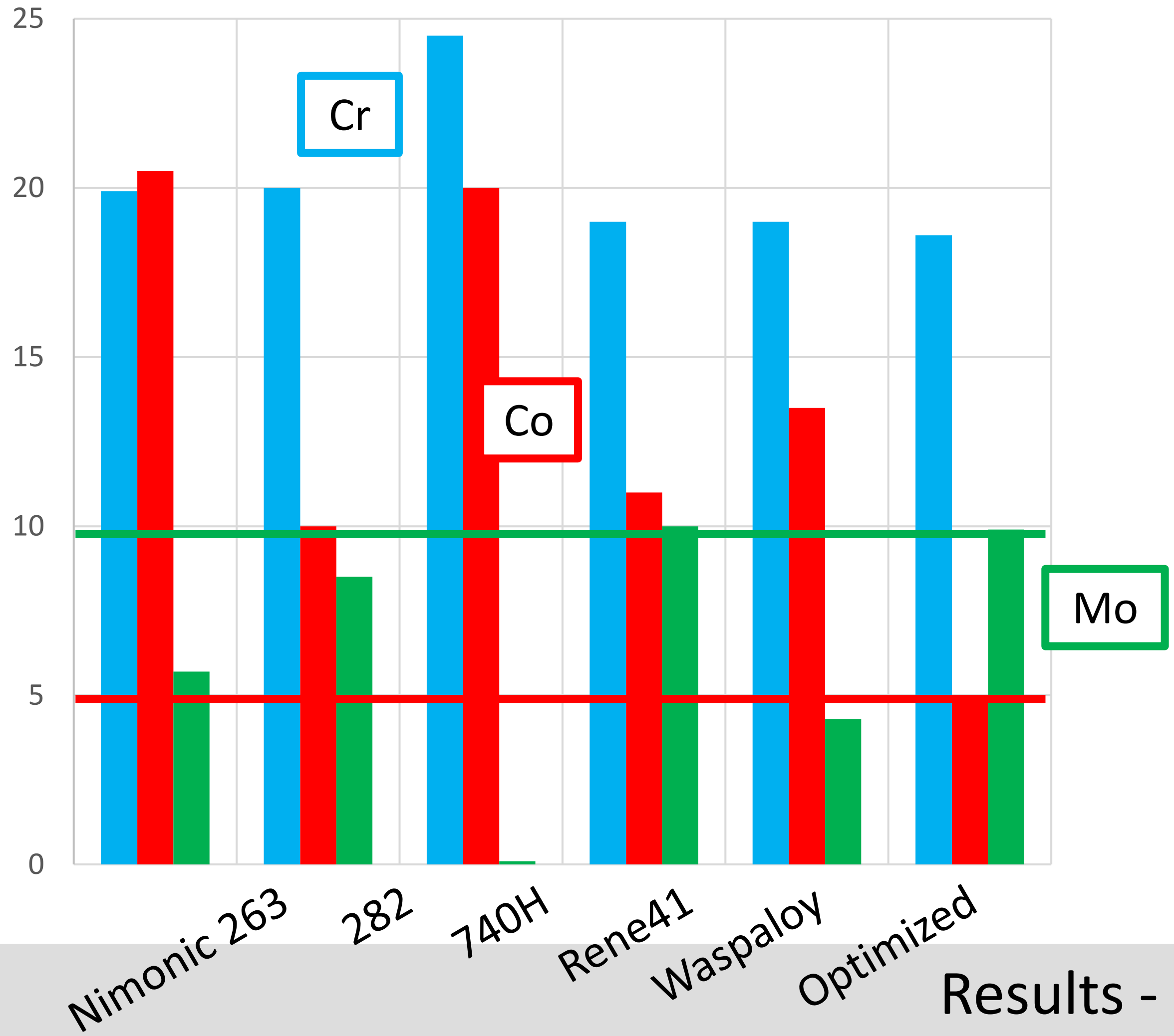
Top ranking alloys from 5wt% Co trials

Rank	Co	Cr	Mo	Al	Ti	C	Ni
1	5.0	21.9	8.4	0.53	2.08	0.06	62.0
2	5.0	18.6	9.9	0.53	2.38	0.06	63.5
3	5.0	19.6	7.0	0.54	2.38	0.06	65.4
4	5.0	18.1	9.5	0.54	2.20	0.06	64.6
Nimonic 263	20.5	19.9	5.7	0.27	2.1	0.07	Bal.

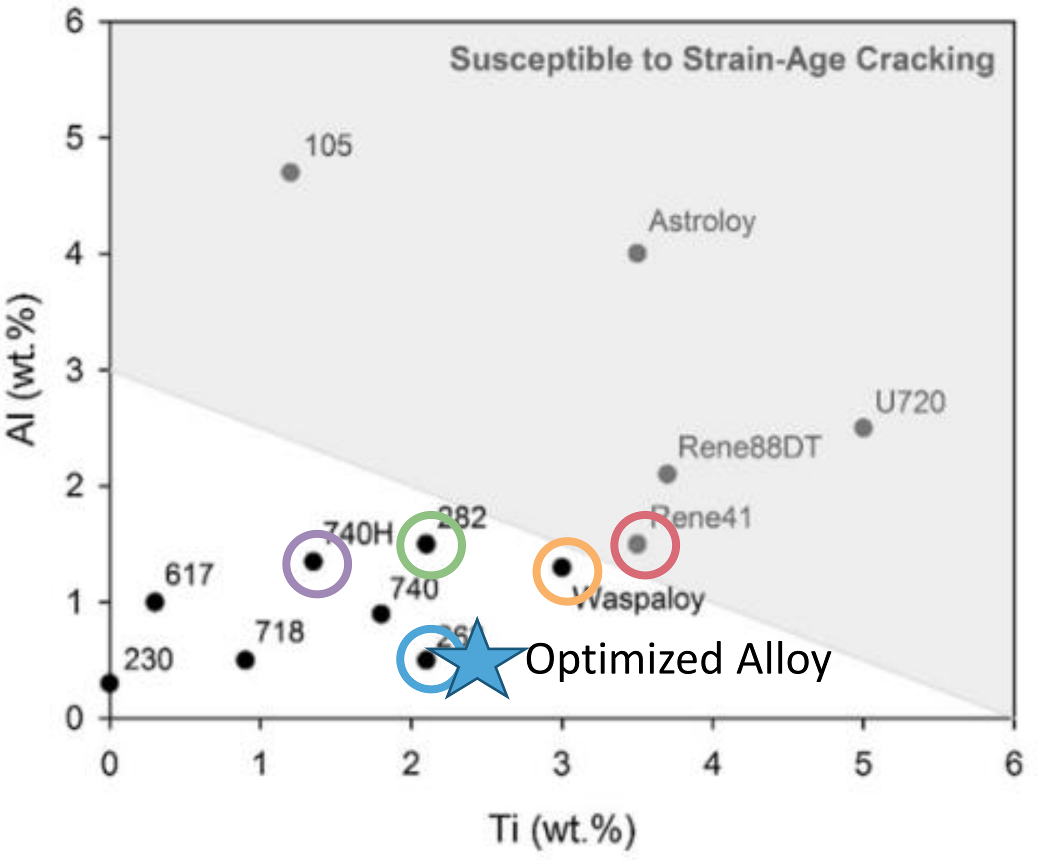
Compositions shown generated with Superalloy MOBO script version 6 (Sv6)

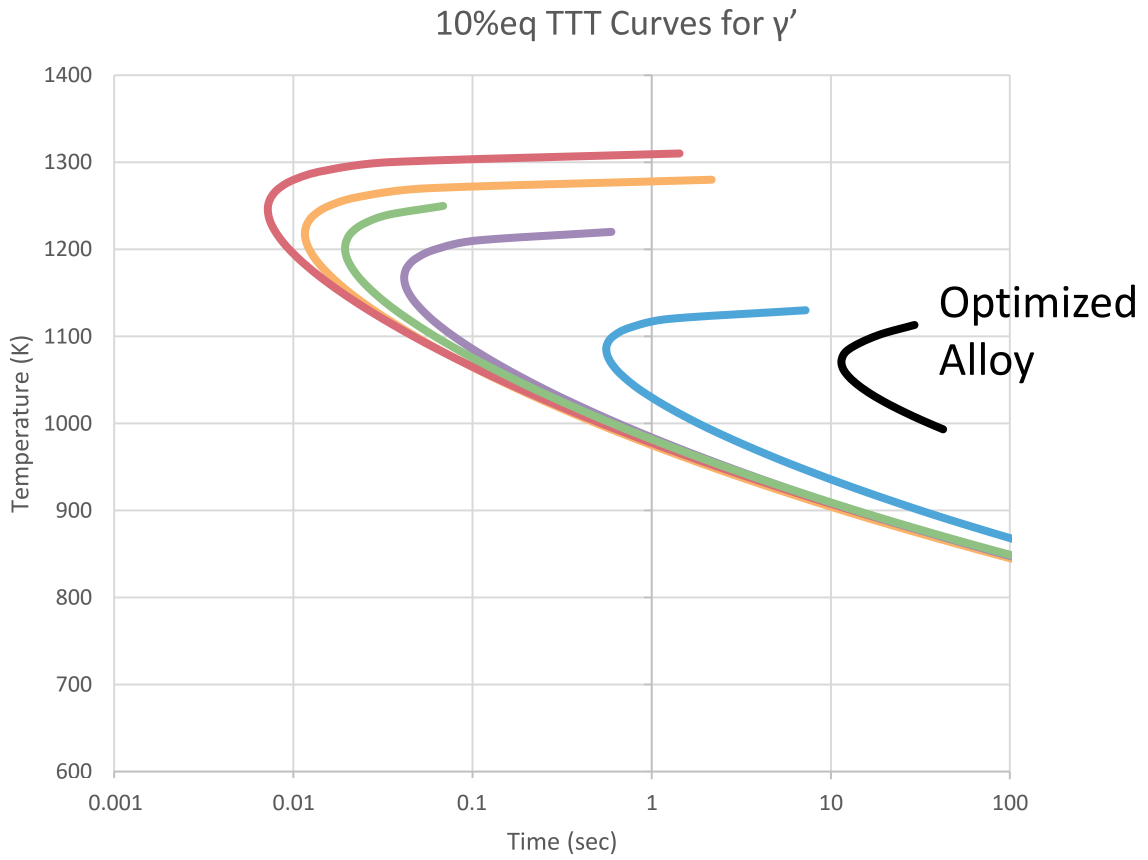
Optimized composition most alike Nimonic 263 with much lower Co content



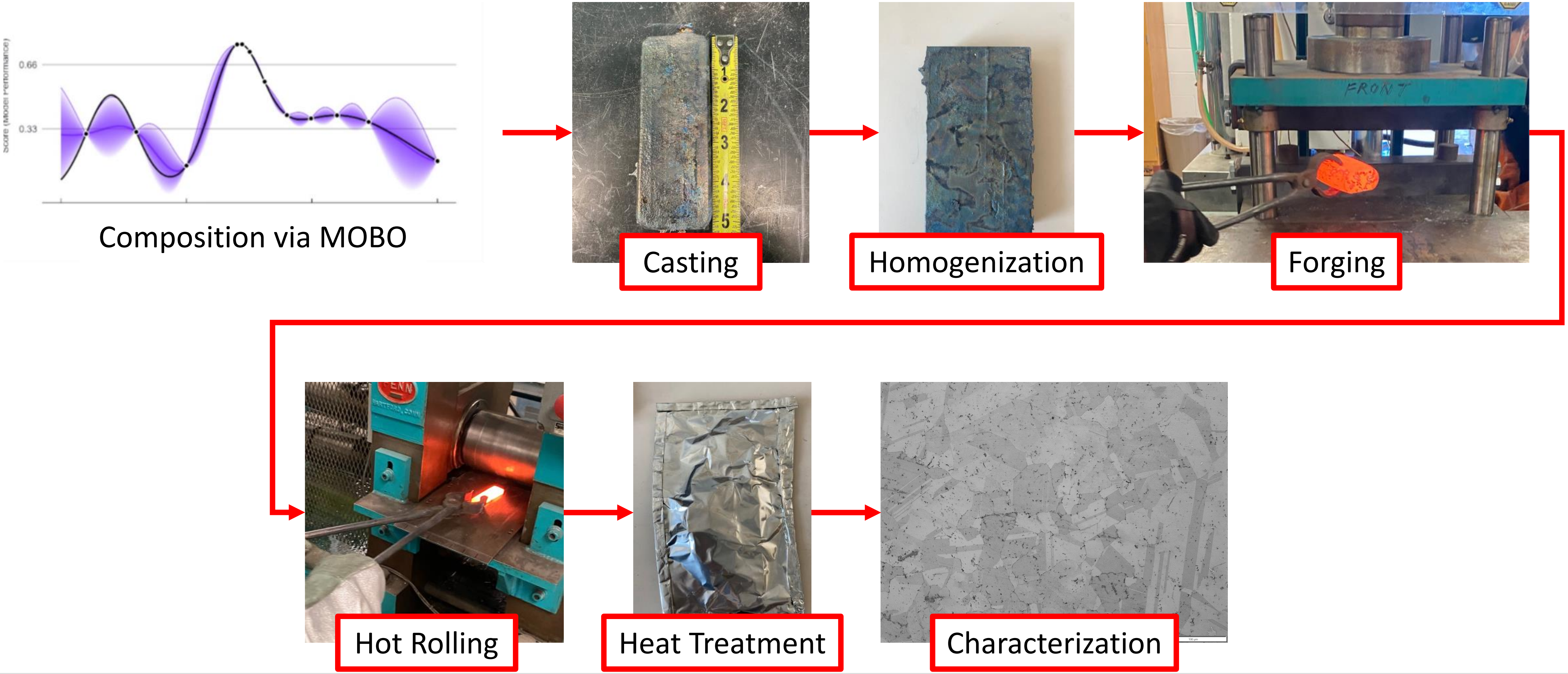


Optimized alloy predicted slower precipitation kinetics other alloys



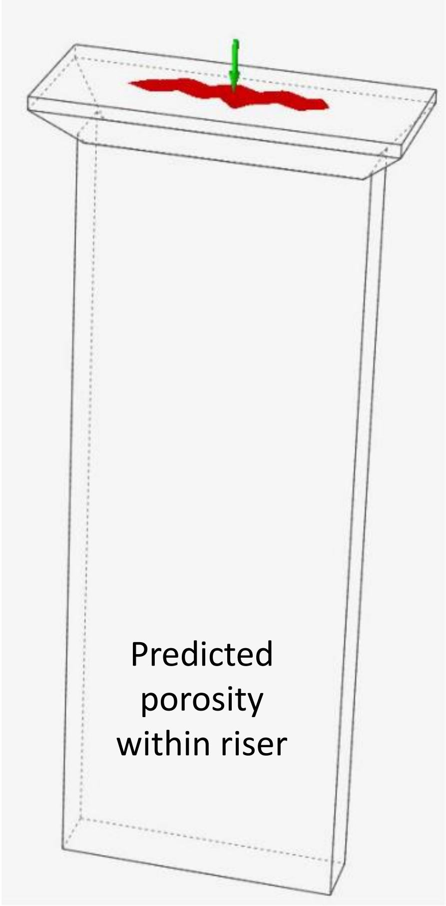


Processing outline

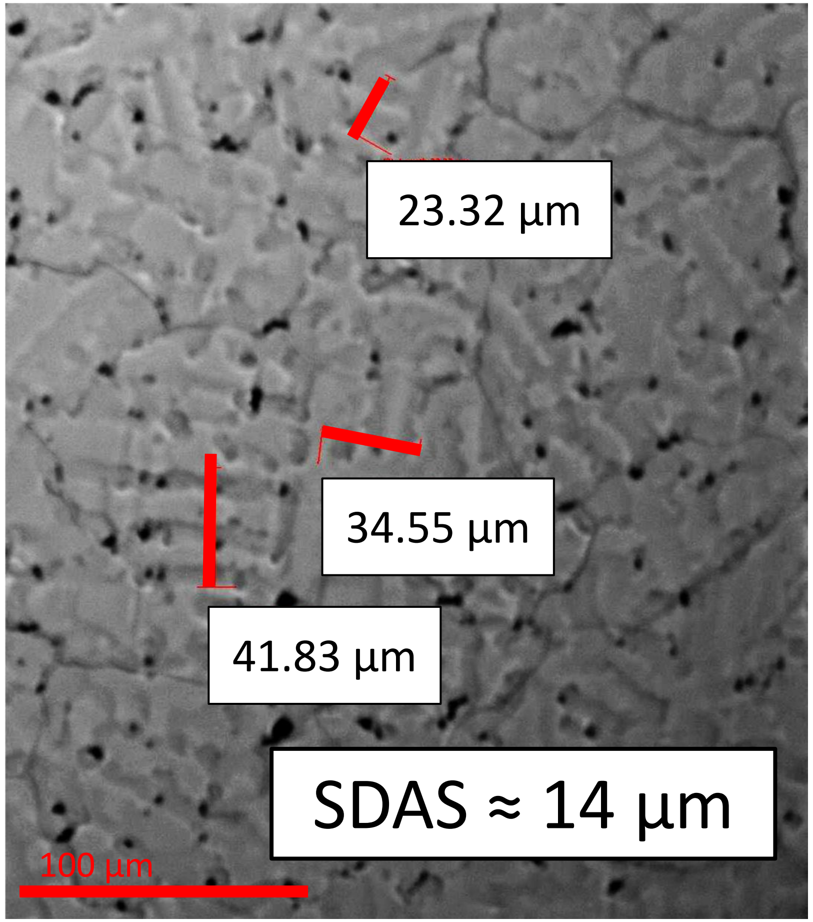


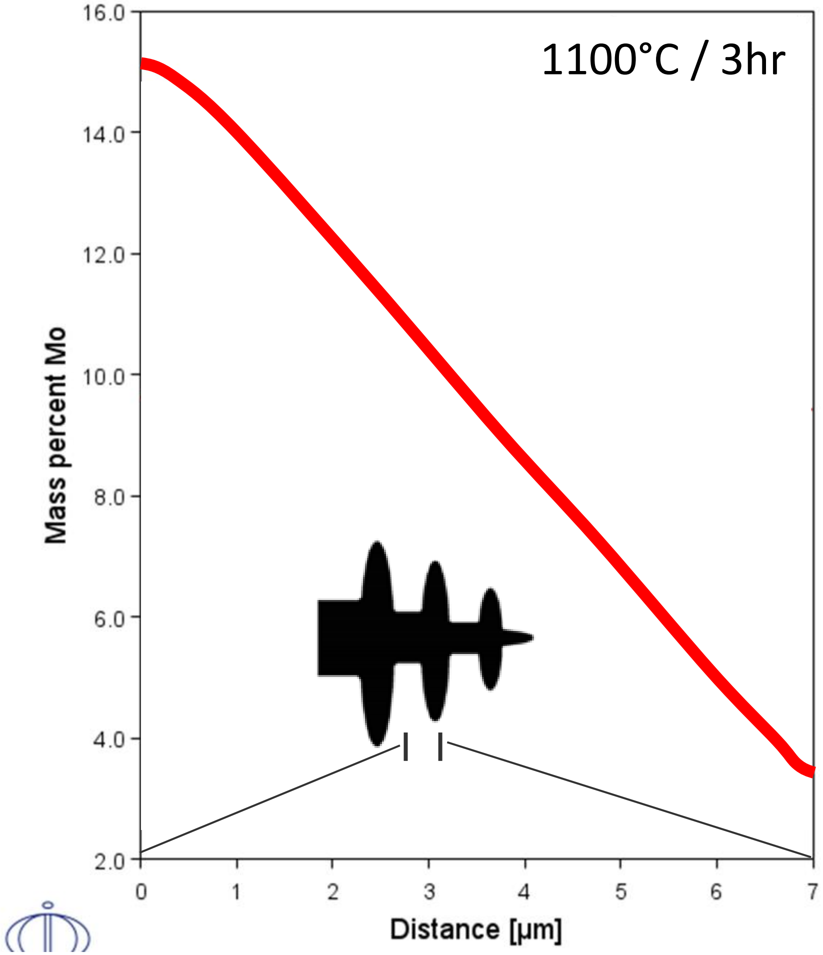
Vacuum Induction Melting (VIM) used for small-scale casting for model validation

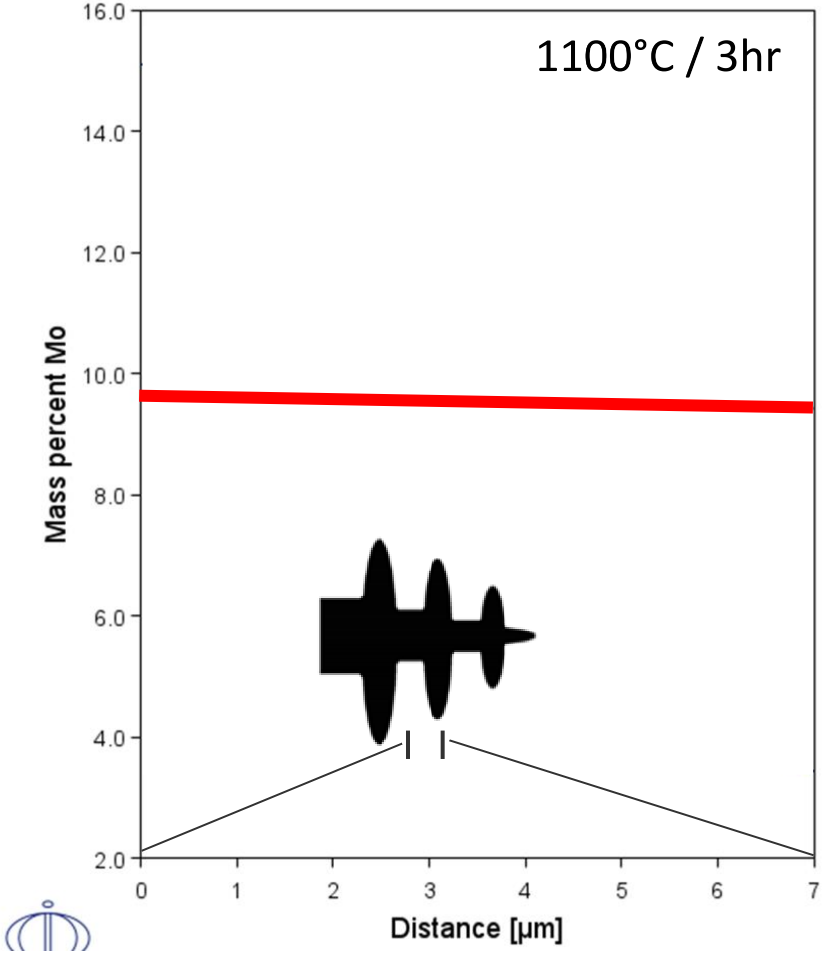
- 744g rectangular sample
- Minimal shrinkage & porosity as seen with Inspire Cast
- OES validation



Mo found to be slowest diffusing element, used to simulate homogenization process

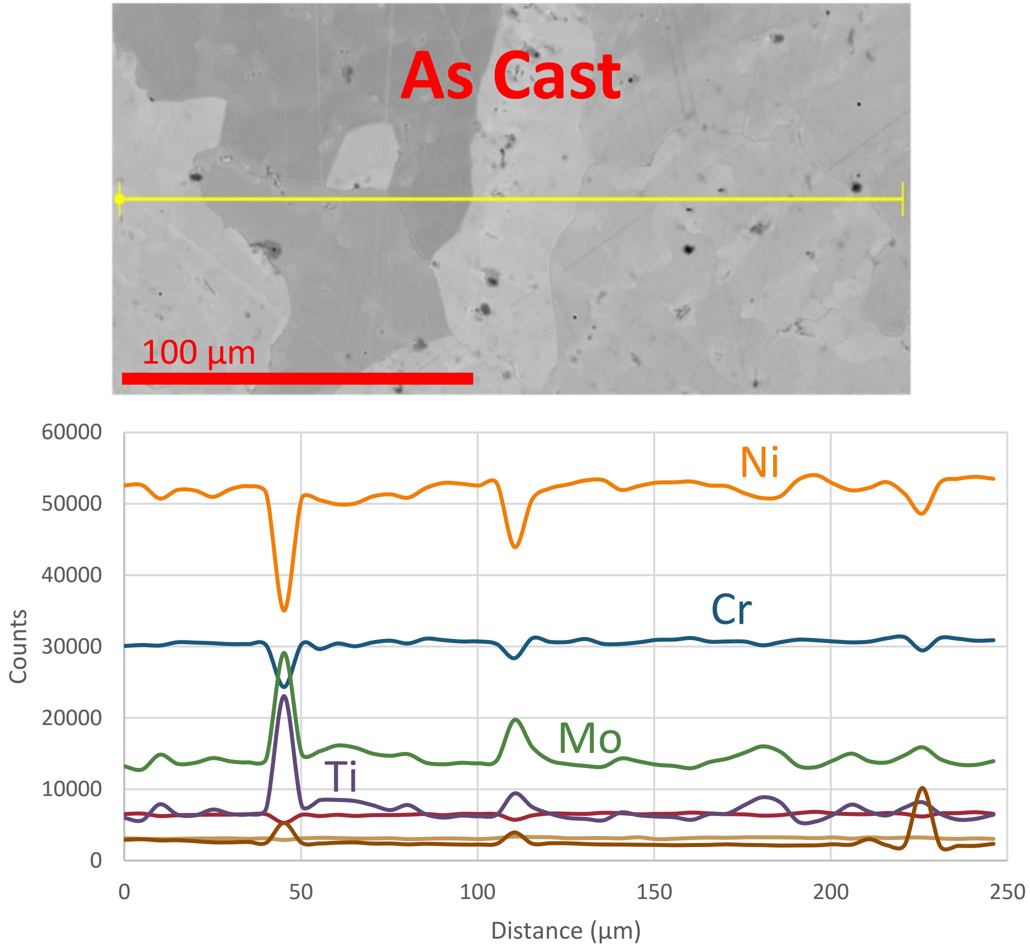


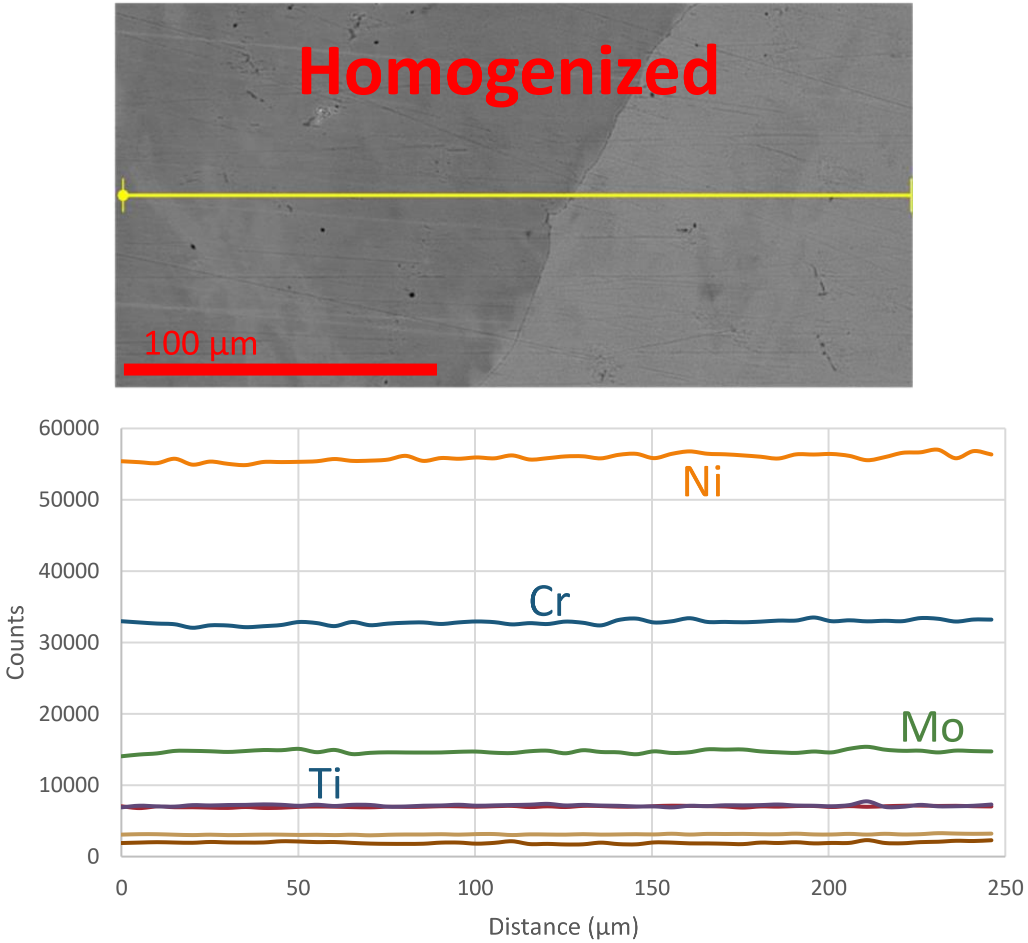




Sample image was etched with a 1:3 ratio of HNO_3:HCl

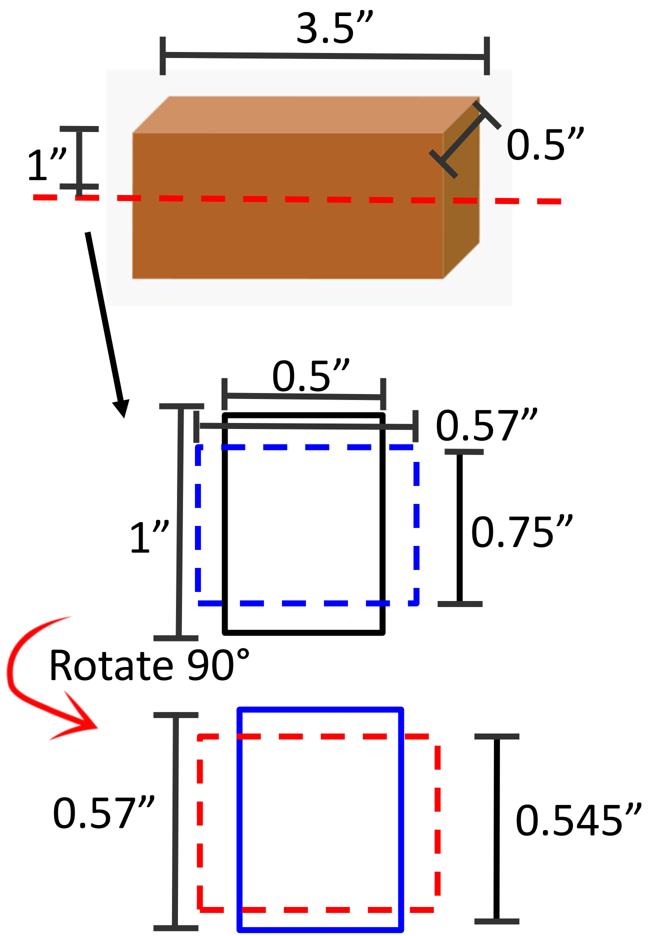
Successful homogenization performed for cast samples (1100°C / 3hr)

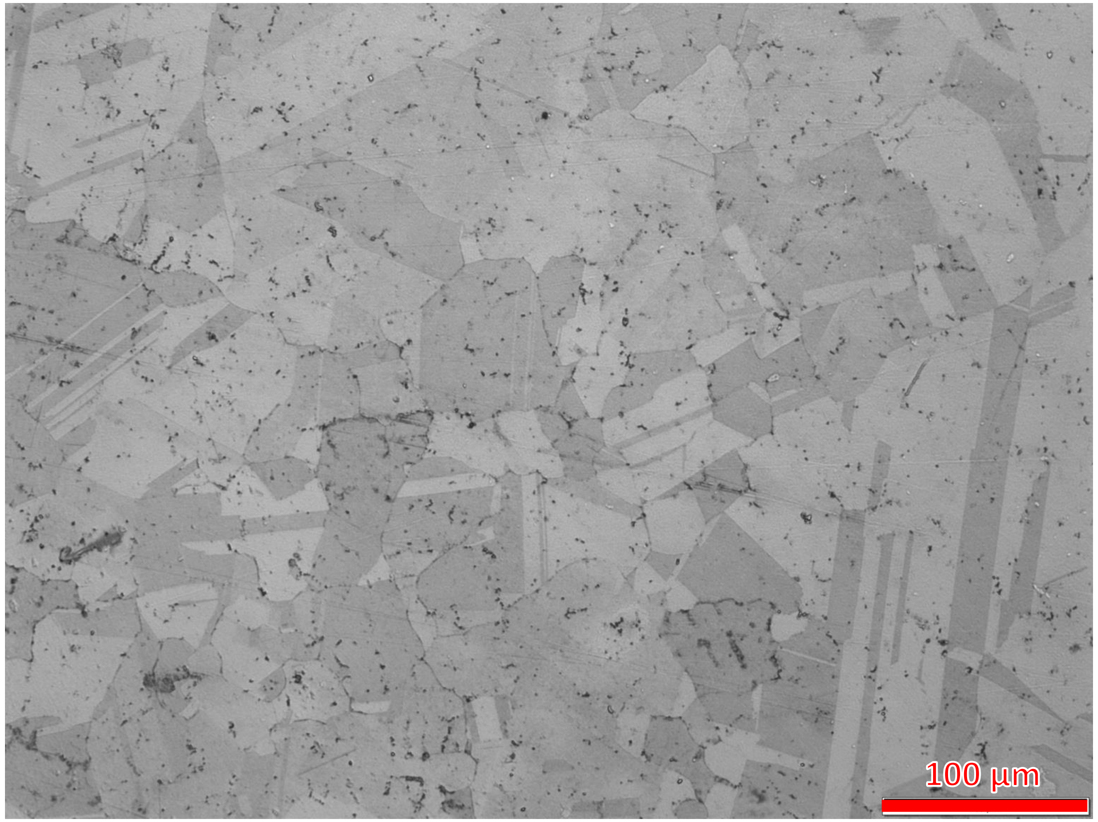




ESEM Settings: BSE, x500, 20kV, Spot Size 7
Continuous line scan

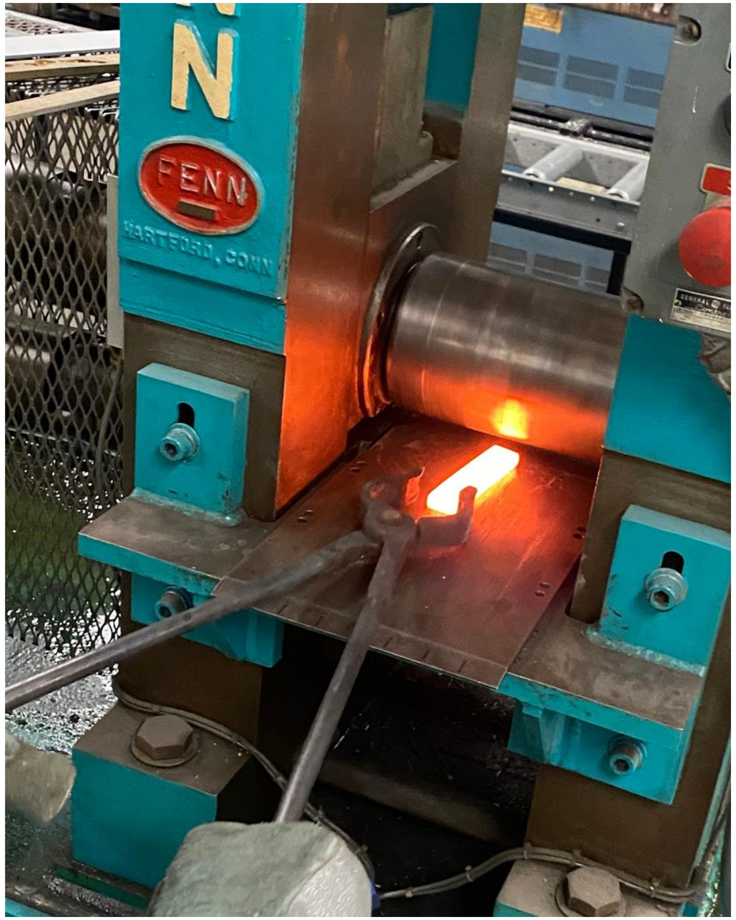
Upset forging done at 1100°C to achieve desired small grain structure

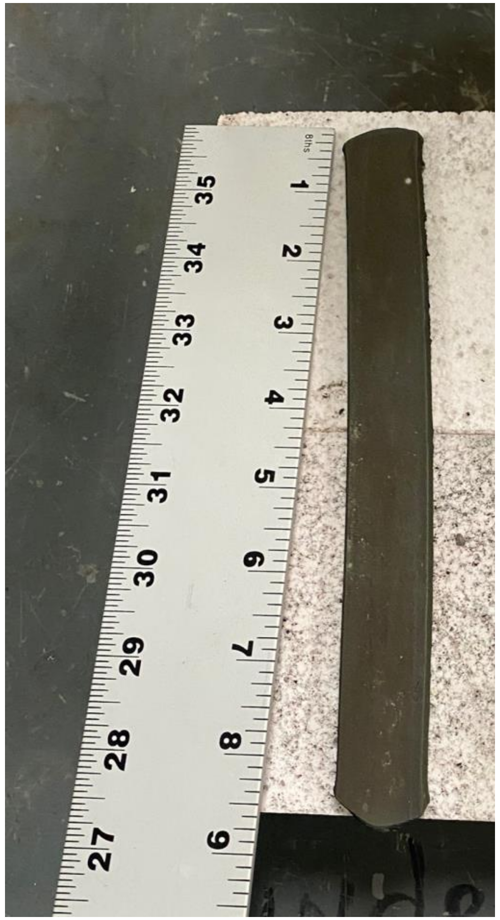


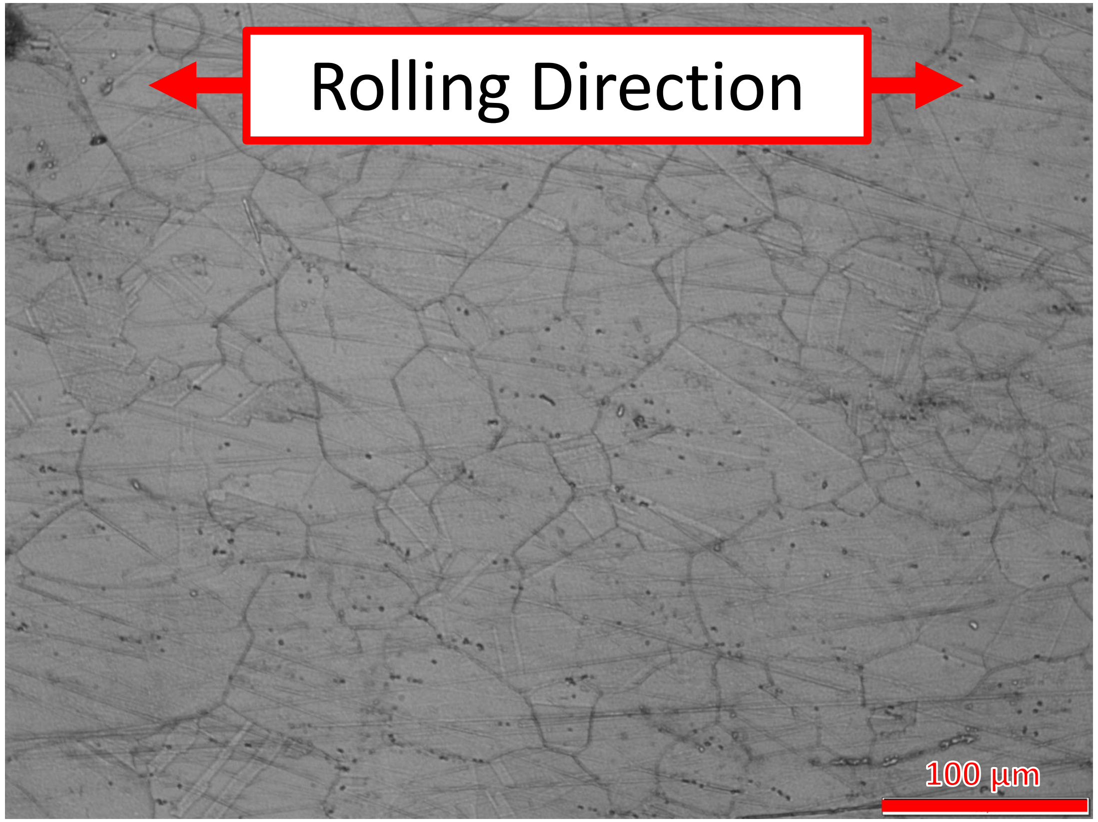


Etched with a 1:3 ratio of HNO3: HCl

Sample hot rolled at 1125°C in 9-10 passes to same thickness of 0.189" with ~60% reduction

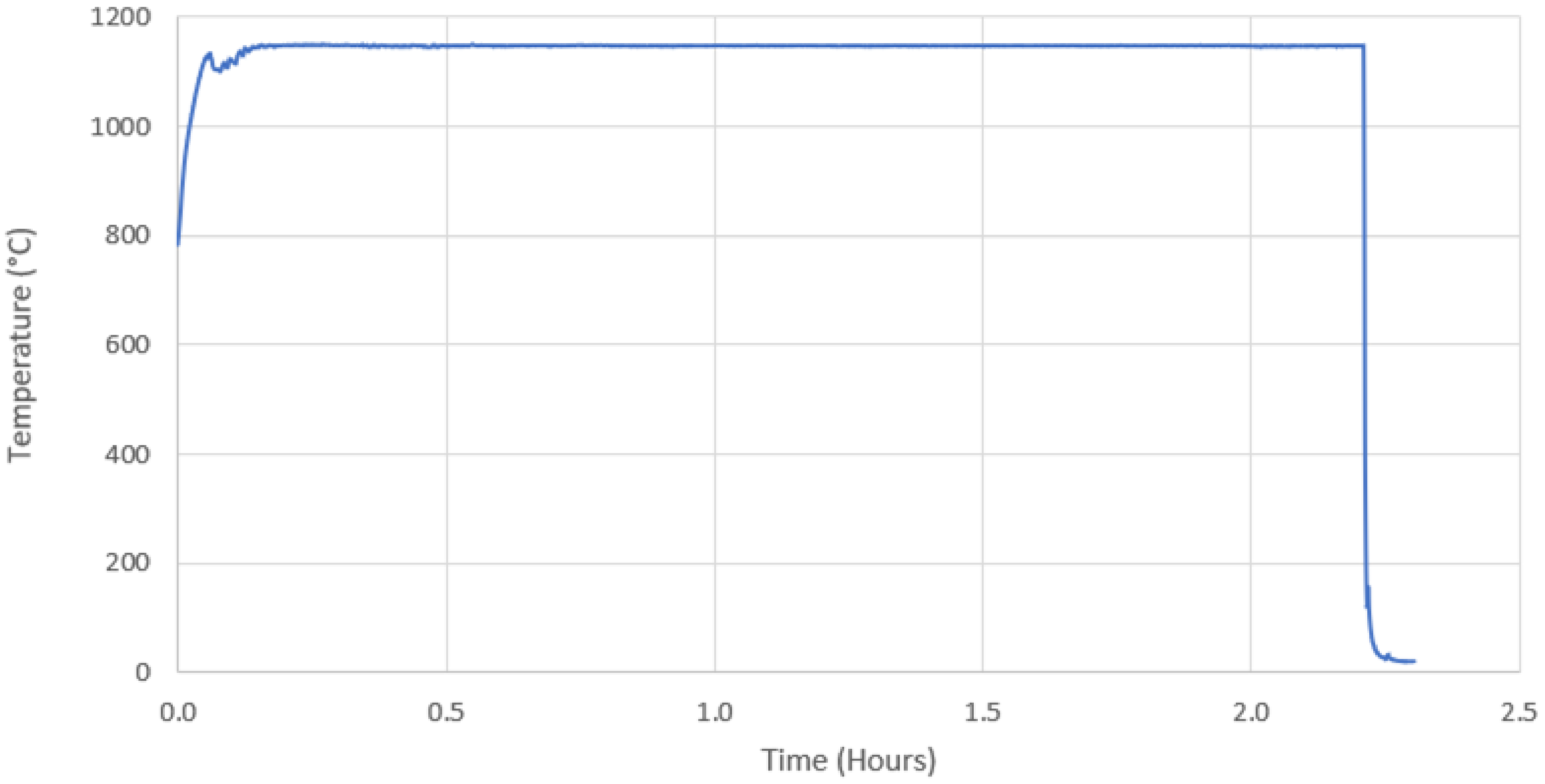




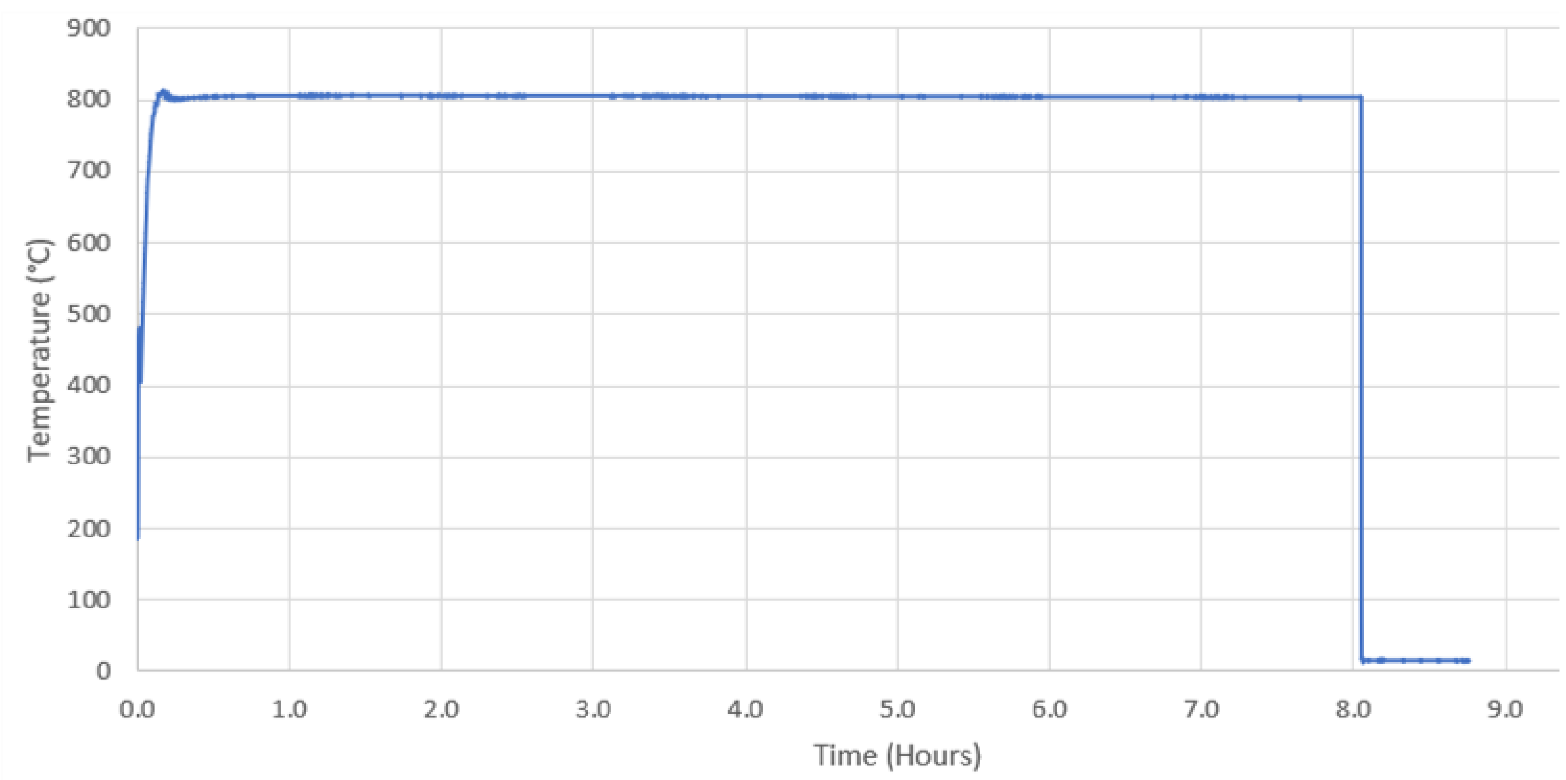


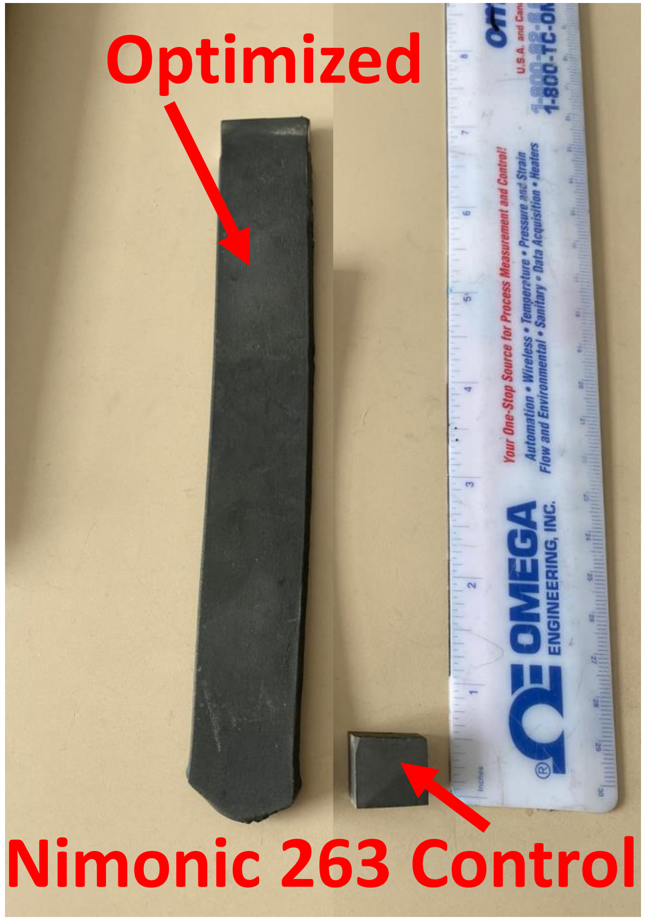
Etched with a 1:3 ratio of HNO3: HCl

Solutionization for 1150°C for 2 hours (based off Nimonic 263)

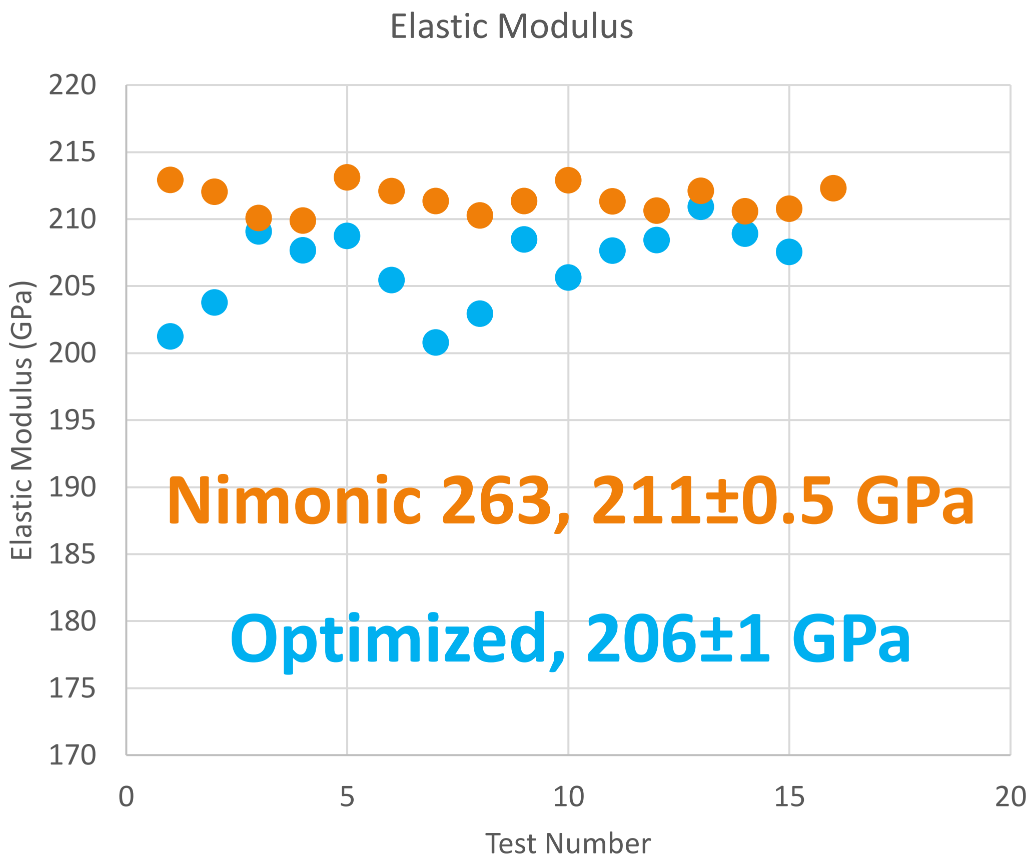


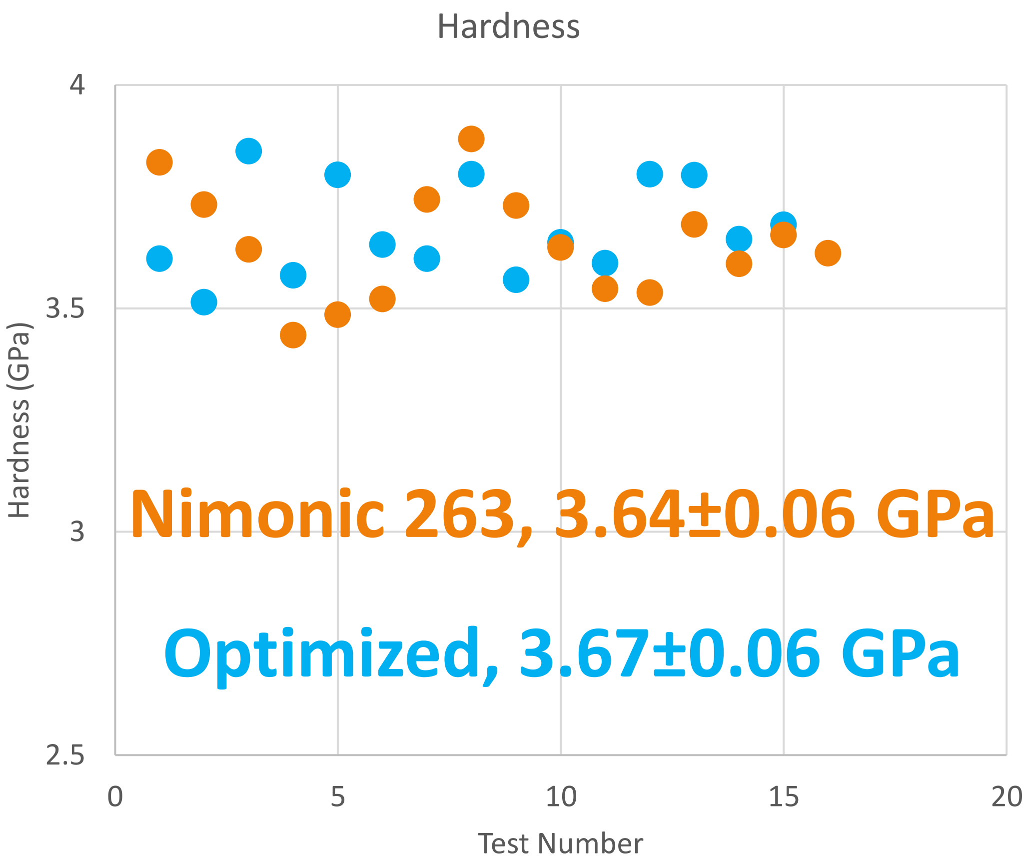
Aging heat treatment at 800°C for 8 hours (based off Nimonic 263)





Optimized alloy meets >10% difference as measured via nanoindentation

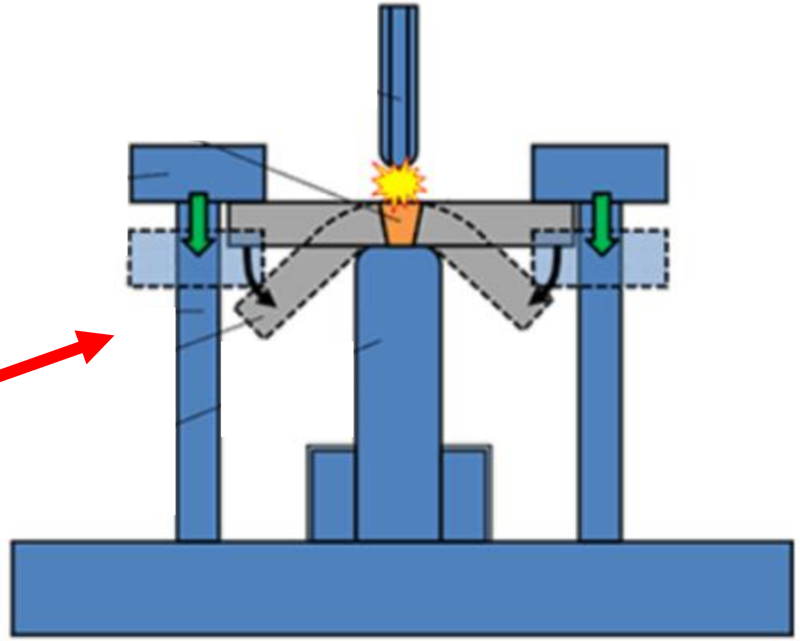




Elastic Modulus measured at a depth of 300nm
Hardness measured at a depth of 1800nm

Next steps/planned characterization:

1. High magnification SEM to confirm precipitate sizes
2. X-Ray Diffraction to confirm volume fractions
3. Hot Hardness mechanical testing
4. Weldability testing via Trans Varestraint test jig
5. Gleeble testing at EPRI



Conclusions

1. Easton model was found to be more computationally reliable
2. Insight to use γ’ kinetics to predict SAC susceptibility
3. Implementation of MOBO to simultaneously optimize several design parameters
4. Experimental casting, processing, characterization performed in-house at Michigan Technological University

Thank you for your time
Questions?

Contact us:
Tanner Olson: tannero@mtu.edu
Dr. Paul Sanders: sanders@mtu.edu
Dr. John Shingledecker: jshingledecker@epri.com