Direct and Inverse Design Optimization of Magnetic Alloys with Minimized Use of Rare Earth Elements

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Status Quo: High performance magnetic alloys use rare earth elements that are expensive and rare in USA.

New Insight: Non-rare earth elements in proper concentrations can create high performance magnetic alloys.

Project Goal: Develop and experimentally verify a computational method for designing optimized chemistries of high strength/high temperature hard magnetic alloys with no rare earth elements.

Main Accomplishments

Why and How

Existing theoretical formulations and accompanying software can predict only certain physical properties of such materials. Since they are currently limited to at most three alloying elements, the use of purely computational tools to predict multiple properties of candidate alloys involving more than three alloying elements is currently infeasible.

We propose to adapt and use advanced semi-stochastic algorithms for constrained multi-objective optimization in combination with experimental testing and verification of candidate alloys to determine optimum concentrations of alloying elements used for magnetic alloys that will simultaneously maximize a number of the alloy's macroscopic conflicting properties.

How and Why

Periodically manufacturing samples of the optimized candidate alloys and testing them will verify the alloy properties predicted by the multi-objective optimization and enhance the accuracy of the entire alloy design process.

An inverse design method will also be developed where the multiple physical properties of a magnetic alloy are specified by the designer, while chemistries of the alloys that can produce these specified values will then be determined.

Publications

E. Inclan, G.S. Dulikravich, "Effective Modifications to Differential Evolution Optimization Algorithm", ECCOMAS Coupled Problems, Ibiza, Spain, June 16-19 (2013).

E. Inclan, X.-S. Yang, G.S. Dulikravich, "Modern Optimization Algorithms and Particle Swarm Optimization", IPDO2013, Albi, France, June 26-28 (2013)

Direct Design Problem

Optimization of chemical composition of alloys for maximum performance

***Purpose**:* Determine Pareto optimal macroscopic properties of an alloy family by finding the corresponding optimal concentrations of the alloying elements.

Problem features:

variable parameters: Concentrations of the alloying elements used

C, S, P, Cr, Ni, Mn, Si, Cu, Mo, Pb, Co, Cb, W, Sn, Al, Zn, Ti

(8,…,17 variables).

Simultaneous objectives (for example):

- Stress (PSI – maximize);
- Operating temperature (T – maximize);
- Time to "survive" until rupture (Hours – maximize).

Mathematical model: Does not exist; hence, use an existing database

- **Direct Design Objectives**

Adapt an advanced semi-stochastic algorithm for constrained multi-objective optimization and combine it with experimental testing and verification to determine optimum concentrations of alloying elements in alloys that will simultaneously maximize a number of alloy's properties.

The proposed algorithm also requires a minimum number of alloy samples that need to be produced and experimentally tested thus minimizing the overall cost of automatically designing high-strength alloys.

Example of "Getting Out-of-the-Box" Alloy Design

- **This work was aimed at optimizing Ni- based heat-resistant alloy castings containing *Ni, C, Cr, Co, W, Mo, Al, Ti*, *B, Nb, Ce, Zr, Y*, and trace amounts of *S, P, Fe, Mn, Si, Pb, Bi.***

- **The technology used in the casting allowed us to alter the chemical composition by varying concentrations of the following elements: *Ni, C, Cr, Co, W, Mo, Al, Ti*.**

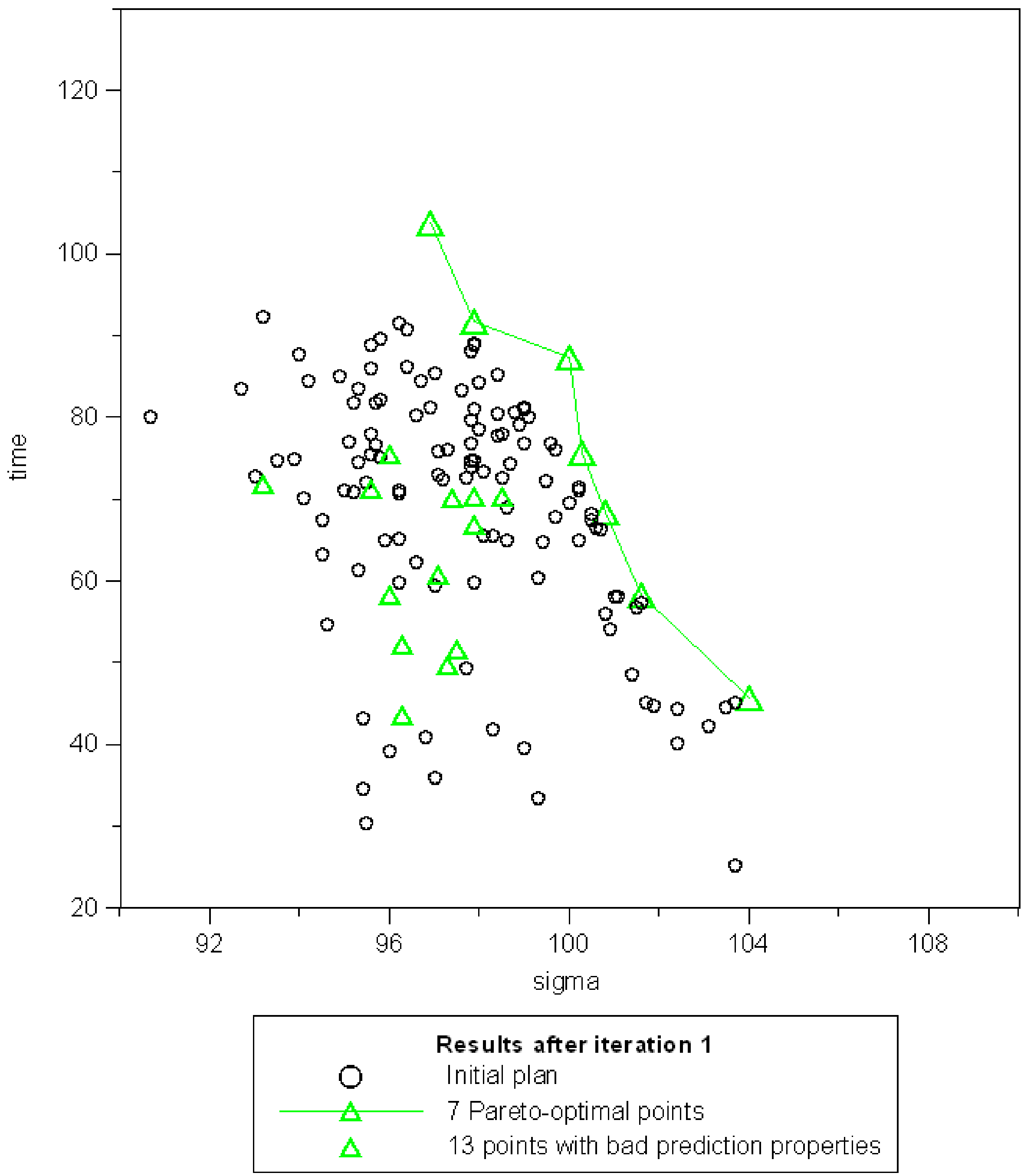
- **The concentrations of *Nb, B, Ce, Zr, Y* in all test samples were 1.1%, 0.025%, 0.015%, 0.04%, and 0.01%, respectively.**

- **In this optimization task the concentrations of seven elements: *C, Cr, Co, W, Mo, Al, Ti* were used as variable parameters.**

- **Thermal treatment of the samples involved heating them to 1210 C, holding for 4 hours, and air cooling.**

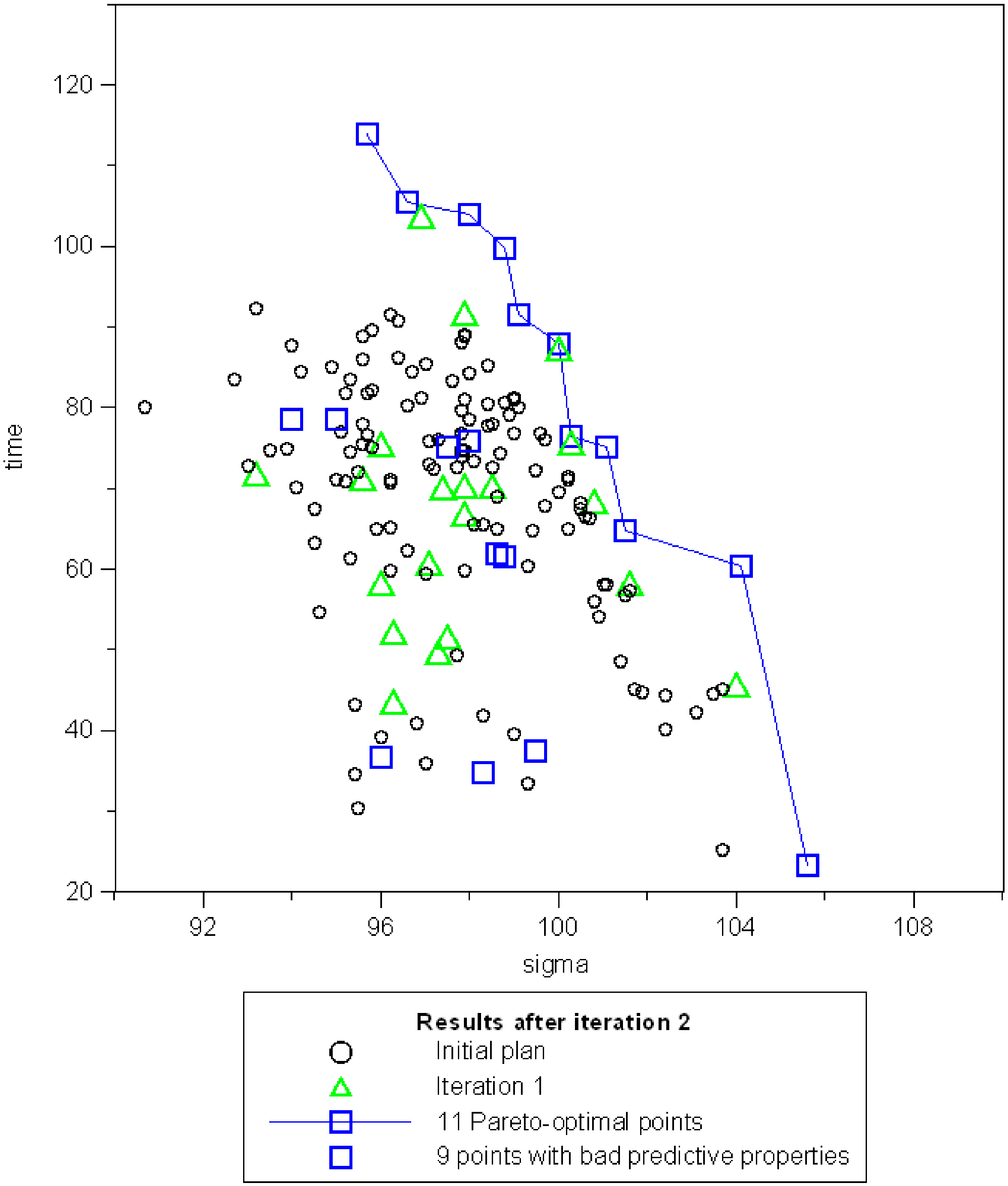
- **During these tests the stress at room temperature (sigma) and the time to survive until rupture (hours) at temperature of 975 C and stress of 2300 N/mm**2 were measured.**

- **The optimization was conducted by simultaneously maximizing stress (SIGMA) and time-to rupture (HOURS).**
- **At each optimization iteration, a two-criterion optimization task with a specified number of Pareto optimal points was solved.**
- **The user-specified number of Pareto points was 20.**
- **At the start, the initial experiment plan including 120 alloys was developed by distributing their chemical compositions via Sobol's algorithm in order to minimize the total number of alloys that need to be tested.**
- **This information was used for building an approximation function (a multi-dimensional response surface) for the first iteration.**
- **This approximation function was then optimized using a variant of IOSO. The result was a set of chemical compositions of 20 new alloys which could be a part of the new Pareto set.**
- **Next step was manufacturing and experimental evaluation of the two properties (maximum stress and time-to-rupture at 975 C) for each of these 20 newly found alloys.**



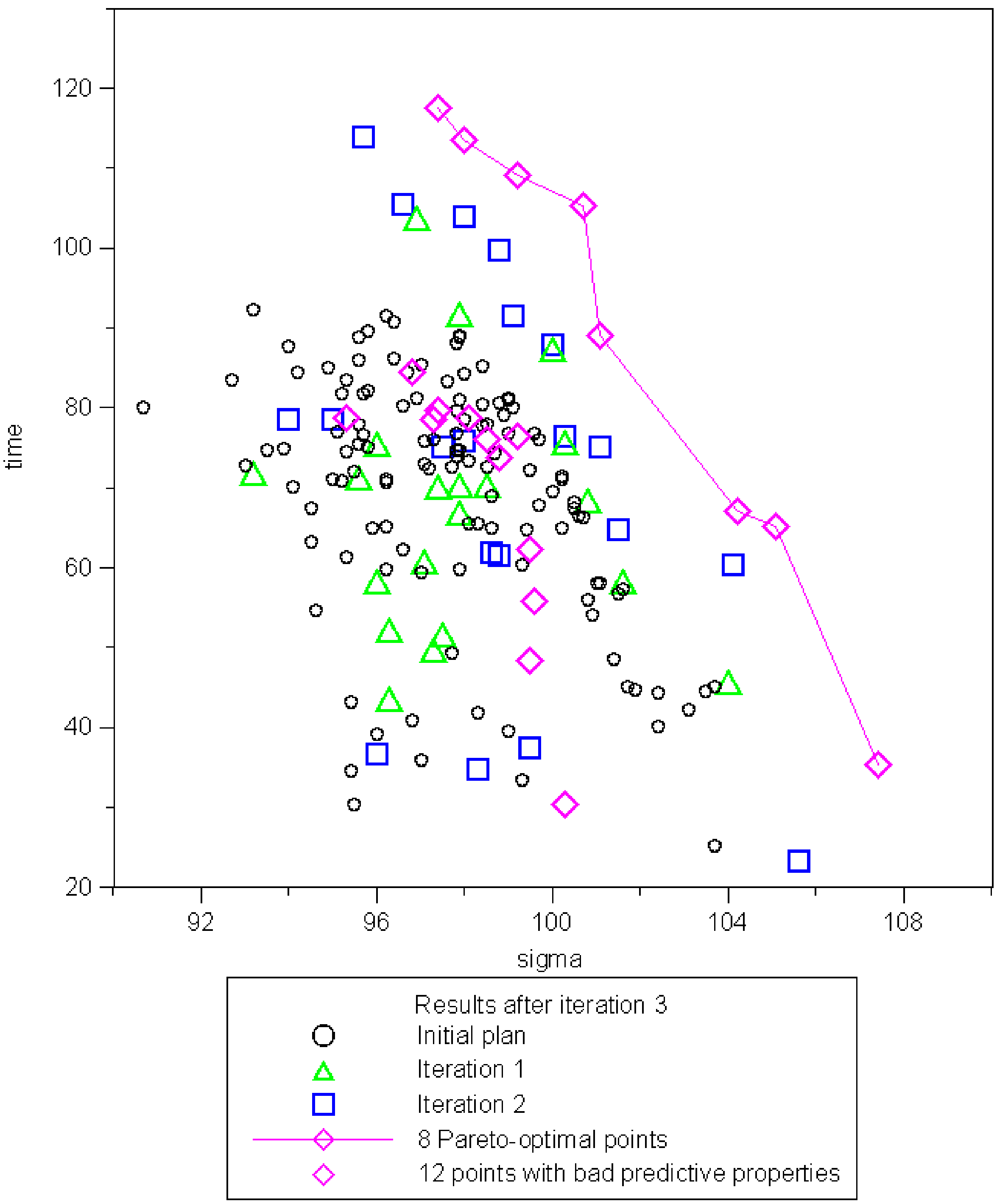
Initial 120 nickel based alloys and 20 alloys predicted by the 1st iteration with IOSO optimizer.

All new alloys were then experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.



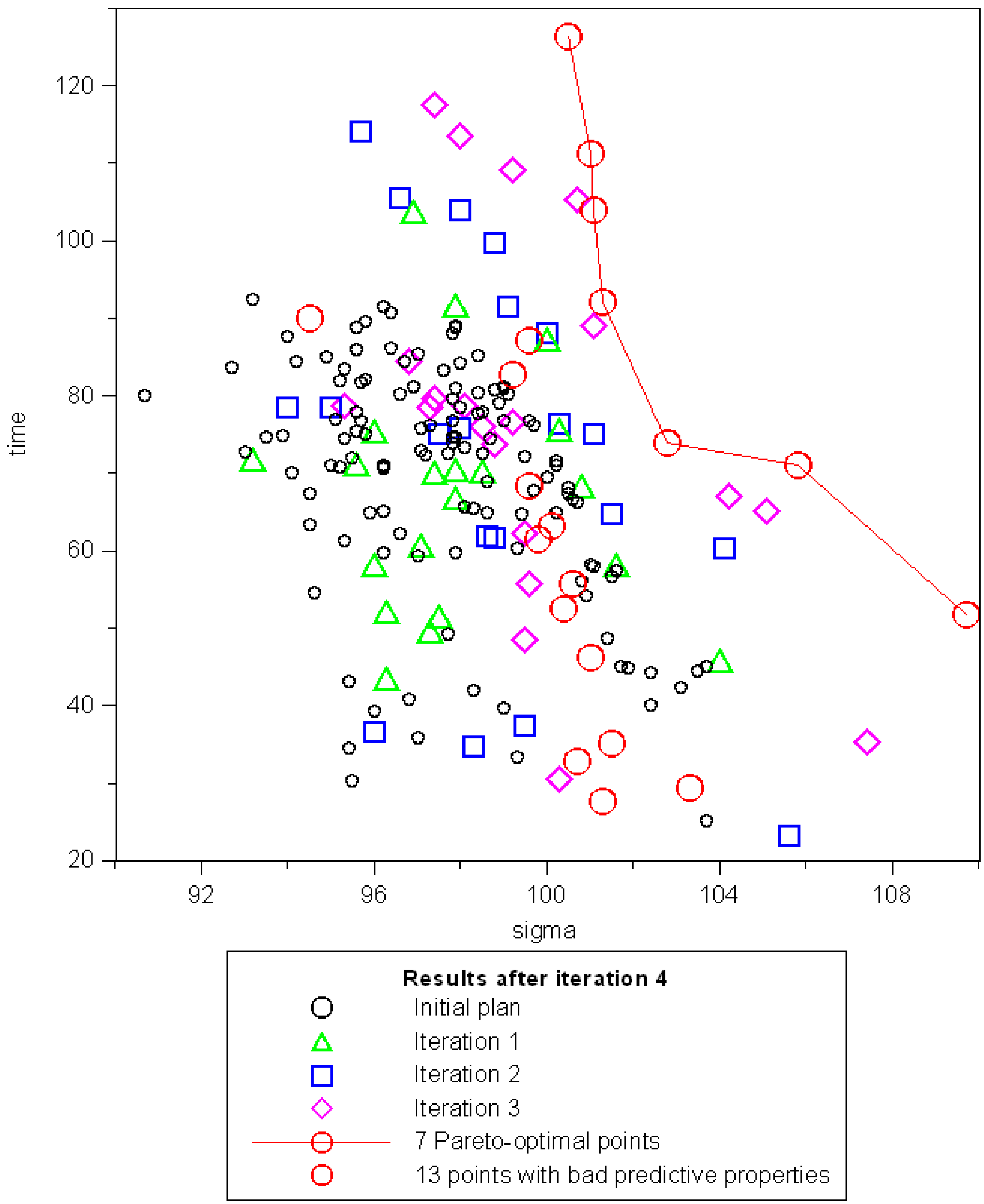
Initial 120 alloys plus 20 alloys from first iteration and 20 alloys predicted by the 2nd iteration with IOSO optimizer.

All new alloys were then experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.



Initial 120 alloys plus 20 alloys from 1st iteration, plus 20 alloys from 2nd iteration, plus 20 alloys predicted by the 3rd iteration with IOSO optimizer.

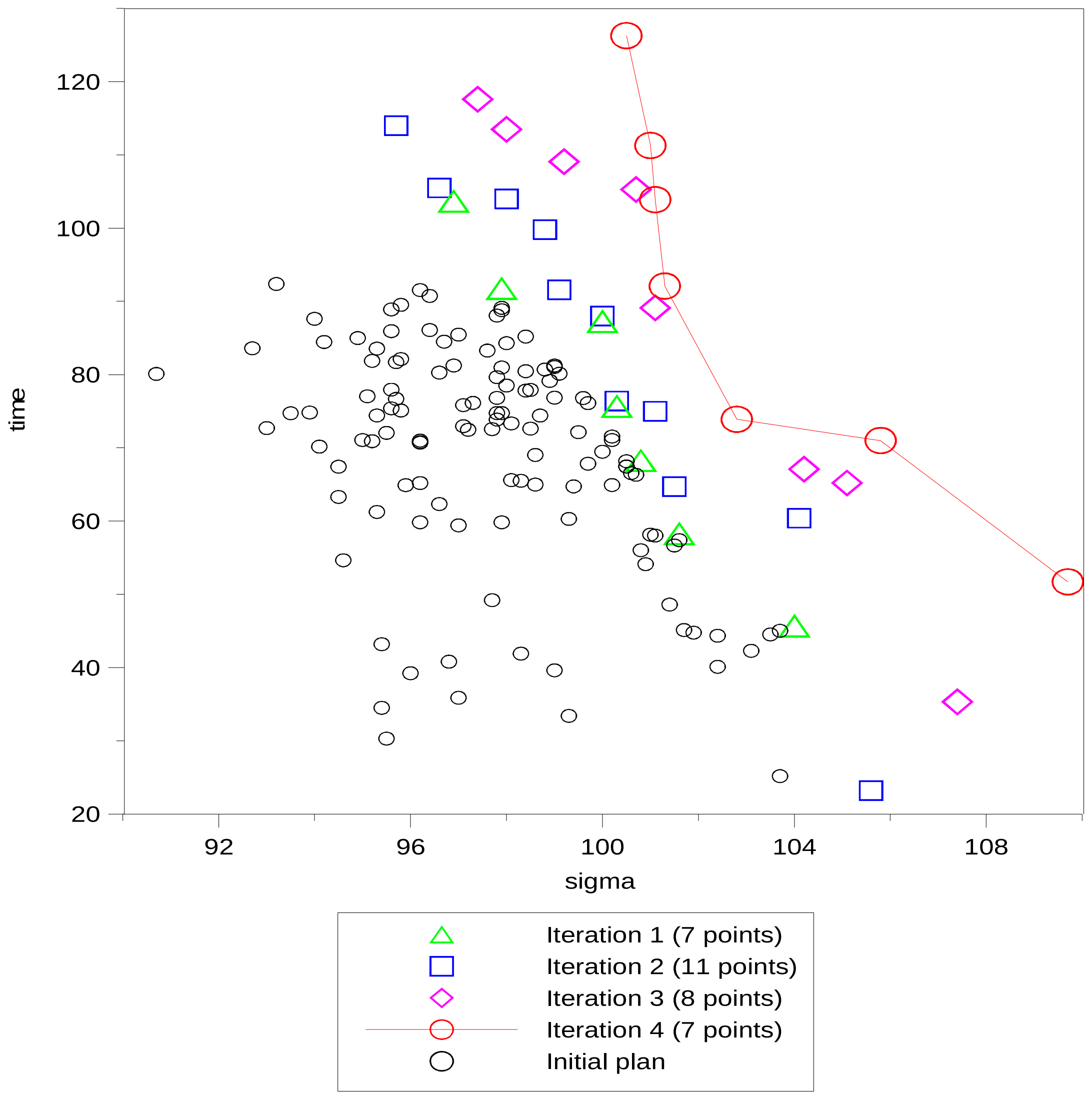
All new alloys were then experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.



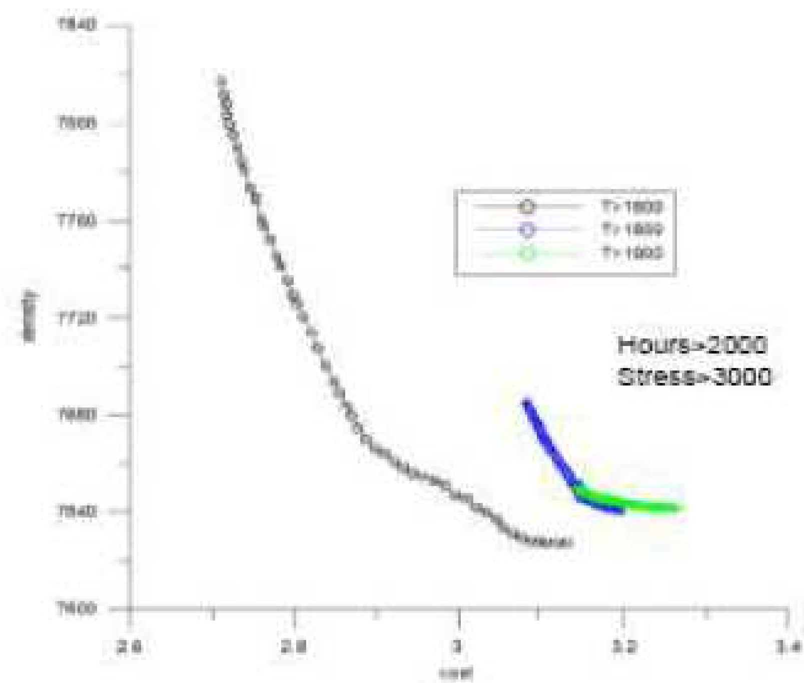
Initial 120 alloys plus 20 alloys from 1st iteration, plus 20 alloys from 2nd iteration, plus 20 alloys from 3rd iteration, plus 20 alloys predicted by the 4th iteration with IOSO optimizer.

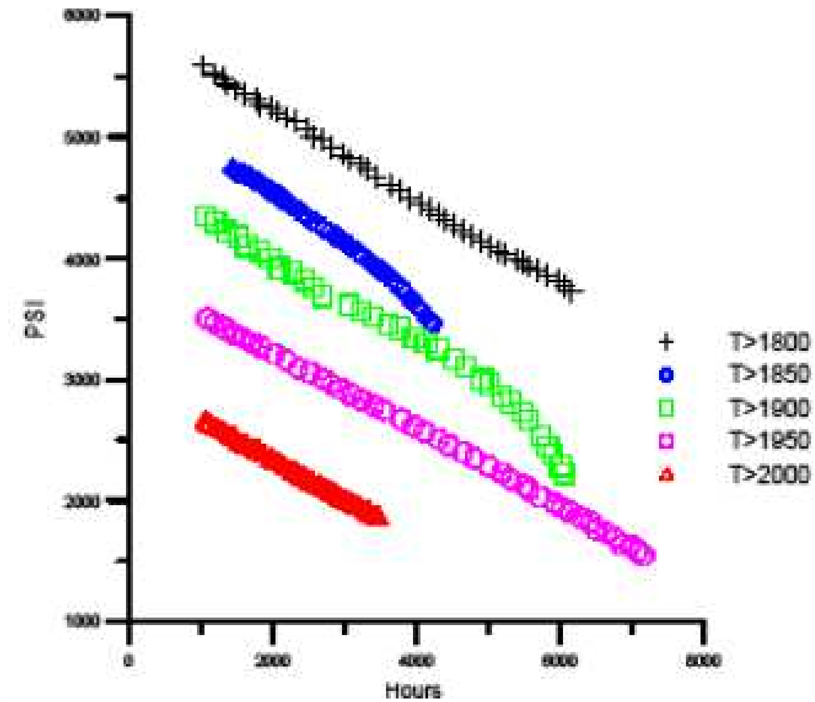
All alloys were experimentally tested for maximum strength and time-to-rupture at 975 degrees Celsius.

Summary of experimentally verified time-to-rupture (at 975 Celsius) and tensile strengths of 120 original steel alloys (black circles) and the four generations of new alloys obtained using IOSO algorithm that optimized their chemical compositions.



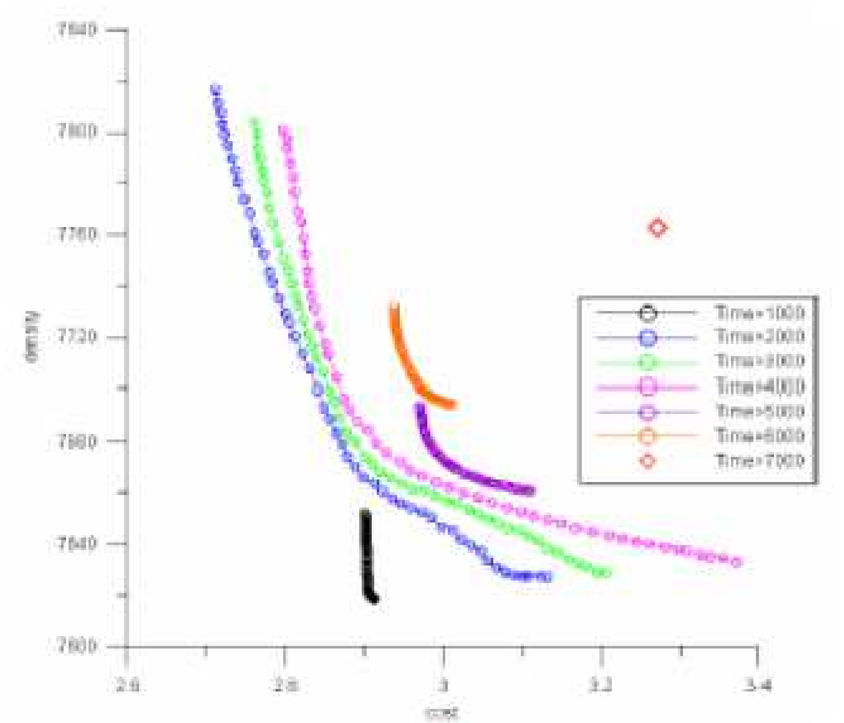
An example of multi-objective design optimization of Ni-based steel superalloys



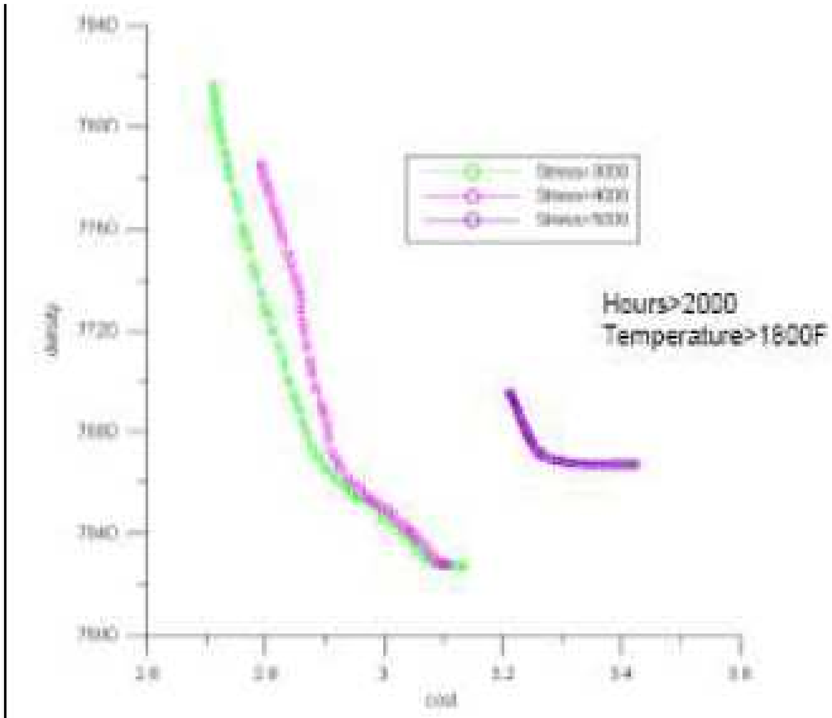


Minimize cost and weight for stress > 3000 psi and TIME > 2000 hours.	Maximize strength and time for cost < 3000 and density < 7800 kg/m^3

An example of multi-objective design optimization of Ni-based steel superalloys



Minimize cost and weight for stress > 3000 psi and temperature > 1800 degrees F.



Minimize cost and weight for time-until-rupture >2000 hours and temperature > 1800 degrees F.

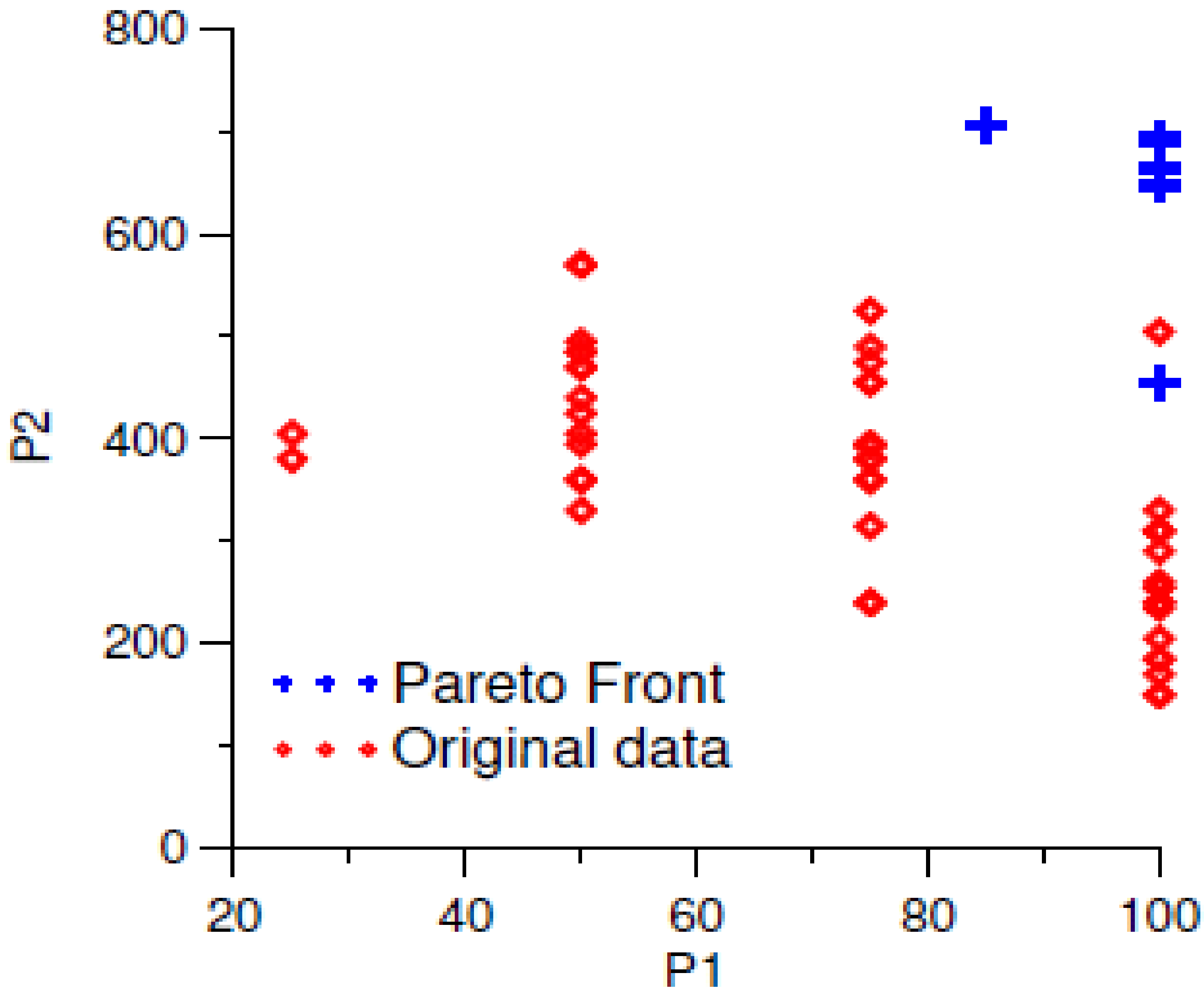
An example of optimization of
Chemical Concentrations
and
Thermal Treatment Protocols

Aluminum Alloys
(Al, Cu, Zn, Mg, Mn)

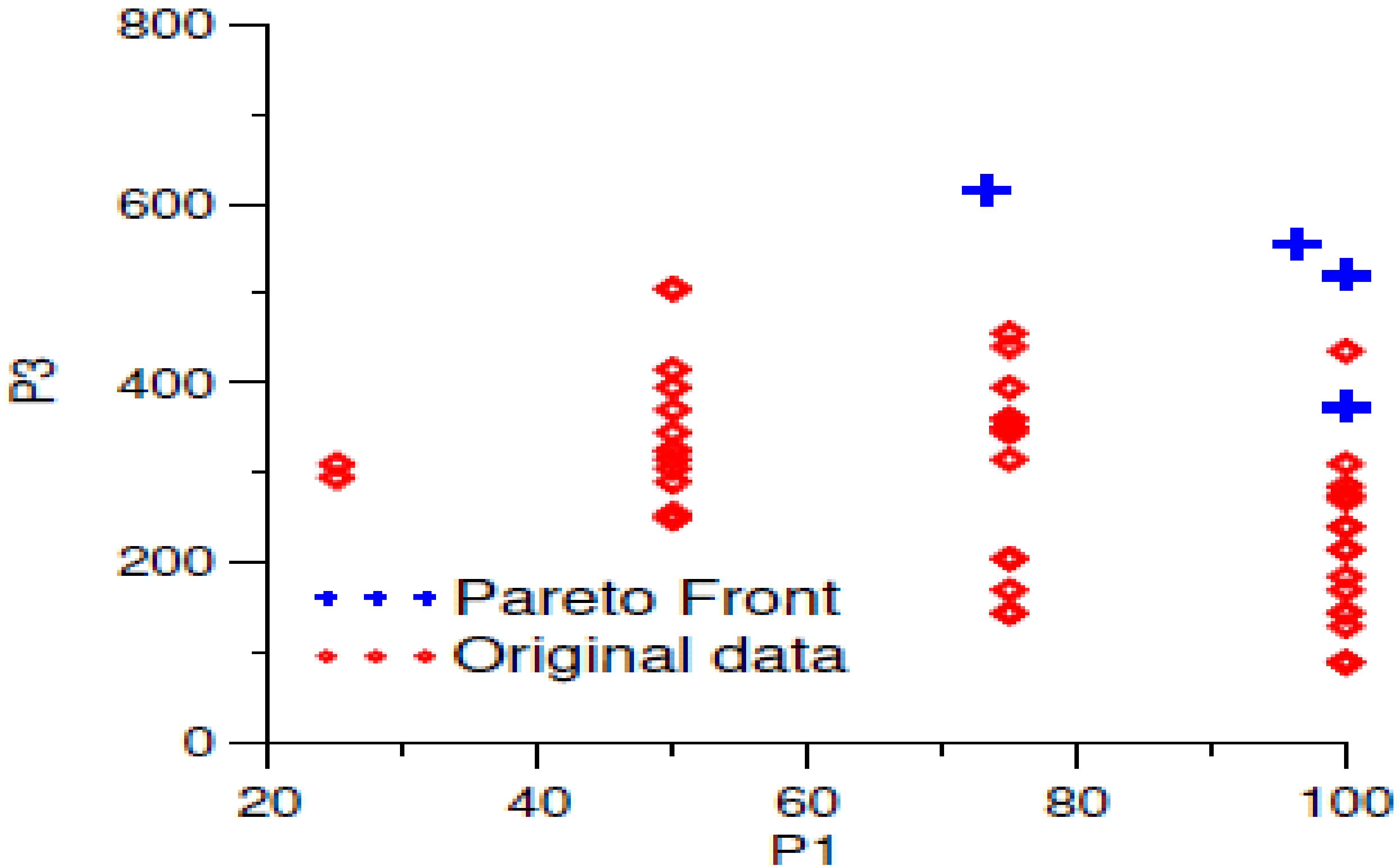
Simultaneous Objectives:

- Maximize Stress Corrosion Crack Resistance (SCCR)
- Maximize Tensile Strength
- Maximize Yield Strength

OPTIMIZATION OF Al-Cu-Zn-Mg-Mn ALLOYS FOR MAXIMUM SCCR (P1) AND MAXIMUM TENSILE STRENGTH (P2) BY DETERMINING PROPER CONCENTRATIONS OF Cu, Zn, Mg, Mn AND TEMPER PROTOCOL



OPTIMIZATION OF Al-Cu-Cn-Mg-Mn ALLOYS FOR MAXIMUM SCCR (P1) AND MAXIMUM YIELD STRENGTH (P3) BY DETERMINING PROPER CONCENTRATIONS OF <u>Cu, Zn, Mg, Mn</u> AND TEMPER PROTOCOL



INVERSE DESIGN OF ALLOYS

FOR A DESIRED (SPECIFIED):

STRESS LEVEL,
TEMPERATURE LEVEL,
LIFE EXPECTANCY

OF A MACHINE PART.

Task:

DETERMINE CONCENTRATIONS OF EACH OF THE ALLOYING ELEMENTS IN AN ALLOY.
ACTUALLY, PROVIDE SEVERAL SUCH ALLOYS SO THAT THE DESIGNER CAN CHOOSE AMONG THEM THE ONE WHICH IS THE CHEAPEST AND MOST OBTAINABLE AT THE TIME OF NEED.

In this problem the percentages of the following 14 elements were treated as independent variables:

C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti.

The ranges of these elements were set as follows. First, minimum and maximum values for existing set of experimental data ($Expmin_i$, $Expmax_i$ = i = 1,..,14) were defined. Then, new minimum and maximum values for each of the 14 elements were obtained according to the following simple dependencies: ($Min_i = 0.9\ Expmin_i$, $Max_i = 1.1\ Expmax_i$ = i = 1,….,14). These ranges are given in Table 1.

Table 1. Ranges of variation of independent variables

	C	**S**	**P**	**Cr**	**Ni**	**Mn**	**Si**
min	0.063	0.001	0.009	17.500	19.300	0.585	0.074
max	0.539	0.014	0.031	39.800	51.600	1.670	2.150

	Mo	**Co**	**Cb**	**W**	**Sn**	**Zn**	**Ti**
min	0.000	0.000	0.000	0.000	0.000	0.001	0.000
max	0.132	0.319	1.390	0.484	0.007	0.015	0.198

Example of an inverse problem of finding chemical composition of an alloy with specified properties

(Problem # 8)

Purpose: **Determine chemical composition of an alloy for specified properties of material by using an existing database**

Problem features:

***variable parameters*: chemical composition of the alloy**

***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti* (14 variables).**

***criteria*: (multi- objective statement – 10 simultaneous objectives)**

- **Specified stress (PSI)** *(PSI-PSI req.)**2 –> minimize*
- **Specified operating temperature (T)** *(T-T req.)**2 –> minimize*
- **Specified time to "survive" until rupture (Hours)** *(Hours-Hours req.)**2 –> minimize*

ALLOY COST MINIMIZATION*:*

Cr -> minimize; Ni->minimize; Mo->minimize; Co->minimize; Cb >minimize;

W >minimize; Sn >minimize; Zn >minimize; Ti >minimize;

constraints: none

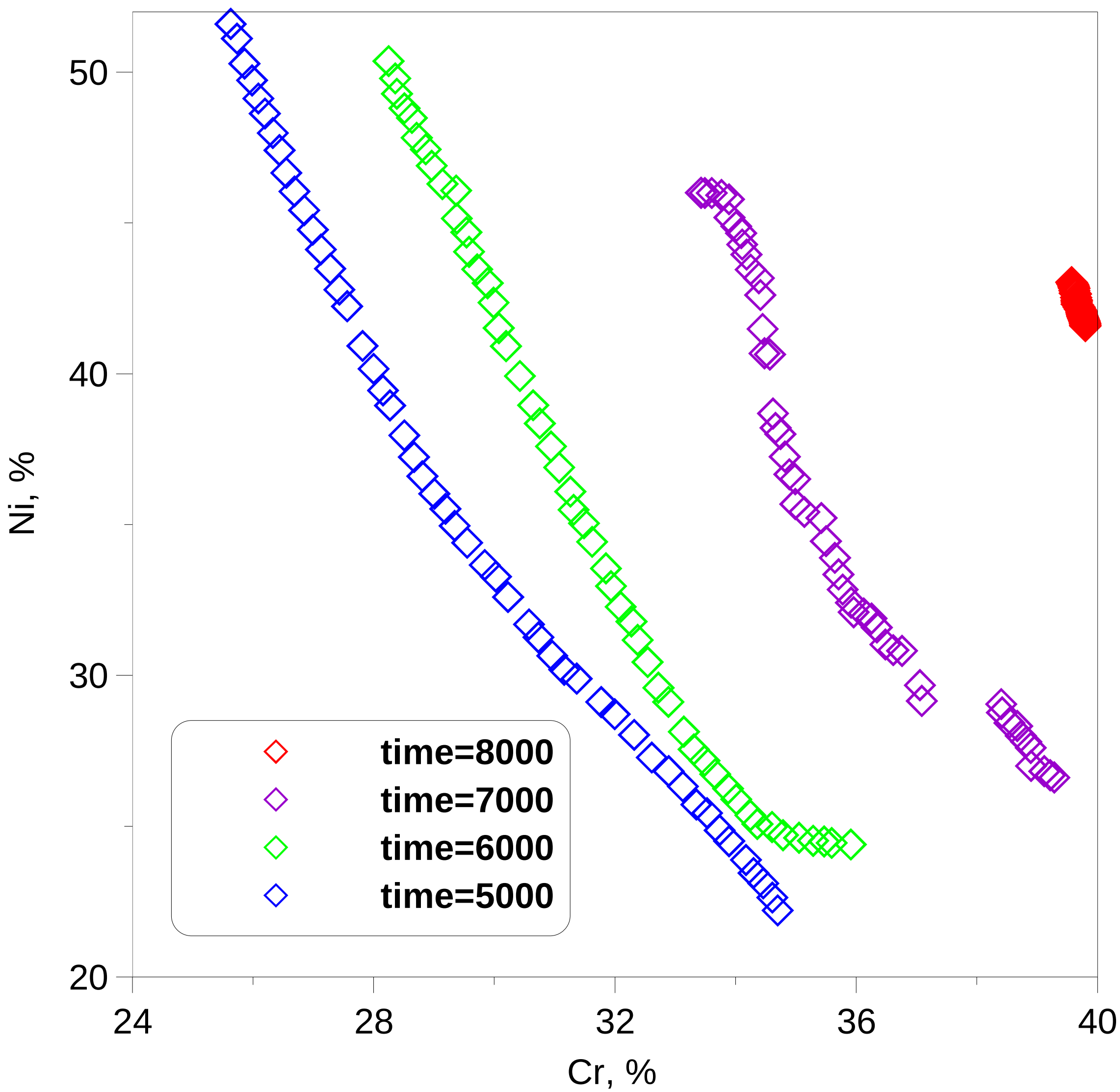
mathematical model: **have none; use an existing experimental database**

Table 1. Eight formulations for objective functions and constraints

		Objectives (minimize)				Constraints (minimize)
Model number	**Number of objectives**	**Stress**	**Operating temperature**	**Time until rupture**	**Low cost alloy**	
1	3	$(\sigma - \sigma_{spec})^2$	$(T - T_{spec})^2$	$(\theta - \theta_{spec})^2$		
2	1	$(\sigma - \sigma_{spec})^2 + (T - T_{spec})^2 + (\theta - \theta_{spec})^2$				
3	3	$(\sigma - \sigma_{spec})^2$	$(T - T_{spec})^2$	$(\theta - \theta_{spec})^2$		$(\sigma - \sigma_{spec}) < \varepsilon$ $(T - T_{spec}) < \varepsilon$ $(\theta - \theta_{spec}) < \varepsilon$
4	1	$(\sigma - \sigma_{spec})^2 + (T - T_{spec})^2 + (\theta - \theta_{spec})^2$				$(\sigma - \sigma_{spec}) < \varepsilon$ $(T - T_{spec}) < \varepsilon$ $(\theta - \theta_{spec}) < \varepsilon$
5	1	$(\sigma - \sigma_{spec})^2$				$(T - T_{spec}) < \varepsilon$ $(\theta - \theta_{spec}) < \varepsilon$
6	1		$(T - T_{spec})^2$			$(\sigma - \sigma_{spec}) < \varepsilon$ $(\theta - \theta_{spec}) < \varepsilon$
7	1			$(\theta - \theta_{spec})^2$		$(\sigma - \sigma_{spec}) < \varepsilon$ $(T - T_{spec}) < \varepsilon$
8	10	$(\sigma - \sigma_{spec})^2$	$(T - T_{spec})^2$	$(\theta - \theta_{spec})^2$	Ni, Cr, Nb, Co, Cb, W, Ti	

Multicriteria optimization of material composition for preset properties (inverse problem) using method #3

Number of variables: 14.
Criteria: Cr and Ni concentration.



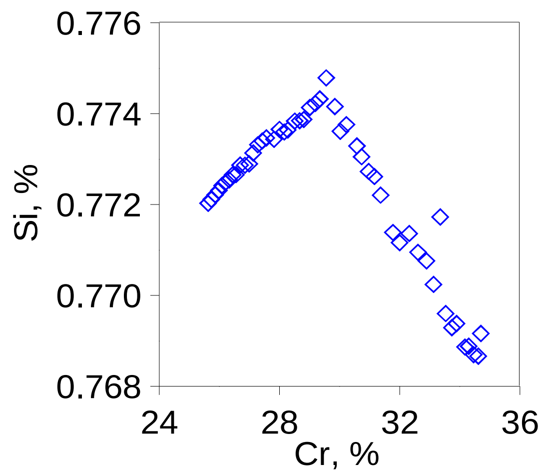
Constraints:
stress=4000 psi;
temperature=1800 F;
time=preset time.

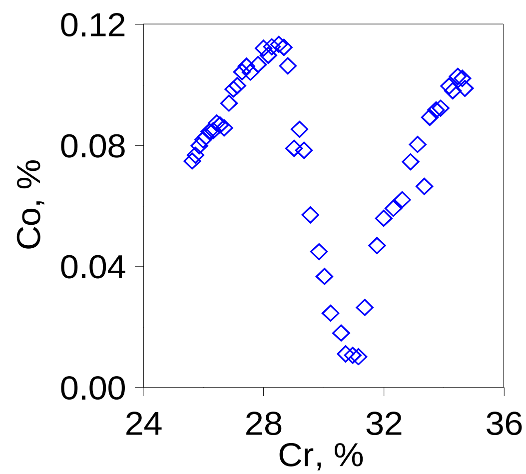
This approach allows us to vary the chemical composition for the same properties !

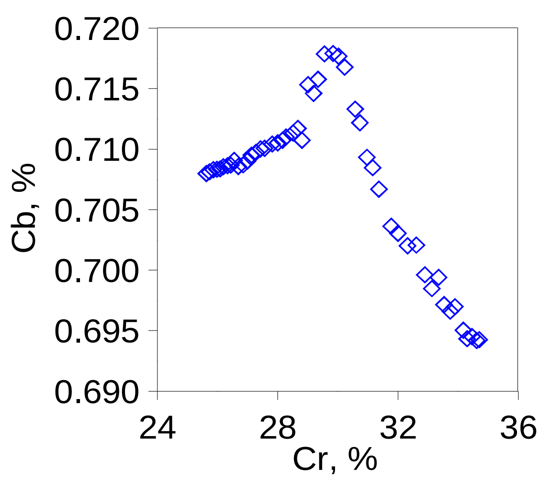
Multi-criteria optimization of material composition for preset properties (inverse problem)

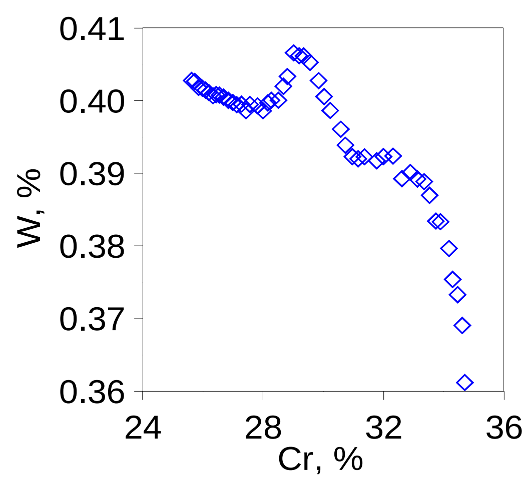
Number of variables (alloying elements): 14.
Criteria: determine Cr and Ni concentrations.

<u>Constraints:</u>
Stress=4000
Temperature=1800
Time=5000.

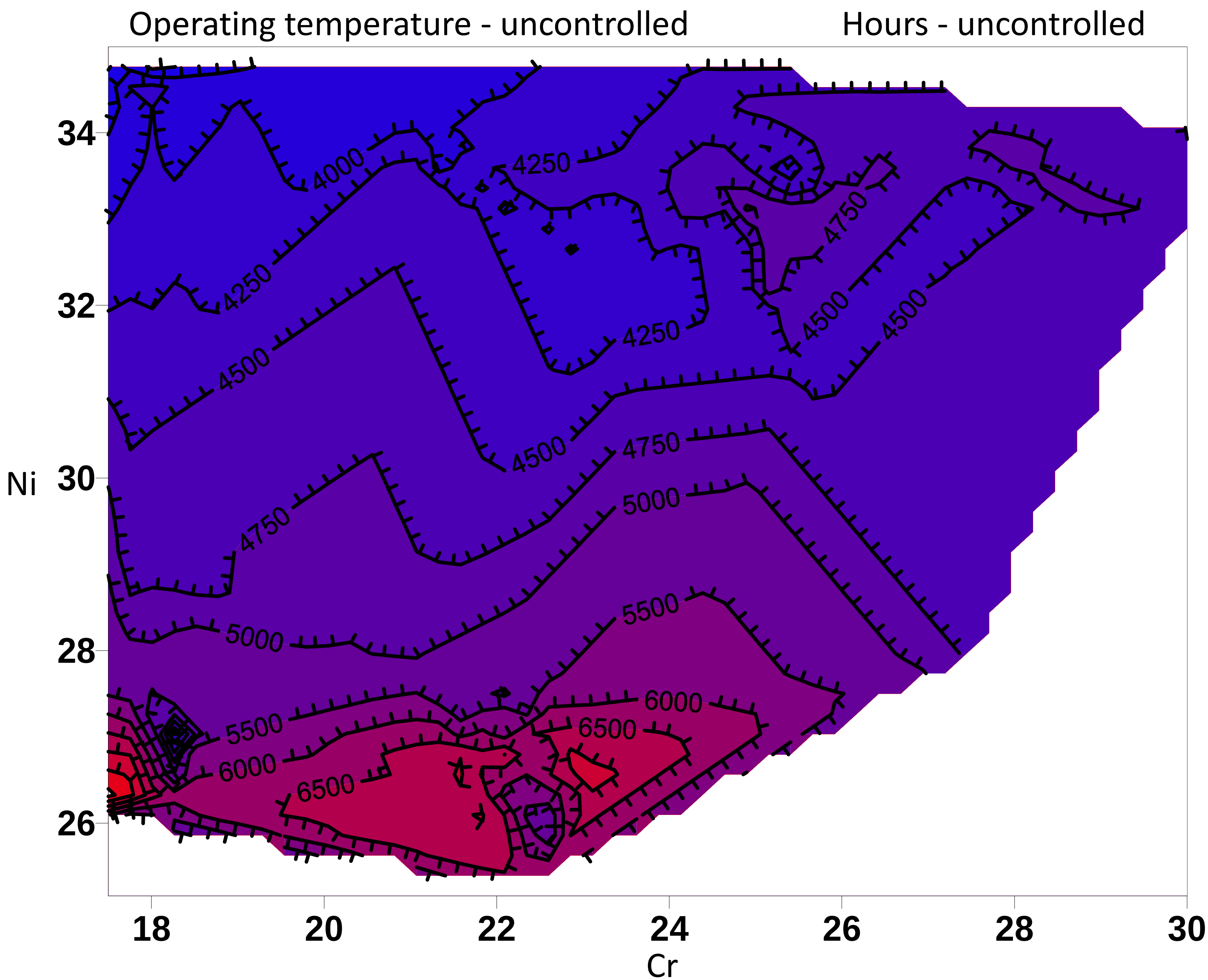




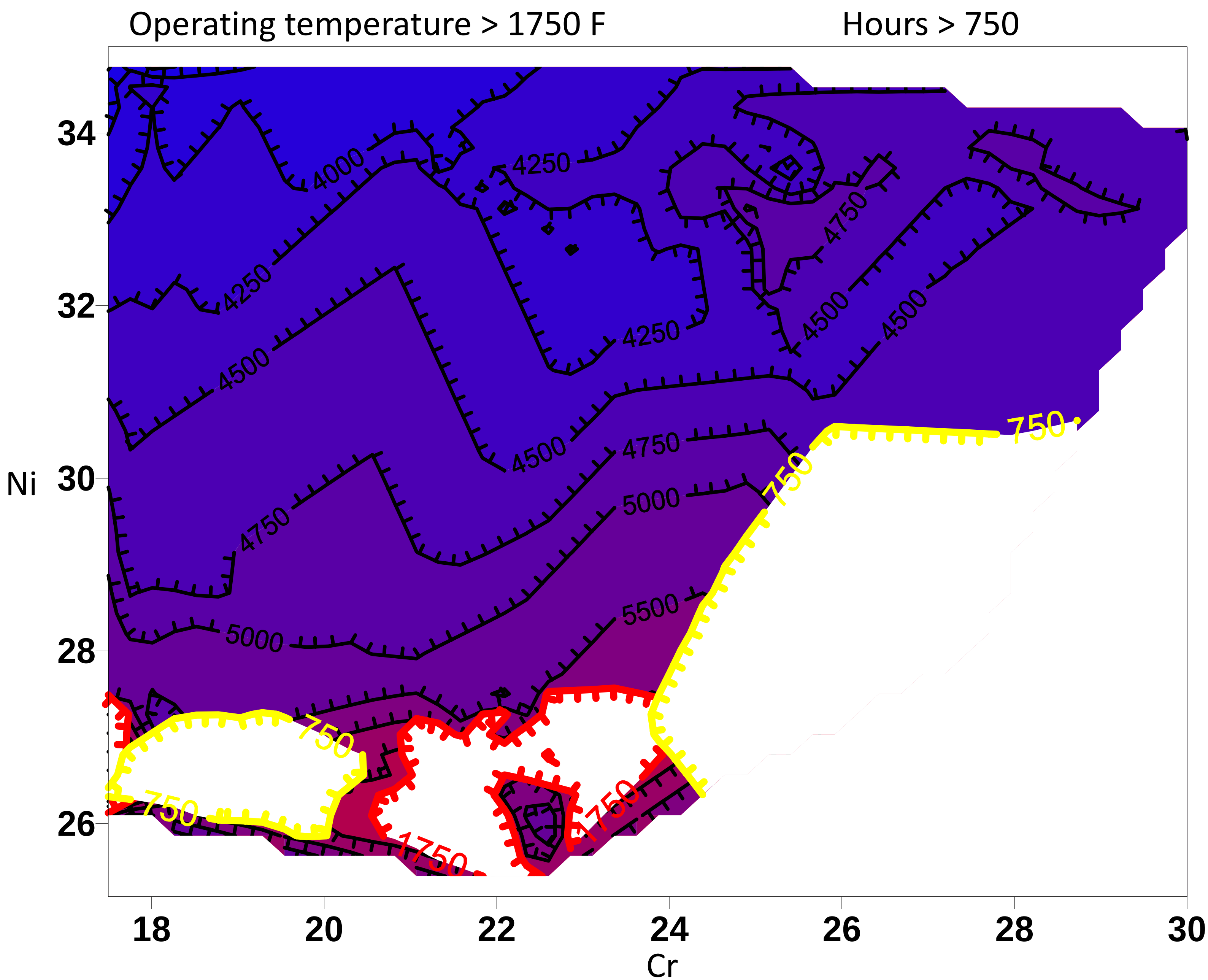




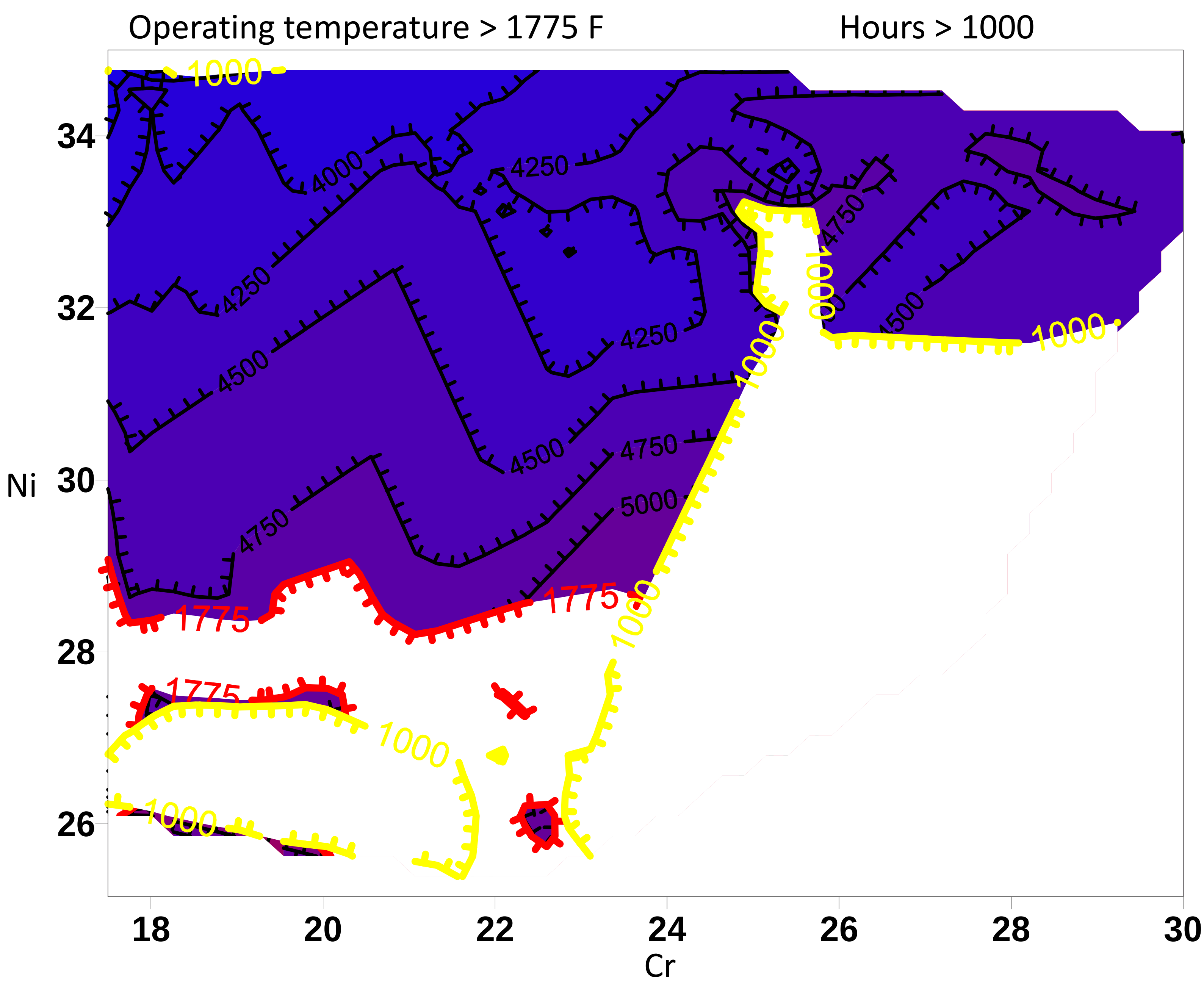
This approach allows us to vary the chemical composition for the <u>same</u> properties !



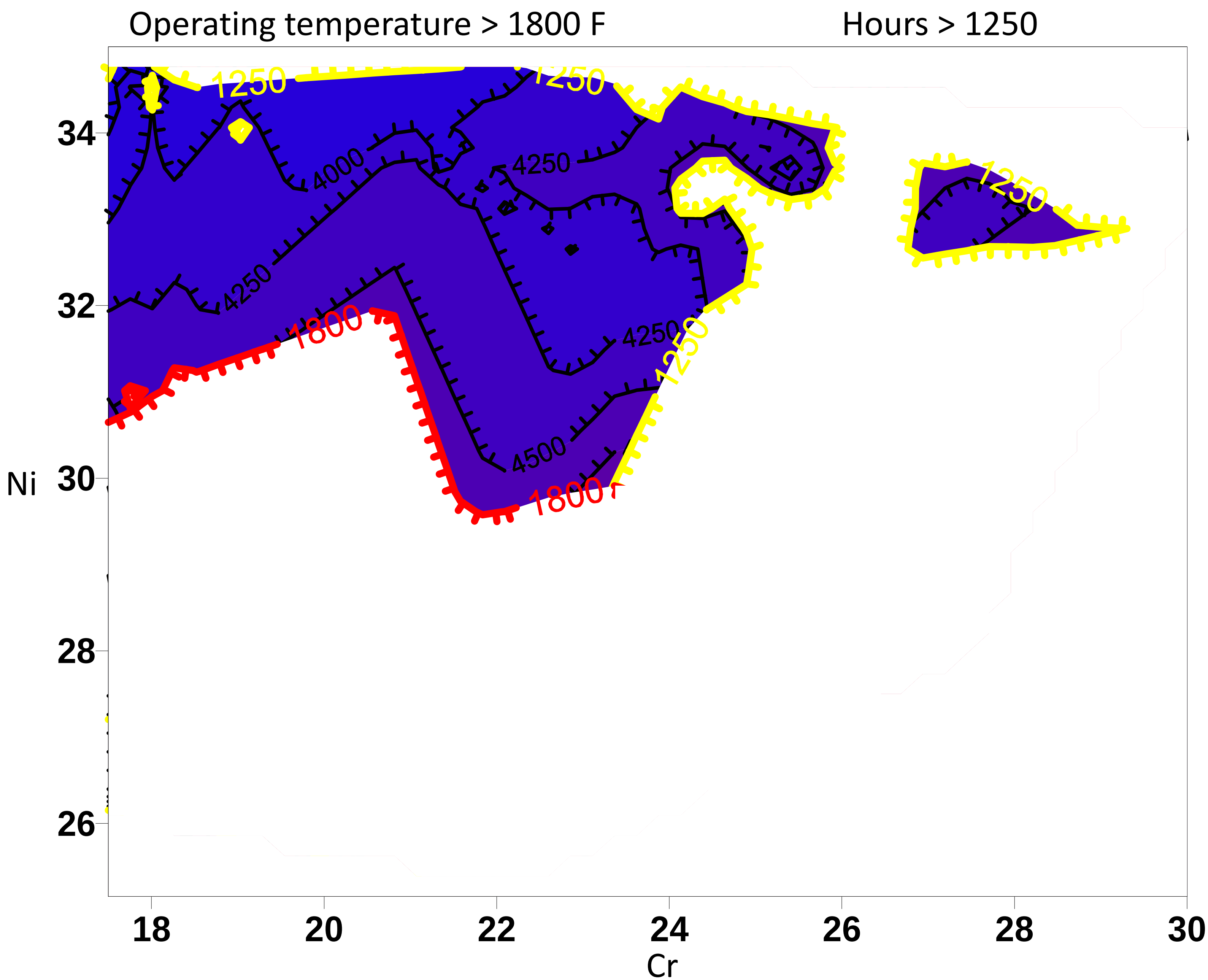
Operating temperature - uncontrolled
Hours - uncontrolled
Ni
Cr
34
32
30
28
26
18
20
22
24
26
28
30
4000
4250
4500
4750
5000
5500
6000
6500



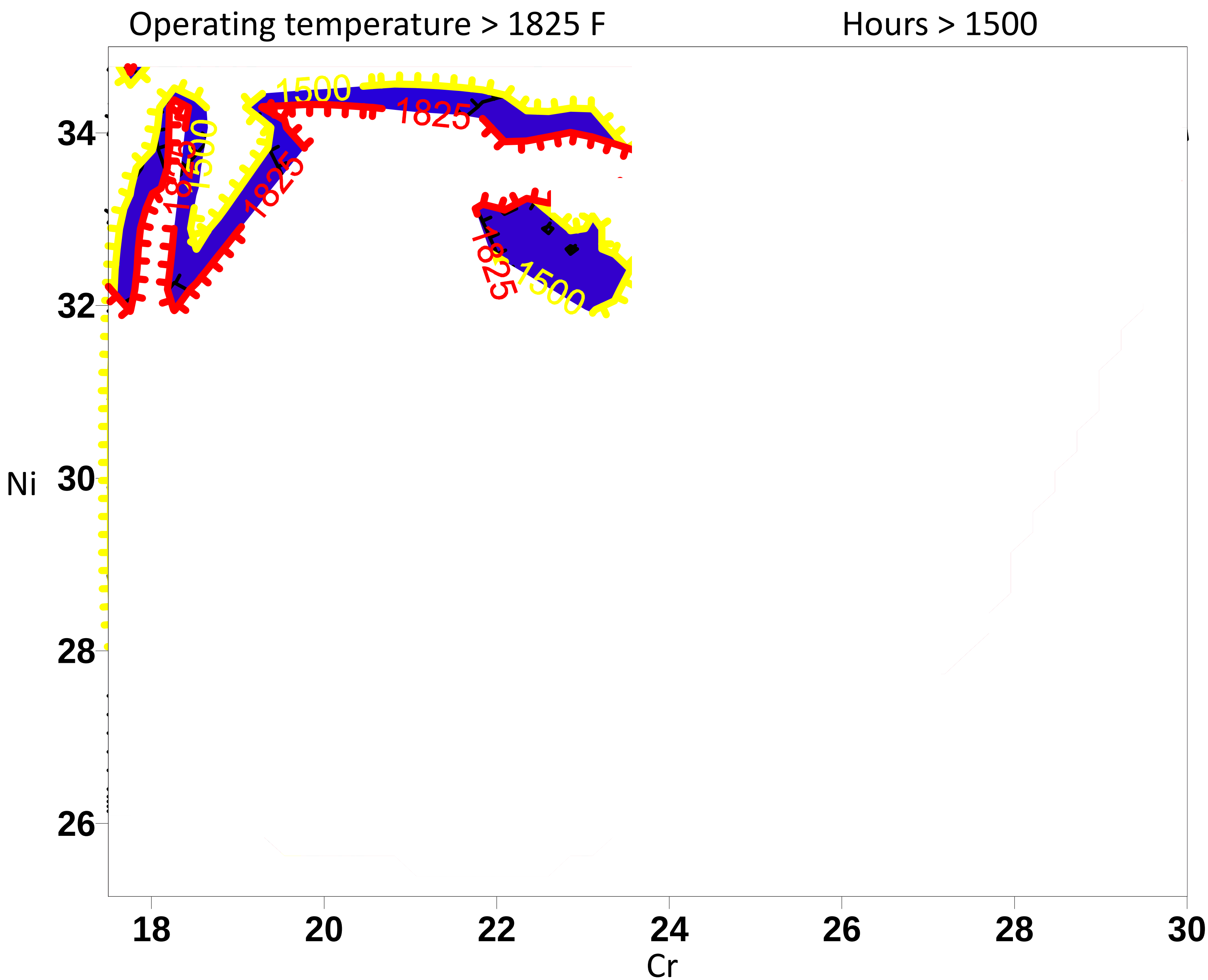
Operating temperature > 1750 F
Hours > 750
Ni
Cr
34
32
30
28
26
18
20
22
24
26
28
30
4000
4250
4500
4750
5000
5500
750
1750



Operating temperature > 1775 F
Hours > 1000
1000
4000
4250
4500
4750
5000
1775
Ni
Cr
34
32
30
28
26
18
20
22
24
26
28
30



Operating temperature > 1800 F
Hours > 1250
1250
1250
1250
1250
4000
4250
4250
4250
4250
4500
1800
1800
Ni
34
32
30
28
26
18
20
22
24
26
28
30
Cr

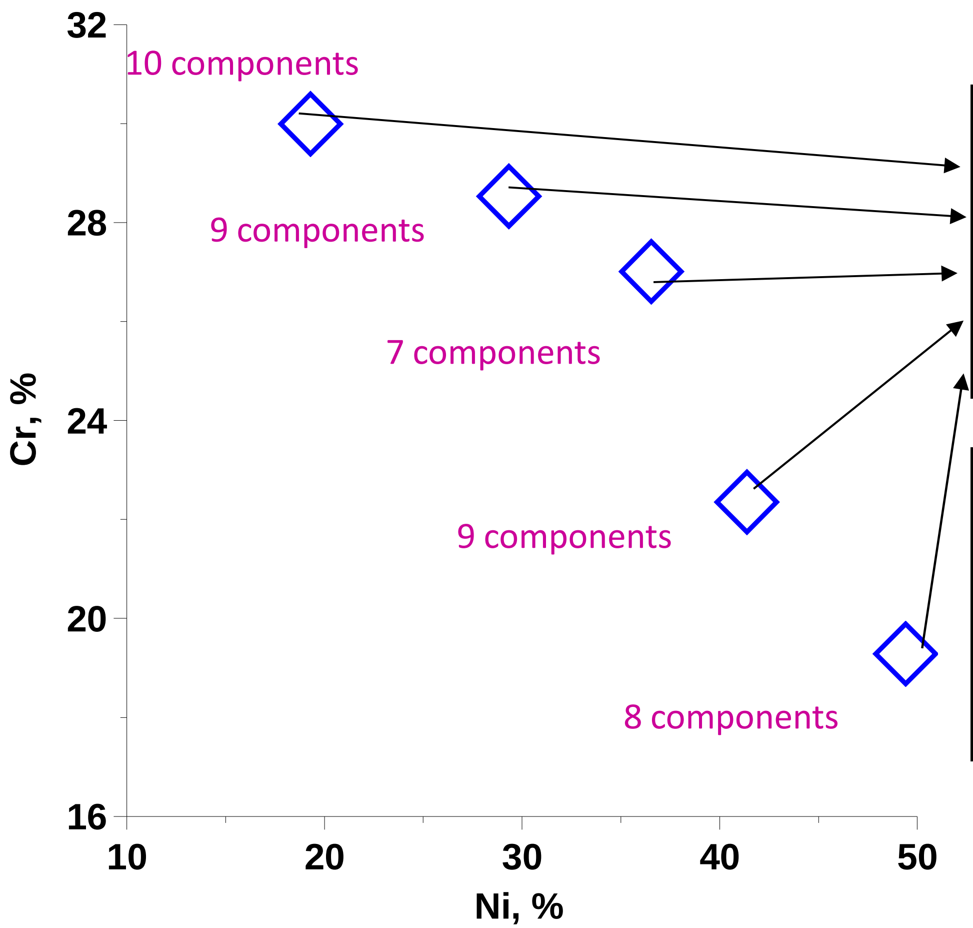


Operating temperature > 1825 F
Hours > 1500
1500
1825
1825
1500
1825
1825
1500
34
32
30
28
26
Ni
18
20
22
24
26
28
30
Cr

Inverse Design Problem

Structural multi-criteria optimization of material composition for preset properties

Example of preset properties: Stress=4000, Temp.=1800, Time=6000;
Criteria: determine Cr and Ni concentrations.



C	S	P	Mn	Si	Cu	Mo
0.529	none	0.02	1.21	none	none	0.065
0.329	none	0.014	0.894	none	none	0.061
0.527	none	none	1.21	none	0.018	0.021
0.506	none	none	0.879	none	none	0.053
0.457	none	none	0.977	none	none	0.013

Pb	Co	Cb	W	Sn	Al	Zn	Ti
0.005	0.003	1.344	0.199	none	0.067	0.001	0.014
0.004	none	1.026	0.188	none	0.074	0.004	0.048
none	none	none	0.281	none	0.074	0.001	0.032
0.005	0.043	0.839	0.37	none	0.034	0.009	0.001
0.003	none	1.367	0.476	none	0.073	0.003	0.059

So, What Exactly is Being Proposed Here?

We propose a novel methodology for predicting the concentration of each of the important alloying elements in magnetic alloys so that the new alloys will have simultaneously maximized:

- **magnetic remanence (Br)** over a range between room temperature and Curie temperature
- **intrinsic coercive field (jH_c)** over a range between room temperature and Curie temperature
- **energy density (BH_{max})** over a range between room temperature and Curie temperature
- **Curie temperature**
- **tensile strength** over a range between room temperature and Curie temperature

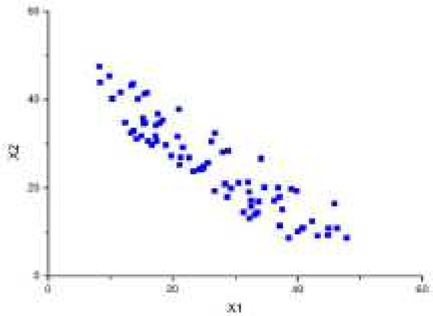
while minimizing the concentration of rare earth elements and other expensive elements.

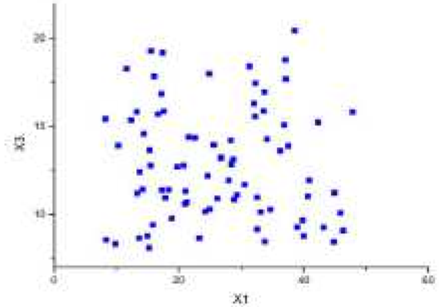
- The proposed optimization method is based on combining experimentally obtained multiple properties of the magnetic alloys (at NCSU) and FIU’s sophisticated, multi-objective, hybrid, evolutionary optimization algorithm.
- It utilizes a polynomial form of radial basis functions and a self-organizational concept to construct multidimensional response surfaces.
- During the iterative computational design process, a small set of new magnetic alloys will be periodically predicted (optimal concentrations of each of the alloying elements in each of them will be predicted), manufactured, and experimentally evaluated for their multiple physical properties in order to continuously verify the accuracy of the entire design methodology.

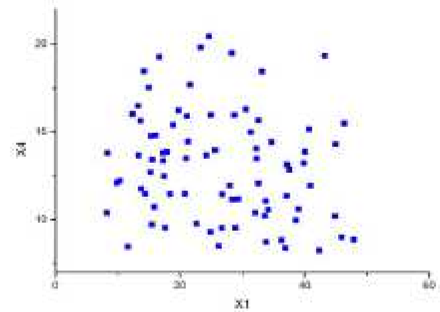
- The proposed alloy design optimization method, thus, will minimize the need for costly and time-consuming experimental evaluations of new alloys.
- This method is capable of exploring alloy concentrations that are outside the initial data set, thus providing a more economical and robust design tool than when using Artificial Neural Networks or Genetic Algorithms alone or in their combination.
- Basic concepts of the proposed method were used by the PI to design H-type steels, Ni-base superalloys, Hf-base BMGs, Ti-base alloys, and Al-base alloys.
- It was shown to be applicable to design optimization of alloys with an arbitrary number of alloying elements and has been tested for up to 12 properties that are simultaneously extremized.

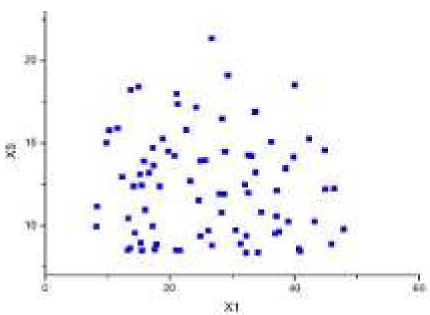
- In this work, an updated version of the FIU's Multi-Objective Hybrid Optimizer (MOHO) will be used.
- The optimizer utilizes several multi-objective, evolutionary optimization algorithms and orchestrates the application of these algorithms to multi-objective optimization problems, using an automatic internal switching algorithm.
- The switching algorithm is designed to favor those search algorithms that quickly improve the Pareto approximation and grades improvements using five criteria.
- A thorough testing of reliability and accuracy of MOHO against a number of prominent multi-objective optimization algorithms and one hybrid optimizer confirmed that MOHO performs reliably and accurately.

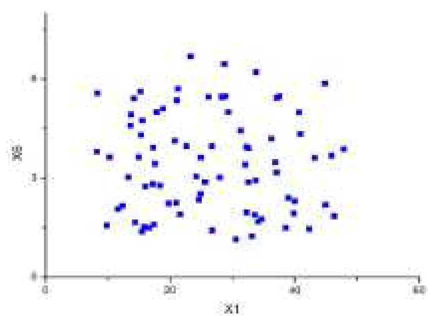
Concentrations at.% for the initial population of 80 candidate alloys, each virtually obtained using Sobol's quasi-random sequence generation algorithm with constraints.

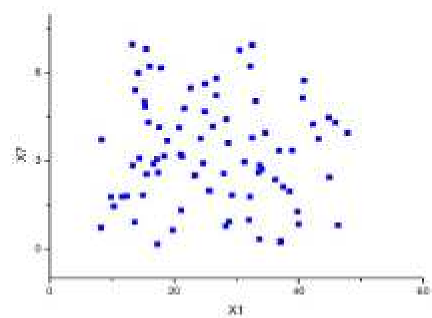


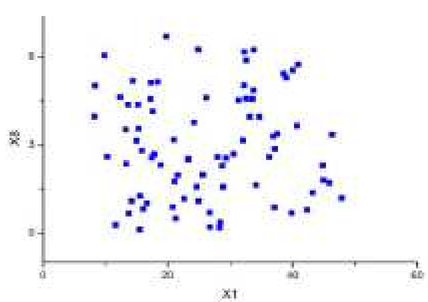






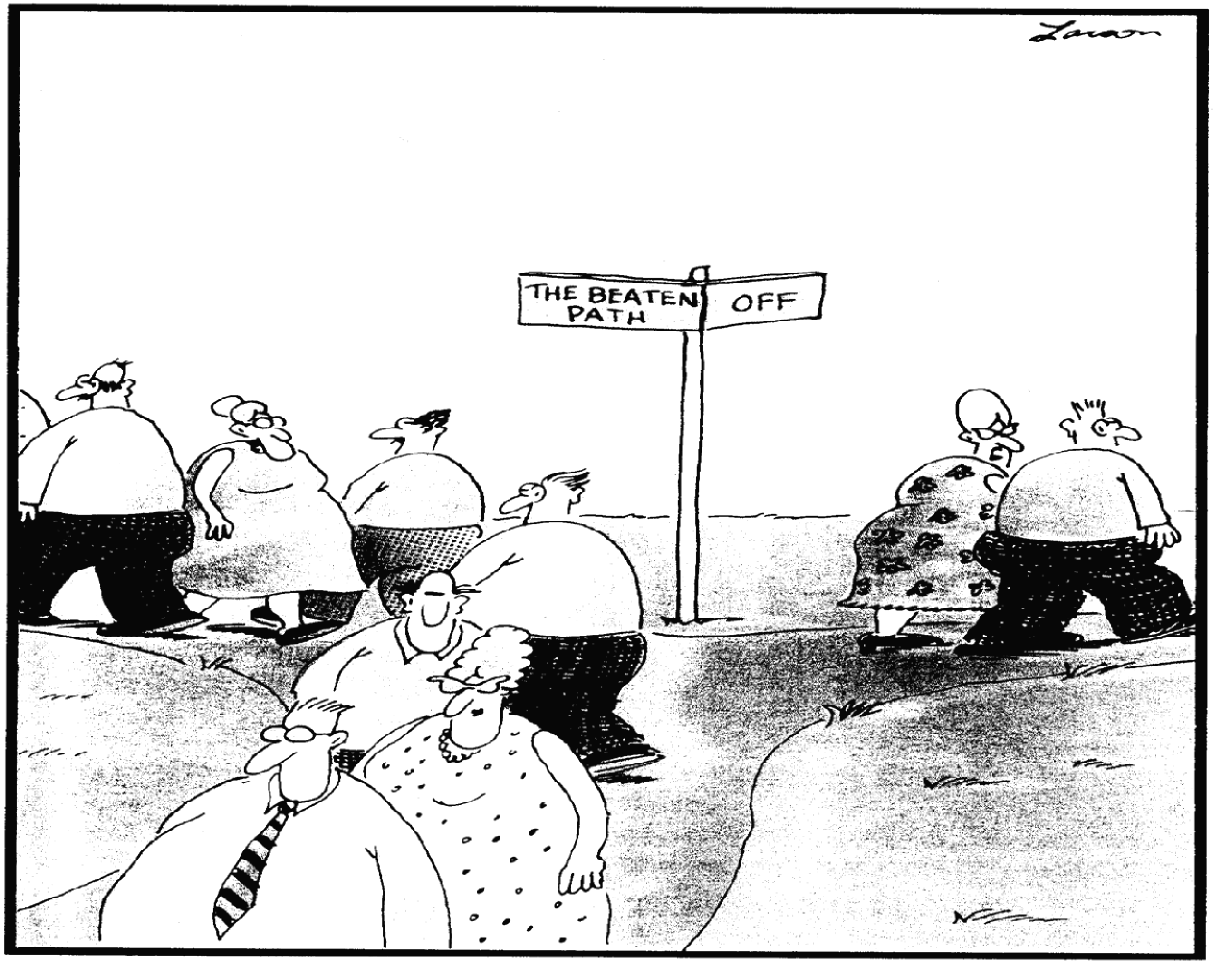






Alloying elements concentrations at.%								
	Fe	Co	Zr	Hf	Ti	B	Si	Mo
Min	7.5	7.5	8.0	8.0	8.0	1.0	0.1	0.1
max	67.3	67.3	22.0	22.0	22.0	7.0	7.0	7.0

Multidisciplinary Research is fun!



"I don't know if this is such a wise thing to do, George."