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DESIGN OPTIMIZATION OFMAGNETIC ALLOYS AND NICKEL-BASED SUPERALLOYS FOR HIGH TEMPERATURE APPLICATIONS

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Abstract. *Developing a new material or even improving properties of an existing material is a complex and time-consuming task. In recent years, materials scientists around the globe proposed a number of ways to speed up the alloy development process by using various computational tools. In this work, we made an attempt to demonstrate the efficacy of using computational tools in design optimization of materials, especially for high-temperature applications. We addressed two different material systems: Alnico alloys (magnetic) and Nickel-based superalloys.*
Alnico type alloys are hard magnetic alloys and well known for high-temperature applications. In this work, we defined the variable range of various elements and generated an initial set of alloys by a quasi-random sequence generation algorithm. These alloys were synthesized and tested for determining various material properties. We used a response surface methodology approach to develop surrogate models (meta-models) that approximately linked alloy chemistry with desired properties for these multi-component systems while being computationally affordable. These models were further used for multi-objective optimization of desired (conflicting) properties by using a number of algorithms based on evolutionary approaches, as well as our hybrid optimizer. Pareto-optimized predictions were experimentally validated and results over the cycles show significant improvement in properties of these alloys.
Nickel-based superalloys are used for high-temperature applications in aerospace, nuclear, and petrochemical industry. In this work, we also developed meta-models for two conflicting objectives, namely Stress to rupture and Time to rupture. Thereafter, we made an attempt to improve these properties by multi-objective optimization. Optimization results show significant improvement in these properties for Nickel-based superalloys.
In both tasks, we used two commercial optimization packages, "modeFRONTIER" and "IOSO", as well as our hybrid optimizer.

Keywords: *Response Surfaces, Multi-objective Optimization, Alnico, Material Properties, Pareto-optimized Predictions*

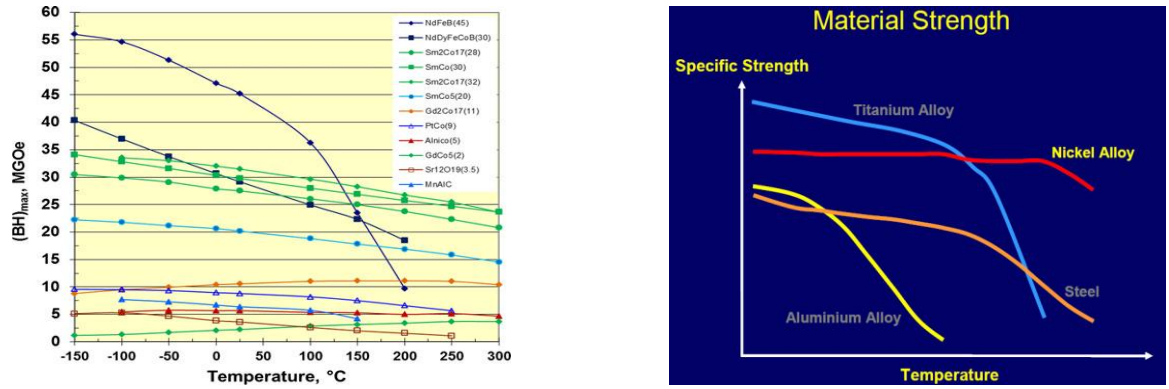
1. INTRODUCTION

A material or an alloy can be termed as a high-temperature material if it is able to maintain its peculiar properties (like physical, mechanical, magnetic, and optical) effectively above 540ºC (1000ºF). Hence, a designer has to be very careful regarding the choice of a particular material for a given application. Researchers around the globe have been constantly working to find new materials that can be more reliable for high-temperature applications. Design of new alloys or even improving the properties of existing alloys is a challenging task mainly due to limited experimental database (Yegorov-Egorov and Dulikravich, 2005, Jha *et al*., 2015). In order to develop a reliable knowledge base (Rajan, 2005, 2013) for design of new alloys, one needs to focus on determining various correlations (composition-property, property-property, and composition-composition) from the available databases (simulated and experimental). This information can be coupled with the theoretical knowledge (atomistic and continuum based theories) to develop a knowledge base. Integrated Computational Materials Engineering (ICME) approach (Horstemayer, 2012), along with the materials genome initiative, highlighted the importance and growing application of computational tools in design of new alloys. It aims at reducing a new alloy development cycle from currently 10 years to two years or even less. In recent years, various data-driven techniques, combined with evolutionary approaches have been successfully implemented in alloy design (Yegorov-Egorov and Dulikravich, 2005; Dulikravich and Egorov, 2012; Jha *et al*. 2014, 2015) and also in improving thermodynamic databases such as "ThermoCalc"(Thermocalc, 2015) for alloy

development. Data mining approaches like principal component analysis (PCA) and partial least square (PLS) regression have been successfully used in designing Magnesium alloys (Toda-Caraballo and Rivera-Diaz-Del-Castillo, 2015), as well as determining properties of Lutetium (Settouti and Aourag, 2015). These applications demonstrate the efficacy of use ofcomputational tools for materials design.

In the present research work, a novel approach is presented for implementation of computational tools in design and multi-objective optimization of materials for high-temperature applications. We addressed two different material systems: Alnico alloys (Magnetic) and Nickel-based Superalloys. Alnico type permanent magnetic alloys are widely popular due to their high-temperature stability and are the only known magnets for applications above 500ºC (Culity and Graham, 2008; Kramer *et al*., 2012). Figure 1(a) shows Magnetic energy density ($(BH)_{max}$) vs. Temperature plots for various magnetic alloys from -150ºC up to 300ºC. It can be seen from the figure that Alnico is least affected among them in this temperature range. Similarly, Ni-based superalloys (Figure 1(b)) was chosen for this work, as it is the preferred choice among superalloys for high-temperature applications (CMSE, 2015, Jha *et al*., 2014, 2015). One can notice in the later part of this text that a few elements (Ni, Co, Al, Ti and Nb) are common in both these alloys. However, Alnico are permanent magnetic alloys while Ni-based superalloys are non-magnetic. High-temperature properties of these alloys are mainly attributed to stability of critical phases in the desired range of temperature of exposure. Hence, heat treatment protocol is basically designed to stabilize the critical phases responsible for desired properties while suppressing the formation of phases which may seem to have an adverse effect. Additionally, there is limited experimental database and literature on phase stability for multi-component system. This demonstrastes the complex problem that an experimentalist faces while designing heat treatment protocol. Hence, meta-modeling may aid the experimentalist in determining the effect of various elements on the desired properties of interest, while multi-objectve optimization may help in improving the properties of the existing alloys before we think of adding or removing an element in the alloy for further improvements.

In this paper, we used actual experimental data to develop metamodels for desired properties for both of the alloys. Desired properties of interest were then further extremized by using our in-house version of hybrid response surface approach (HYBRID) (Colaço *et al*., 2008, Dulikravich and Colaço, 2013).



(a) (b)

Figure 1: Temperature dependence of various alloy systems (a) magnetic alloys, (b) superalloy systems.

1.1 Alnico alloys

Rare earth elements (REE) based magnets have much higher magnetic energy density ($(BH)_{max}$) than any other known magnets (Culity and Graham, 2008). Higher $(BH)_{max}$ aids in designing smaller magnets without compromising on other magnetic properties. REE magnets possess higher coercivity (H_c), that is, it can withstand stronger external magnetic fields than most materials without demagnetizing. They also have a high magnetic remanence (B_r), that is, the amount of magnetic flux density left in the magnet after removal of external magnetic field. However, they loose their superior magnetic properties rapidly as temperature increases beyond 150 ºC as it can be seen in Figure 1(a). Another problem is that deposits of most of the rare earth elements used for synthesizing these magnets are located in China. Hence, due to depleting resources and stringent trade rules from the suppliers, it is important to look at other options to synthesize these magnets as well as look for its alternatives. Alnico magnets(Culityand Graham, 2008), are permanent magnetic alloys based on the Fe-Co-Ni-Al system without REEs. Alnico magnets have very high Br values, comparable to REE magnets. Alnico magnets have lower Hc values, and can be demagnetized in the presence of an external magnetic field. However, low Hc also means that these magnets can be easily magnetized to saturation. A high Br and low Hc value help to cast this material in complex shapes while magnetizing it in the production heat treatment stages. Alnico magnets offer excellent corrosion resistance and high-temperature stability and are the only magnets that can be used up to 800 ºC.

At present, researchers around the globe are working on designing magnetic alloys that will be able to cover the gap between the properties achieved by Alnico magnets and the rare-earth magnets, basically by adding small amount of

those rare-earth elements that are less critical in the sense of supply (Ronning and Bader, 2014). This will help in addressing a few important energy conversion applications. Sellmayer *et al*., 2014 worked on a few rare-earth free alloys and the properties were found to be in the vicinity of Alnico alloys. Zhou *et al*. (2014) manufactured a few commercial Alnico alloys to demonstrate the scope of improvement in this field. However, the difference between the theoretically calculated and the experimentally measured properties were quite large for $(BH)_{max}$ and H_c. Hence, random experimentation may be misleading in terms of improvement in alloy properties while being both expensive and time-consuming.

Alnico magnets were discovered in 1931 by Mishima in Japan (Culity and Graham, 2008). Initially, these magnets were based on Fe-Co-Ni-Al system. Magnetic properties in these materials are attributed to the presenceof a two-phase system of BCC (Body Centered Cubic) α_1 and α_2 (Dilon, 2014). It was later observed that separation of α_1 and α_2 isdueto a metallurgical phenomenon popularly known as "spinodal" decomposition. Phase α_1 is Fe-Co rich ferromagnetic phase, while α_2 is Ni-Al rich phase. These phases are stable upto 850^{o}C. Curie temperature is about 860°C (Curie temperature is the temperature above which ferromagnetic behavior disappears as a result of thermal agitation of atoms). Above 850°C, FCC (face centered cubic) phase begins to appear. An FCC γ phase was observed in a few compositions. This phase is quite detrimental for magnetic properties. In later years, attempts were made to stabilize the magnetic α_1 and α_2 phases while at the same time eliminate or reduce the amount of FCC γ phase. These attempts include modification of heat treatment protocol and an addition of other elements to enhance various magnetic properties of these materials. Since 1980, there has been limited research on Alnico magnets mainly due to the discovery of powerful REE-based magnets. The recent rise in prices of rare-earth elements led to search of rare-earth free magnets. In recent years, there has been a significant amount of work (Sellmayer *et al*., 2014; Dilon, 2014; Ronning and Bader, 2014; Zhou *et al*., 2014) in this field. Due to their proven high-temperature stability and related properties, Alnico magnets are a popular choice for research.

Currently, Alnico alloys contain 8+ elements. In our work, we used 8 alloying elements. These elements include Iron (Fe), Cobalt(Co), Nickel(Ni), Aluminum(Al), Titanium(Ti), Hafnium(Hf), Copper(Cu) and Niobium(Nb). Variable bounds of these elements have been tabulated in Table 1. It is important to know the role of these alloying elements during manufacture of alloys for targeted properties. Later, this information can be utilized to select meta-models for a certain property. This is done with a purpose to develop a knowledge base for discovery of new materials while improving properties of existing materials. In this section, we addressed the effect of various elements on $(BH)_{max}$, H_c, and B_r.

Numerically, $(BH)_{max}$, is the area of largest rectangle that can be inscribed in the second quadrant of B-H curve. H_c and B_r are conflicting. That is, one has to sacrifice on one of these properties to improve the other property. Therefore, in order to increase $(BH)_{max}$, one needs to maximize both H_c and B_r. Role of various alloying elements and their individual effects on H_c and B_r have been addressed (Dilon, 2014) with the following conclusions:

1. Cobalt: It is a γ stabilizer. Hence, a solutionization anneal is needed to homogenize it to a single α phase. Cobalt increases coercivity and Curie temperature.
2. Nickel: It is also a γ stabilizer. It increases H_c (less than Cobalt), but at expense of B_r.
3. Aluminum: It is a α stabilizer. Hence, it will help in reducing the solutionization temperature. It affects H_c positively.
4. Copper: It is also a α stabilizer. It affects H_c positively and increases it. Additionally, it also increases B_r. In Alnico 8 and 9, Cu precipitates out of the α_2 phase into particles and increases the phase separation between α_1 and α_2 phases. It results in an increase in H_c. In Alnico 5-7, Cu remains in α_2 phases and it leads to an increase in H_c while decrease in Curie temperature.
5. Titanium: It is also a α stabilizer. It is one of the most reactive elements. It reacts with impurities such as S and N and precipitates out or purifies the magnet. It also eliminates Carbon. Carbon is a strong γ stabilizer and hence needs to be eliminated at any cost. Titanium helps in grain refining and assists columnar grain growth. It is to be noted that, due to columnar grain growth, majority of grains are aligned perpendicular to the chill plate. Large shape anisotropy can be achieved if spinodal decomposition occurs in this direction. Titanium increases H_c while it decreases B_r.
6. Niobium: It is also a α stabilizer. It helps in neutralizing the affects of Carbon. Like Titanium, Nb assists in columnar grain growth. Nb increases H_c, while it decreases B_r. But decrease in Br due to Nb is less than that observed due to Ti.
7. Hafnium: It is used for enhancing high-temperature properties. Hf usually precipitates at the grain boundary and helps in improving creep properties. Recent studies related to Co-Hf magnets motivated us to use Hf in this work.

1.2 Nickel-based superalloys

Multi-component superalloys are the preferred choice for high-temperature applications mainly due to their superior high-temperature and corrosion-resistant properties. They are extensively used in many specialized high-tech applications such as aeronautical, nuclear and petrochemical industry. Superalloys are most often used for high-

temperature applications, which are in excess of 70 percent of the absolute melting temperature. Hence, such alloys must be resistant to oxidation and hot corrosion. Additionally, they must resist mechanical forces such as creep, fatigue and thermo-mechanical fatigue. Superalloys can be based on Iron, Cobalt, Titanium, Nickel, *etc*. Nickel based alloys and Ti based alloys are best suited for high-temperature applications. At the same time, further retention of high-performance properties at extremely high temperatures implies use of expensive rare earth elements (Jha *et al*., 2014, 2015).

Modern Ni-based superalloys usually contain more than ten alloying elements along with some impurities. Various alloying elements enhance different properties of the alloys as follows (CMSE, 2015, Jha *et al*., 2014).

1. Cobalt, Chromium, Iron, Molybdenum, Tungsten, Tantalum, and Rhenium basically enhance solid solution strengthening;
2. Chromium, Titanium, Niobium, Hafnium, Molybdenum, Tungsten, and Tantalum enhance grain boundary strengthening with carbides;
3. Aluminum and Titanium generate a two-phase equilibrium microstructure with Nickel; gamma (γ) and gamma-prime (γ'), which enhance the elevated-temperature strength of the alloy and is also responsible for resistance to creep deformation;
4. Aluminum, Chromium, Yttrium, Cerium and Lanthanum improve the oxidation resistance;
5. Chromium, Cobalt, Silicon, Thorium and Lanthanum improve hot corrosion resistance;
6. Boron, Carbon, Zirconium and Hafnium act as grain boundary strengthening (refining) agents.

The concentration of various alloying elements is very important in determining the microstructure of an alloy and consequently multiple macroscopic properties of the alloy. Even a slight deviation in the concentration may affect the composition of phases responsible for the desired property.

2. ALLOY SYSTEMS UNDER STUDY

As mentioned before, we used actual experimental data for this work. Following section describes the nature of the dataset used for the two systems.

2.1 Alnico system

In this work, we used a set of computational tools to develop a novel approach for design and optimization high temperature and high-intensity magnetic alloys.

The steps involved in the proposed approach can be listed as follows:

1) Initial dataset: From the open literature, we defined the variable bounds of 8 alloying elements in the alloy. We used one of the best-known quasi-random number generators, Sobol's algorithm (Sobol, 1976), to generate chemical concentrations for each of the 80 candidate alloys (see Table 1 and Table 2). The initial set of alloys was screened on the basis of limited knowledge of phase equilibrium and magnetic property from a commercial thermodynamic database,"Factsage" (Factsage, 2015).
2) Manufacture and testing: The alloys were manufactured and tested for various properties of interest as shown in Table 3.
3) Response surface generation: From the available data, response surfaces were developed for the measured and calculated properties listed in Table 3. We used various modules available in optimization package," modeFRONTIER (ESTECO, 2015).
4) Multi-objective optimization: The most accurate response surfaces were used to extremize various properties as per the objectives specified in Table 3.
5) This work was independently carried out at two different place using:
    1) Commercial optimization package, "Indirect Optimization based on Self-Organization algorithm (IOSO)"(Egorov, 1998).
    2) Our Hybrid response surface (Colaço *etal*., 2008, Dulikravichand Colaço, 2013).

Predictions from both the optimization packages were merged and a set of alloys were selected for further manufacture and testing.

6) The work is performed in cycles. That is, steps 2-5 will be repeated until the improvements of multiple macroscopic properties of such magnetic alloys become negligible.
7) Sensitivity analysis: Various statistical tools were used to determine composition-property relations. This was done in order to find the most and the least influential alloying element.

This work is aimed at developing a knowledge base that will help the research community in designing new alloys.

In data-driven material science, knowledge discovery (Rajan, 2005, 2013) for designing new materials requires:

1. Data: In this work, our database is a combination of experimentally verified data predicted by a well-known random number generator and data from Pareto-optimized predictions as discussed above.
2. Correlations: Here, we used various linear and nonlinear correlation, clustering, and principal component analysis tool to discover various trends in the dataset.

3. Theory: The above information can be coupled with theoretical knowledge to motivate the experimentalist to move forward with the manufacture of new alloys.

Table 1: Concentration bounds for alloying elements in AlNiCo type alloys

	Alloyingelements	**Variablebounds (Wt %)**		
		Alloysnumber		
		1 – 85	**86 – 143**	**144-173**
1	Cobalt (Co)	24 – 40	24 – 38	Variableboundsrelaxedby 5 % for eachoftheseelements
2	Nickel (Ni)	13 – 15	13 – 15	
3	Aluminum (Al)	7 – 9	7 – 12	
4	Titanium (Ti)	0. 1 – 8	4 – 11	
5	Hafnium (Hf)	0. 1 – 8	0. 1 – 3	
6	Copper (Cu)	0 – 6	0 – 3	
7	Niobium (Nb)	0 – 2	0 – 1	
8	Iron (Fe)	Balance to 100		

Table 2: Design cycle and alloy number

Cycle no.	**Alloys Designed**	**Best alloy**
1	1-80	#30
2	81-85	#84
3	86-90	#86
4	91-110	#95
5	111-120	#117
6	120-138	#124
7	139-143	#139
8	144-150	#150
9	150-160	#157
10	160-165	#162
11	166-173	#169

Table 3: Quantities to be simultaneously extremized using multi-objective optimization

	Properties	**Units**	**Objective**
1	Magnetic energy density ($(BH)_{max}$)	kg m^{-1} s^{-2}	Maximize
2	Magnetic coercivity (H_c)	Oersted	Maximize
3	Magnetic remanence (B_r)	Tesla	Maximize
4	Saturation magnetization (M_s)	Emu/g	Maximize
5	Remanence magnetization (M_r)	Emu/g	Maximize
6	$(BH)_{max}$/mass	m^{-1} s^{-2}	Maximize
7	Magnetic permeability (m)	kg m A^{-2} s^{-2}	Maximize
8	Cost of raw material (cost)	$/kg	Minimize
9	Intrinsic coercive field (jH_c)	Am^{-1}	Maximize
10	Density(ρ)	Kgm^{-3}	Minimize

2.2 Ni-based superalloy system

Concentrations for an initial batch of 120 Ni-based superalloys were generated using Sobol's quasi-random sequence generation algorithm (Sobol, 1976). These alloys were then manufactured and their mechanical properties evaluated using standard experimental procedures. The chemical elements that were considered to be important were identified as Ni, C, Cr, Co, W, Mo, Al, Ti, B, Nb, Ce, Zr, Y, while elements such as S, P, Fe, Mn, Si, Pb, Bi were treated as extraneous impurities. Hence, in the present system, twelve alloying elements can be treated as significant alloying elements. Out of these, a total of seven alloying elements appear to be major property changers. These elements were chosen for developing response surfaces and further for optimization. Thus, the chosen elements whose concentrations were optimized were Ni, C, Cr, Co, W, Mo, Al, Ti. Their compositional bounds are presented in Table 4. Concentrations of Nb, B, Ce, Zr, Y in all sample alloys were kept constant at 1.1%, 0.025%, 0.015%, 0.04%, and 0.01%. All 120 initial alloys were tested for their stress-to-rupture (N/mm2) and the time-to-rupture (hours). It should be noted that in the present case, the stress-to-rupture was measured at the room temperature while the time-to-rupture was measured for a constant stress of 230 N/mm2 at a temperature of 975ºC (Yegorov-Egorov and Dulikravich, 2005, Jha *et. al.* 2014, 2015).

Multi-objective optimization problem was formulated to

Simultaneously maximize stress-to-rupture at room temperature and time-to-rupture at 975 ºC at a fixed stress of 230 N/mm2.

Higher stress would lead to accelerated rupture; hence, the objectives are mutually conflicting. This will lead to a Pareto-optimal solution, that is, the best trade-off solutions. Hence, we can proceed towards meta-modeling and subsequent optimization for both of these alloys.

Table 4: Upper and lower bounds of the major alloying elements in Ni base superalloy design (Yegorov-Egorov and Dulikravich, 2005)

	Elements (wt %)							Objective	
	C	Cr	Co	W	Mo	Al	Ti	Stress to rupture (N/mm^2)	Time to rupture (Hours)
Min	0.13	8.0	9.0	9.5	1.2	5.1	2.0	907	25.17
Max	0.20	9.5	10.5	11.0	2.4	6.0	2.9	1037	92.38

3. META-MODELING AND MULTI-OBJECTIVE OPTIMIZATION

In this work, we used a commercial optimization package,"modeFRONTIER". The response surfaces were tested on various accuracy measures and the most accurate one was chosen for further study. Various approaches to develop response surfaces include Radial basis functions (RBF), Kriging, Anisotropic Kriging and Evolutionary Design.

Multi-objective optimization: Most accurate response surfaces developed above were used to extremize various properties as per the objectives specified in Table 3 for Magnetic alloy and the multi-objective problem formulation for Ni-based superalloy. It was observed that most of the optimization tasks yielded alloys with similar chemical composition for a set of objectives. Hence, several optimization runs were performed to get a diverse pool of results. The optimization algorithms used in modeFRONTIER include Non-dominated Sorting Genetic Algorithm II (NSGA2), Multi-Objective Particle Swarm Optimization (MOPSO), Multi-Objective Simulated Annealing (MOSA) and FAST (FAST optimizer uses response surface models (meta-models) to speed up the optimization process using search algorithms like NSGA2, MOPSO, MOSA).

This work was independently carried out at two different place using:

1) Commercial optimization package, "Indirect Optimization based on Self-Organization algorithm (IOSO)".
2) Hybrid response surface (HYBRID) (Colaço *et al*., 2008, Dulikravichand Colaço, 2013). NSGA2 was used for optimization.

4. RESULTS

Pareto-optimized predictions from HYBRID approach were plotted along with the experimentally verified predictions from various approaches. This is done for both Alnico alloys as well as Ni-based superalloys. Screening of candidate alloys from a large set of Pareto-optimized predictions is a tricky task. This task has been addressed in this work for Alnico alloys. Similar approach can be followed for Ni-based superalloys.

4.1 Alnico alloy

As discussed in the previous section, $(BH)_{max}$ is the maximum area of the rectangle that can be inscribed in the second quadrant of B-H curve. Hence, B_r and H_c are conflicting in nature. In this case, we used the meta-models developed in the previous section and attempted to maximize $(BH)_{max}$, B_r and H_c altogether. Pareto-optimized predictions from HYBRID have been plotted in Figure 2. Top 10 alloys have been marked on the figure for comparison.

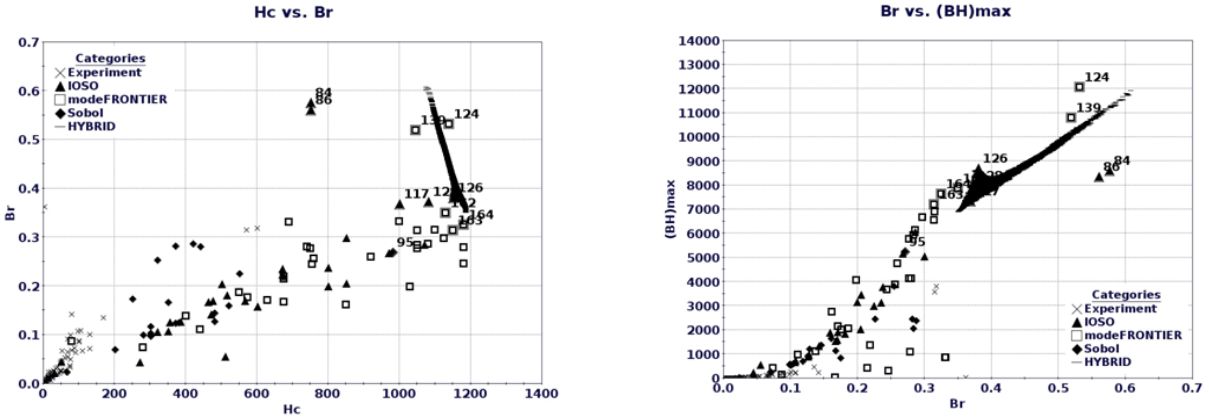


Figure 2: Comparison of Pareto-optimized prediction from HYBRID with various other techniques.

From the figures above, we can see that alloys predicted by HYBRID approach are in the vicinity of the experimentally verified alloys predicted by various methods. Hence, we can use a few alloys predicted by HYBRID approach before moving towards rare-earth addition.

One of the major challenges in using alloys predicted by HYBRID approach is screening of suitable candidates for manufacture. It is due to large number of Pareto-optimized candidates predicted by the optimizer. Another problem is that the alloys are in close composition ranges, hence making the work more complex.

In order to address this, we used a popular statistical measure,"Multi-Criterion Decision making (MCDM)" approach. This module is available in modeFRONTIER. Fifteen alloys were selected for this analysis.

To further validate that these 15 alloys will perform as expected, we used Principal Component Analysis (PCA), which is usually used to reduce the dimensionality of the dataset. PCA analysis test has been successfully used in the past for materials discovery as we have mentioned in Section 1. In the present case, these alloys were further clustered to discover any pattern in the dataset by K-nearest point method. Figure 3 shows the results obtained from PCA analysis.

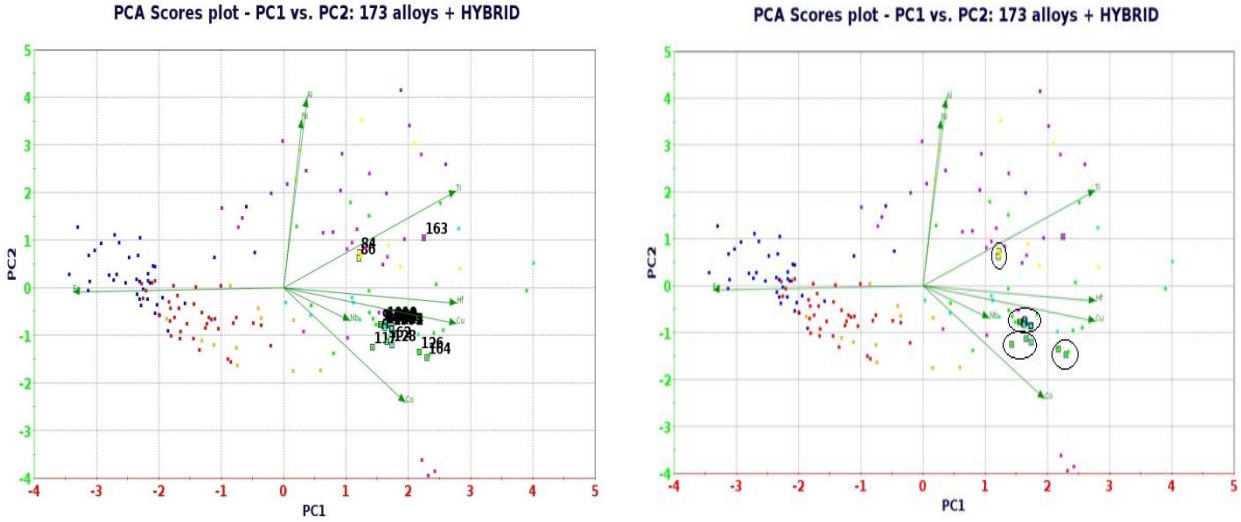


Figure 3: PCA analysis of selected datapoints: top 10 alloys are marked in the figure

From PCA analysis, we can see that the alloys predicted by HYBRID and screened by MCDM are included in the clusters of the top 10 alloys. Hence, these alloys are expected to perform as per our expectations. Consequently, we can proceed towards manufacture of a few candidate Pareto optimized alloys to validate our findings.

4.2 Nickel-based superalloys

Meta-models were developed for Stress to rupture and Time to rupture. In HYBRID method, we used NSGA2 for optimization. In modeFRONTIER, we used Radial Basis function to develop meta-models and NSGA2 for optimization. Figure 4 shows a comparison between results obtained by various approaches.

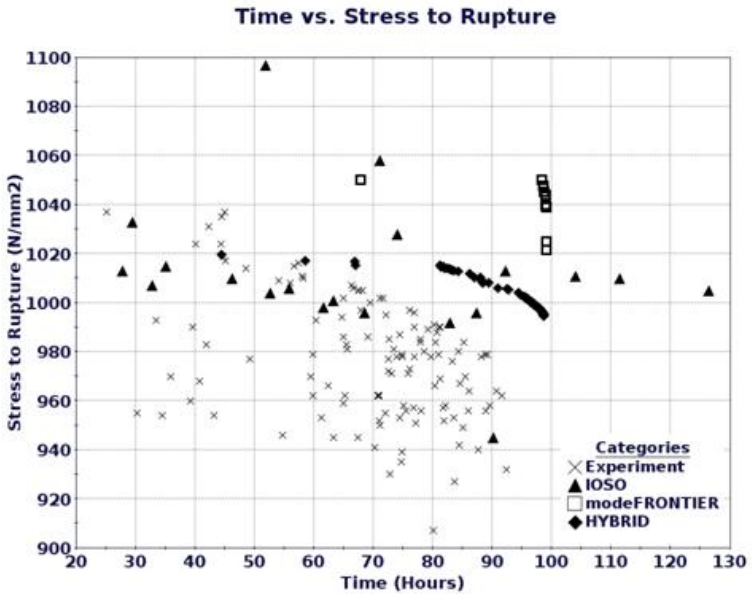


Figure 4: Comparison of Pareto-optimized prediction using HYBRID and other algorithms

Figure 4 shows that the HYBRID approach is able to generate data points that are superior to the initial set of alloys. Additionally, a few of these points are in the vicinity of experimentally verified IOSO predictions.

5. CONCLUSION

The main purpose of this work was to test a few additional alloys before we proceed towards rare-earth addition in case of Alnico alloys. Even for Ni-based superalloys, to further improve the properties one has to proceed towards rare-earth addition. Hence, in this work, we were able to demonstrate the efficacy of HYBRID approach in design optimization of two different systems of alloys for high-temperature applications.

A few unique contributions from this work can be listed as follows:

1. In this work, we were able to generate alloys with a unique composition and comparatively superior properties when compared to the dataset used for meta-model development.
2. Screening of candidate alloys were done by MCDM approach.
3. Further classification was done by PCA analysis. Hence, the decision maker will be confident while selecting the alloy for experimentation.
4. Above findings will be beneficial in the development of database/ knowledge base for design optimization of other alloy systems.

6. FUTURE WORK

The main purpose of computational materials science is to boost the confidence of a curious experimentalist. He must have enough confidence in the proposed methodology so that he can think of altering the alloy development protocol for improved results. Above analysis, theoretical knowledge, evolutionary approach combined with standard statistical tests will be able to address various concerns an experimentalist may have before making changes in standard alloy development protocol. Any further concern can be addressed by implementing it in our meta-model.

7. ACKNOWLEDGEMENTS

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8. REFERENCES

Cullity, B.D. and Graham,C.D., 2008, Introduction to Magnetic Materials, 2nd ed., New York, Wiley-IEEE Press.

Colaço, M.J.; Dulikravich, G.S. and Sahoo, D.; 2008, A response surface method-based hybrid optimizer, Inverse Problems in Science and Engineering, 16:6, 717 – 741.

Colaço, M.J.; Silva, W.B.; Magalhães, A.C. and Dulikravich, G.S., 2008, Response surface methods applied to scarce and small sets of training points – a comparative study, EngOpt 2008 - International Conference on Engineering Optimization, Rio de Janeiro, Brazil, June 1-6, 2008.

Colaço, M.J.; and Dulikravich, G.S., 2008, A hybrid RBF based method for highly multidimensional response surfaces using scarce data sets, paper AIAA-2008-5892, 12th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Victoria, British Columbia, Canada, September 10-12, 2008.

CMSE, http://www.cmse.ed.ac.uk/AdvMat45/SuperEng.pdf (accessed on May 1, 2015)

Dilon, H.M., 2014, Effects of heat treatment and processing modifications on microstructure in alnico-8H permanent magnetic alloys for high temperature applications". Graduate Thesis and Dissertations. Paper 13867, Iowa State University, http:/lib.dr.iastate.edu/etd/13867

Dulikravich, G.S.; and Egorov, I.N., 2012, Inverse design of alloys' chemistry for specified thermo-mechanical properties by using multi-objective optimization. Chapter 8 in Computational Methods for Applied Inverse Problems (eds: Wang, Y.F.; Yagola, A.G.; Yang, C.C.), De Gruyter and Higher Education Press, China, ISBN: 978-3-11-025905-6.

Dulikravich, G.S. and Colaço, M.J., 2015, Hybrid optimization algorithms and hybrid response surfaces, Chapter 2 in *Advances in Evolutionary and Deterministic Methods for Design, Optimization and Control in Engineering and Sciences*(eds.: Greiner, D.; Galván, B.; Periaux, J.; Gauger, N.; Giannakoglou, K.; Winter, G.), Computational Methods in Applied Sciences Series, Springer Verlag, pp. 19-47.

Egorov, I.N., 1998, Indirect optimization method on the basis of self-organization, Proceedings of Optimization Techniques and Applications (ICOTA'98), Curtin University of Technology, Perth, Australia, 2, 683-691.

ESTECO, 2015, http://www.esteco.com/home/mode_frontier.html (accessed May 1, 2015)

FactSage, 2015, http://www.factsage.com/ (accessed May 1, 2015)

Sobol, I.M., 1976, Uniformly distributed sequences with an additional uniform property, USSR Computational Mathematics and Mathematical Physics, (16) 236-242.

Horstemeyer, M.F., 2012, Integrated Computational Materials Engineering (ICME) for Metals: Using Multiscale Modeling to Invigorate Engineering Design with Science,(Hoboken, New Jersey,TMS - The Minerals, Metals & Materials Society, John Willey & Sons, Inc.).

Jha, R.; Dulikravich, G.S.; Pettersson, F.; Saxen, H.; Chakraborti, N., 2015, Evolutionary Design of Nickel Based Superalloys Using Data-Driven Genetic Algorithms and Related Strategies. Materials and Manufacturing Processes, 30:4,488-510, http://dx.doi.org/10.1080/10426914.2014.984203.

Jha, R.; Dulikravich, G.S.; Pettersson, F.; Saxen, H.; Chakraborti, N., 2014, A Combined Experimental-Computational Approach to Design Optimization of High Temperature Alloys. ETS2014-1008, ASME Symposium on Elevated Temperature Application of Materials for Fossil, Nuclear, and Petrochemical Industries, Seattle, WA, March 25-27.

Jha, R.; Dulikravich, G.S.; Fan, M.; Shwartz, J.; Koch, C.; Egorov, I.N.; Poloni, C., 2014, A Combined Computational-Experimental Approach to Design of High-Intensity Permanent Magnetic Alloys, CONEM2014, Uberlandia, Brazil, August 10-15, 2014.

Kramer, M.J.; McCallum, R.W.; Anderson, I.A.; Constantinides, S., 2012, Prospects for non-rare earth permanent magnets for traction motors and generators, JOM, Vol. 64, No. 7, 752-763

Ronning, F. and Bader, S., 2014, Rare earth replacement magnets, J. of Physics: Condensed Matter 26 060301 (3pp).

Sellmyer, D.J.; Balamurugan, B.; Zhang, W.Y.; Das, B.; Skomski, R.; Kharel, P.; and Liu, Y., 2013, Advances in rare-earth-free permanent magnets (edited by: Fernand Marquis), The 8th Pacific Rim International Congress on Advanced Materials and Processing, John Wiley & Sons, Inc., Hoboken, NJ, USA.

ThermoCalc, http://www.thermocalc.com/solutions/by-application/alloy-development/ (accessed on May 1, 2015)

Yegorov-Egorov, I.N.; and Dulikravich, G.S., 2005, Materials and Manufacturing Processes, 20, 569-590.

Yegorov-Egorov, I.N.; and Dulikravich, G.S., 2005, Design of alloy's concentrations for optimized strength, temperature, time-to- rupture, cost and weight, Sixth International Special Emphasis Symposium on Superalloys 718, 625, 706 and Derivatives (ed: Loria, E.A.) TMS - Minerals, Metals & Materials Society Publ., Pittsburgh, PA, Oct 2-5, 419-428.

Zhou, L.; Miller, M.K.; Lu, P.; Ke, L.; Skomski, R.; Dillon, H.; Xing, Q., Palasyuk, A.; McCartney, M.R.; Smith, D.J.; Constantinides, S.; McCallum, R.W.; Anderson, I.A.; Antropov, V.; Kramer, M.J., 2014, Architecture and magnetism of Alnico, ActaMaterialia, 74, 224-233.

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