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

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#### 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





Augusto Di Gianfrancesco - Materials for Ultra-Supercritical and Advanced Ultra-Supercritical Power Plants

## 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  $\eta$  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 strainage cracking resistance
- 3. Maintain material properties within 10% nano-indentation and hothardness values of a comparable superalloy (Nimonic 263)





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### Design space limited by Thermo-Calc TCNI12 database

1 H Hydrogen 1008	2 IIA											13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	<sup>18</sup> VIIIA <sup>2</sup> Helium 4.002602
<sup>3</sup> Li Lithium	Beryllium											5 Boron	6 C Carbon	7 Nitrogen	8 Oxygen	P Fluorine	Neon
11 Na Sodium 22.98976928	12 Mg Magnesium 24.305	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIIIB	9 VIIIB	10 VIIIB	11 IB	12 IIB	13 Al Aluminium 26.9815385	14 Si Silicon 28.065	15 P Phosphorus 30.973767998	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Argon 39.948
19 R Potassium	Calcium 40078	Scandium	22 <b>Ti</b> Titanium 47,867	23 Vanadium 50.9415	Chromium 51.9961	25 Mn Manganese 54,938044	Fe Iron	27 Cobalt 58,933794	28 Nickel 58.6934	29 Cu Copper 63.546	<sup>30</sup> <b>Zn</b> Zinc 65.38	Gallium 69,723	Germanium 72.630	33 Ass Arsenic 74,921595	Selenium	Bromine	Krypton 83,798
Bubidium	38 Strontium	39 Yttrium	<sup>40</sup> Zr <sub>Zirconium</sub>	41 Niobium	42 Molybdenum	TC Technetium	Ruthenium	Rhodium	Palladium	47 Ag Silver	48 Cadmium	49 In Indium	<sup>50</sup> Sn	Sb Antimony	Tellurium	53	54 Xenon
55 Caesium	56 Ba Barium	57 - 71 Lanthanoids	72 Hafnium	92.90637 73 Tantalum	74 Tungsten	75 <b>Re</b> Rhenium	76 OS Osmium	77 Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Thallium	82 Pb Lead	83 Bi Bismuth	84 Polonium	Astatine	Be Badon (312)
87 Francium (223)	88 Radium (226)	89 - 103 Actinoids	104 Ref Rutherfordium	105 Dubnium (268)	106 Sg Seaborgium (209)	107 Bh Bohrium (270)	108 Hassium (209)	109 Mt Meitnerium (278)	110 Darmstadtium (281)	Boentgenium (282)	Copernicium (285)	113 Nhonium (286)	114 Flerovium (289)	115 Mc Moscovium (289)	Livermorium (293)	117 TS Tennessine (294)	118 Oganesson (294)
	57 L Lanti 138.1 89 Acti (2	.a 58 Sanum 20047 14 14 14 14 14 14 14 14 14 14	59 Praseoc 140.9 Th 91 Priver 140.9 Priver 140.9 Protec 231.0	Pr 800 Symium Neody 144 2000 200	d <sup>61</sup> Prom. <sup>242</sup> <sup>93</sup> J N <sup>100</sup> <sup>100</sup> <sup>100</sup> <sup>100</sup> <sup>100</sup> <sup>100</sup> <sup>100</sup>	m Sam sthium 99 punium 99 Punium 27)	63 Eurium 236 PU 440 840	Eu 64 cpium Gadu 196 m 26 196 Cu Cu Cu Cu	id Jinium Tert 158. 97 98 Berk Berk (2	bium bium 22535 Bk celium 477	by Holts Posium Holts Stoo 99 Cf Einst. (2)	100 100 100 100 100 100 100 100	Er <sup>69</sup> Th Th Th Th Th Th Th Th Th Th	ијшт 193422 102 102 102 102 Nob (2)	10 10 10 10 10 10 10 10 10 10	.U tium 9668 .r	



Design Space - 9

### 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

Design Space - 10

## Most nonmetals are not optimized, carbon cannot be ignored

1 H Hydrogen 2 Lithium 6.64 11 Na Sodium 22.9997029	2 IIA 4 Beyflum sotztast 12 Magnesium sz.305	3 111B	4 IVB	5 VB	6 7 VIB VII	B VII	9 18 VIII	в 10 в VIIIВ	11 18	12 118	13 IIIA Bacon total 13 Aluminium 20.9875385	14 IVA 6 C Carbon 12011	15 VA Narogen Licost	16 VIA 8 Oxygen 15399 16 Suthur 12,06	9 <b>F</b> 19 19 19 17 17 17 17 10 19 19 19 19 19 19 19 19 19 19 19 19 19	18 VIIIA 2 Неішт 4005002 10 Neon 201797 18 Аст 20150
<sup>19</sup> <b>K</b> Potassium 39.0983	20 Ca calcium 40.078	21 Scc Scandium 44.955908	22 Ti Titanium 40 Tr	23 V Vanadium 50.9415 42	Cr M romium 12961 43 43 43 43 43 43 43 4	n 26 Intese 1044 Iro 558	e <sup>27</sup> C <sup>coba</sup> <sup>coba</sup> <sup>coba</sup> <sup>56,933</sup>	0 28 Ni Nickel 58.6934	<sup>29</sup> Cu <sub>Copper</sub> <sub>63.546</sub>	<sup>30</sup> Zn <sub>Zinc</sub> 65.38	Gallium Gallium 60.723	Germanium 72.630	<sup>33</sup> As Arsenic 74.921595	<sup>34</sup> Se Selenium 78.971	35 Bromine 79,904	36 Krypton 83.798
Rubidium 85.4678	Strontium 87.62	Yttrium 88.90584	Zirconium 91224 72	Niobium Moly 92.90637 73 73 74	ybdenum 95.95 Techno (98 75	ptium Puther 1011 76	u Rhodii 102.905 77	ium Palladium 550 78	Ag silver 107.8682	Cadmium 112.414 80	Indium 114.818	311 Tin 118.710	3D Antimony 121.760 83	Tellurium 127.60 84	lodine 126.90447 85	Xenon 131.293
Caesium 132.90545196 87	Barium 137.327 88	57 - 71 Lanthanoids	HT Hafnium 178.49	Tantalum Tu 160.94788 105 106	N Rheni 183.84 105.2	e O 108 007 108	S If um tridiu 192.21	Platinum 17 195.084	Gold 196.966569	Hg Mercury 200.592	Thallium 204.38	PD Lead 2072	Bismuth 208.98040	Polonium (209)	At Astatine (210)	Rn Radon (222)
Francium (223)	Radium (226)	89 - 103 Actinoids	Rf Rutherfordium (267)	Db Dubnium (268) Sea	borgium (200) Bohri (270	h H	S M Meitner	rium ) t Darmstadtiu (281)	m Roentgenium	Copernicium (285)	Nihonium (286)	Flerovium (289)	Mc Moscovium (289)	LV Livermorium (293)	TS Tennessine (294)	Oganesson (294)
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- 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 ( $\gamma' + \eta$ )

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n<br/>ogical<br/>tyAkca, Gursel – A Review on Superalloys and IN718 Ni-Based INCONEL SuperalloyBelan – GCP and TCP phases presented in Ni-base superalloysSims, Stoloff, Hagel – Superalloys & Superalloys II

#### Design Space - 12

#### 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
  - $T_o = \text{coherency} @ f_{s,co} = 0.98$
  - $f_s(T) = fraction of solid$

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





**Benoit, Zhu, Abbott, Easton** – Evaluation of the effect of RE additions on the hot tearing susceptibility of Al7150 ... **Easton, Gibson, Zhu, Abbott** – An a priori hot-tearing indicator applied to die-cast magnesium-rare earth alloys

## Better performance as compared to Kou solidification model

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

$$Score_{Kou.Solid} = max(|dT/d(f_{s})^{1/2}|)$$
$$Score_{Easton.Solid} = \int_{To}^{Tco} f_{s}(T)dT$$



## Strain-age cracking (SAC) traditionally measured as function of $\gamma'$ 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%

Hardy, Detrois, et al – Solving Recent Challenges fro Wrought Ni-Base SuperalloysSims, ITang, Reed, et al – Alloys-By-Design: Application to new superalloys for additive manufacturing

Sims, Hagel – The Superalloys

#### Strain-age cracking resistance correlates with slower $\gamma^\prime$ kinetics





Hardy, Detrois, et al – Solving Recent Challenges fro Wrought Ni-Base Superalloys Sims, I Tang, Reed, et al – Alloys-By-Design: Application to new superalloys for additive manufacturing

Sims, Hagel – The Superalloys

## Utilize Bayesian Optimization to efficiently optimize utility functions



#### Explore high variance regions Exploit high reward regions



**Optimization - 18** 

## Bayesian Optimization can only be used for single target optimization





**Optimization - 19** 

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



w<sub>m</sub>: scaling/normalization term calculated from the inverse of the parameter range

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



#### Optimization - 20

## 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



#### Best compositions from optimizations

#### Top ranking alloys from 5wt% Co trials

	Rank	Со	Cr	Мо	Al	Ti	С	Ni
	1	5.0	21.9	8.4	0.53	2.08	0.06	62.0
$\left\{ \right.$	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





Results - 24

#### Processing outline







Casting & Processing - 25

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



Casting & Processing - 27

Michigan Sample image was etched with a 1:3 ratio of HNO<sub>3</sub>:HCI Technological

University

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











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

Casting & Processing - 28

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







#### Casting & Processing - 29

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



Michigan Technological Etched with a 1:3 ratio of HNO3: HCl

niversitv

#### Casting & Processing - 30

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







Casting & Processing - 31

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





Casting & Processing - 32

## Optimized alloy meets >10% difference as measured via nanoindentation





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

Property Analysis - 33

#### 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





Next Steps - 34

#### Conclusions

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



# Thank you for your time Questions?

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



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