

OPTIMIZATION OF CONCENTRATIONS OF ALLOYING ELEMENTS IN STEEL FOR MAXIMUM TEMPERATURE, STRENGTH, TIME-TO-RUPTURE AND MINIMUM COST AND WEIGHT

Key words: Multi-objective optimization; Metal alloys; Alloy design.

Abstract: This prospect is based on the use of experimental data and a new evolutionary truly multi-objective optimization algorithm for simultaneously optimizing several properties of steel alloys while minimizing the number of experimental evaluations of the candidate alloys. This approach has been shown to have the potential of identifying new chemical compositions for significantly superior performance alloys requiring as few as 80 new alloy samples that otherwise could not be identified with classical techniques without requiring thousands of new alloys. Furthermore, this approach has been demonstrated to have the potential for determining concentrations of alloying elements for a specified set of alloy's properties for specific applications, thereby maximizing their utilization. Cost and weight are two of the objectives in addition to the more standard objectives such as maximized operating temperature, tensile stress and time-to-rupture.

1 INTRODUCTION

This prospect is based on the use and a special adaptation of a multi-objective constrained Indirect Optimization based upon Self-Organization (IOSO). This multi-objective optimization algorithm allows for concentrations of a number of alloying elements to be optimized so that a finite number of properties (maximum tensile strength, maximum operating temperature, maximum time-until-rupture, minimum weight, minimum cost, etc.) of the alloy are simultaneously extremized, while satisfying a number of equality and inequality constraints.

IOSO multi-objective optimization algorithm is of a semi-stochastic type incorporating certain aspects of a selective search on a continuously updated multi-dimensional response surface. Objective function evaluations in this particular project were obtained utilizing experimental testing and verification of the initial alloy samples and all newly created alloys in order to determine optimum concentrations of each of the alloying elements. This novel alloy design tool is expected to minimize the need for the addition of expensive alloying elements and still obtain the optimum properties needed to design the components. The main benefits of IOSO algorithm are its outstanding reliability in avoiding local minimums, its computational speed, and a significantly reduced number of required experimentally evaluated alloy samples as compared to more traditional gradient-based and genetic optimization algorithms. Also, the self-adapting multi-dimensional response surface formulation used by IOSO allows for incorporation of realistic non-smooth variations of experimentally obtained data and allows for accurate interpolation of such data.

2 OPTIMIZING ALLOYS FOR MAXIMUM PERFORMANCE BY UTILIZING AN EXISTING DATABASE

An initial database was obtained containing experimentally measured mechanical properties on 201 H-type cast steel alloys. However, certain alloys did not have complete information on alloy chemical composition. These alloys were deleted from the set. This resulted in the final database having only 158 steel alloys.

Concentrations of the following 17 elements were taken as independent variables:

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

The minimum and maximum values for the concentrations of each element were determined from the existing set of experimental data ($Exp_min_i, Exp_max_i, i = \overline{1,17}$). Then, new minimum and maximum values for each of the 17 elements were obtained as follows:
 $Min_i = 0.9 \cdot Exp_min_i, Max_i = 1.1 \cdot Exp_max_i, i = \overline{1,17}$ (Table 1).

Table 1. Ranges of concentrations of 17 independent design variables
(chemical elements in the steel alloy)

	C	S	P	Cr	Ni	Mn	Si	Cu	Mo
min	0.063	0.001	0.009	17.500	19.300	0.585	0.074	0.016	0.000
max	0.539	0.014	0.031	39.800	51.600	1.670	2.150	0.165	0.132

	Pb	Co	Cb	W	Sn	Al	Zn	Ti
min	0.001	0.000	0.000	0.000	0.000	0.001	0.001	0.000
max	0.006	0.319	1.390	0.484	0.007	0.075	0.015	0.198

The following parameters were then used as optimization objectives:

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

During this research the solution of a simultaneous three-objective optimization problem and a series of two-objectives problems were accomplished when one of the considered parameters was constrained.

During the first stage, the problem of simultaneously optimizing three objectives was solved with 100 points of Pareto optimal solutions (Fig. 1). Analysis of this result allowed us to extract an area of admissible combinations of different optimization objectives since results were distributed in the admissible part of the objectives' space quite uniformly.

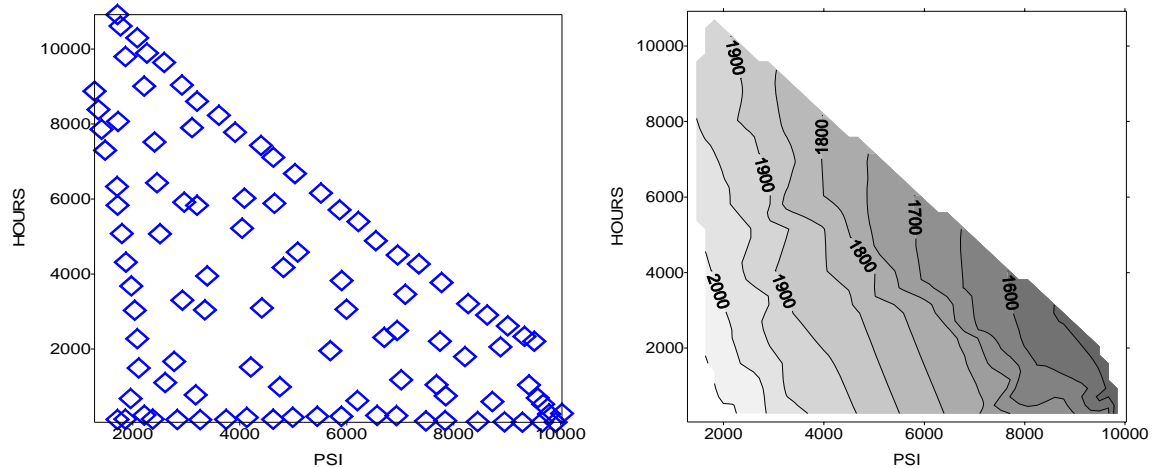


Fig.1. Time-to-rupture vs. strength for three-objectives Pareto set using 17 design variables. Constant temperature contours are also indicated in degrees Fahrenheit.

Such a distribution offers a possibility for a significant improvement of accuracy of response surfaces on condition that the experiments will be carried out at the obtained Pareto optimal points. Then, in accordance with the elaborated technique, it is necessary to conduct experiments at the obtained Pareto optimal points, evaluate accuracy of prediction of values of partial optimization objectives, and either complete the process or perform another iteration.

3 DESIGN OPTIMIZATION OF NEW GENERATIONS OF STEEL ALLOYS UTILIZING EXPERIMENTAL VERIFICATION

This work represents the first experimentally verified attempt to step out of the initially available database when optimizing nickel based heat-resistant alloy castings containing *Ni, C, Cr, Co, W, Mo, Al, Ti, B, Nb, Ce, Zr, Y*, and *S, P, Fe, Mn, Si, Pb, Bi* as trace elements. Heat treatment of the samples of such alloys involved heating to 1210 C, holding for 4 hours, and air cooling to room temperature. During these tests the maximum stress at room temperature (σ) and the time to survive until rupture at 975 C and 230 N/mm² load were measured. Manufacturing of all of the alloys involved in this case and experimental testing of their properties were carried out in the same certified metallurgical institute. Chemical

compositions of these alloys differed by varying concentrations of the following seven elements: *C, Cr, Co, W, Mo, Al, Ti* (Table 2). The concentration of *Nb* in all tests was 1.1%, while concentrations of *B, Ce, Zr, Y* were 0.025%, 0.015%, 0.04%, and 0.01% respectively. The concentration of nickel made the rest of 100% of the alloy. Average percents of the addition agents were negligible.

Table 2. Ranges of design variables (concentrations of 7 major alloying elements)

	C	Cr	Co	W	Mo	Al	Ti
min	0.13	8.0	9.0	9.5	1.2	5.1	2.0
max	0.20	9.5	10.5	11.0	2.4	6.0	2.9

During each IOSO iteration, a two-criterion optimization task with 20 Pareto optimal points was solved. The two simultaneous optimization objectives were: maximize stress and maximize time-to-rupture at elevated temperature. The initial database contained 120 experimentally tested steel alloys whose concentrations were specified using Sobol's algorithm so that they are as uniformly distributed as possible. After that, 4 iterations were conducted using IOSO with 20 new (Pareto optimal) alloys predicted and consequently experimentally tested after each iteration. Thus, the total number of experimentally tested alloys during the solution of the entire optimization problem using IOSO was only 200 which is considered a significant improvement over the current alloy design methodologies. The accuracy and predicting capabilities of the self-adapting response surfaces generated by IOSO were constantly improving during the optimization process. A summary of the evolution of the Pareto front through four IOSO iterations (Fig. 2) demonstrates that IOSO is capable of reliably predicting concentrations of alloying elements that create superior performance steel alloys after each application of IOSO. Notice that all data presented in these figures are the results of experimental evaluations involving 120 original database alloys and four sets of 20 alloys each predicted by the IOSO algorithm.

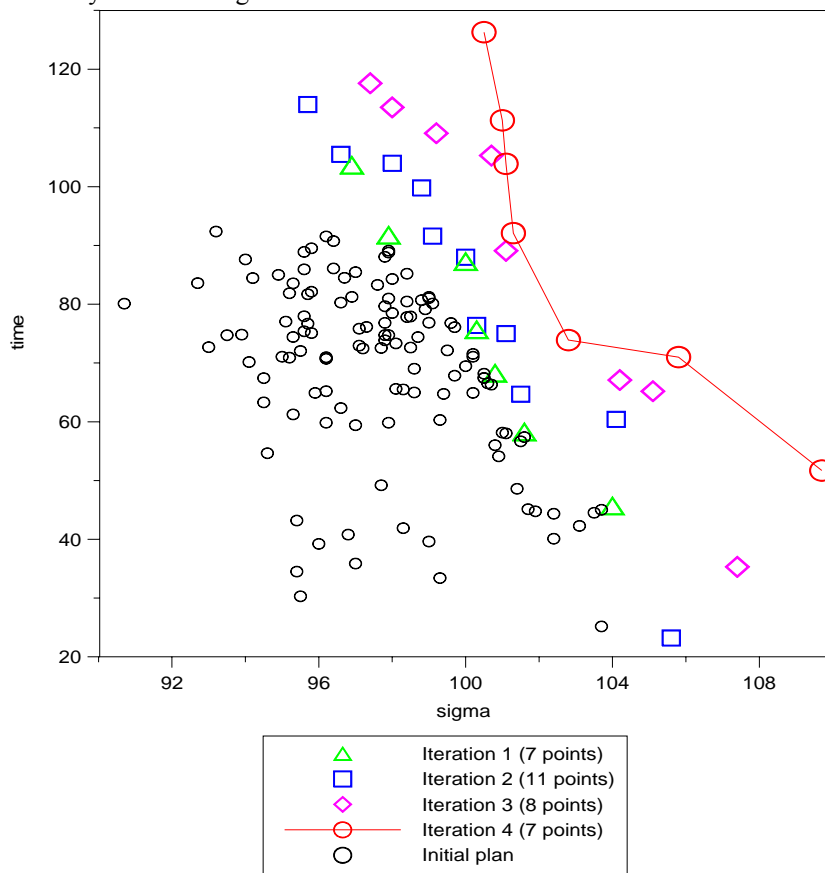


Figure2: The dynamics of change of Pareto optimal solutions after each of the four iterations with IOSO.

4 INCLUDING MINIMUM COST AND WEIGHT OBJECTIVES

In many applications it is highly desirable to use as light alloys as possible. Yet, it is well-known that high temperature resistant alloys require ingredients that have the highest melting points. However, these alloying elements are also very dense, thus heavy. This is an obvious example of a multi-objective optimization where some of the objectives (in this case high temperature resistance and weight) are highly opposing.

Furthermore, certain alloying elements are considerably more expensive than other elements. In direct response to a rapidly increasing demand from industry and military to develop high performance alloys that will also be affordable, we obtained a standard daily price list of typical alloying elements available on the metals market. We also obtained a list of densities of these alloying elements. The original idea was to optimize simultaneously the following five objectives: maximum stress, maximum temperature, time-to-rupture, minimum cost of the raw ingredients, and minimum volume-specific weight (density) of the resulting metal alloy. However, we reformulated it as a sequence of five different multi-objective optimization problems that are depicted in Fig. 3-6.

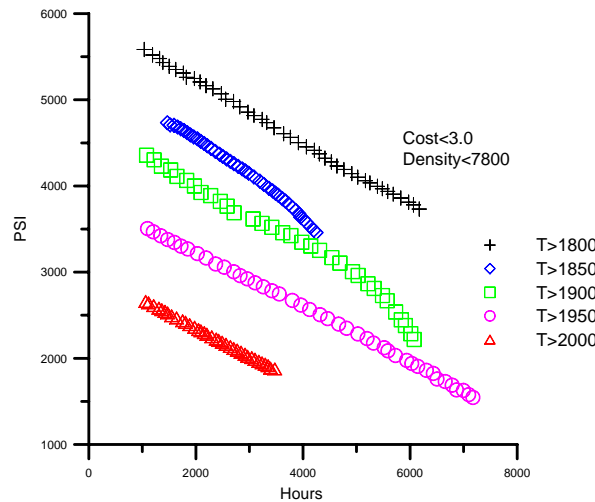


Figure 3: Pareto fronts for two primary constraints (minimum cost and minimum specific weight) and five secondary constraints (maximum temperature).

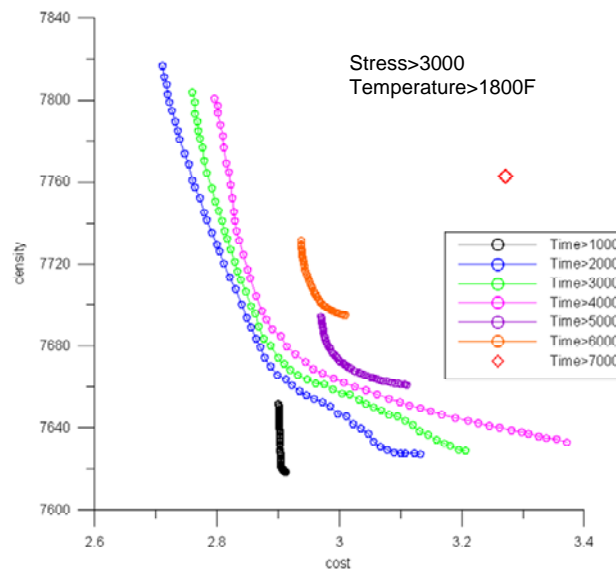


Figure 4: Pareto fronts for two primary constraints (maximum stress and maximum temperature) and seven secondary constraints (time-to-rupture).

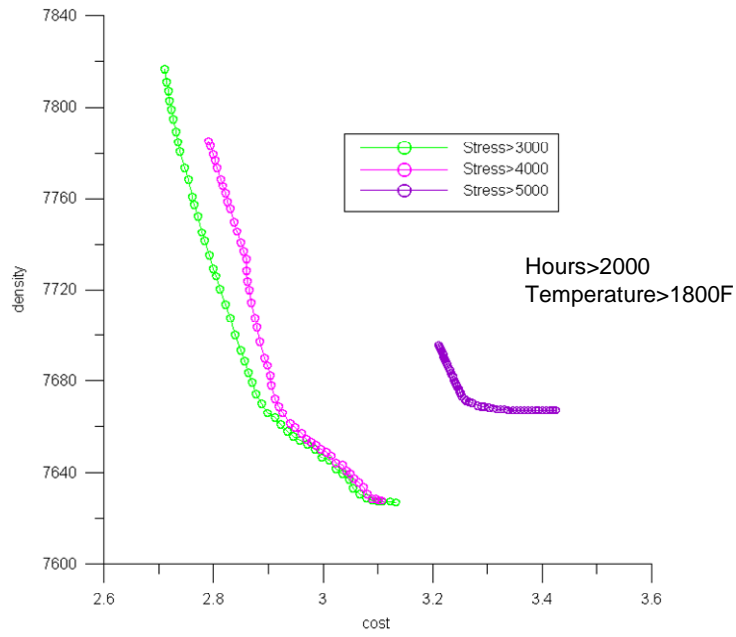


Figure 5: Pareto fronts for two primary constraints (time-to-rupture and maximum temperature) and three secondary constraints (maximum stress).

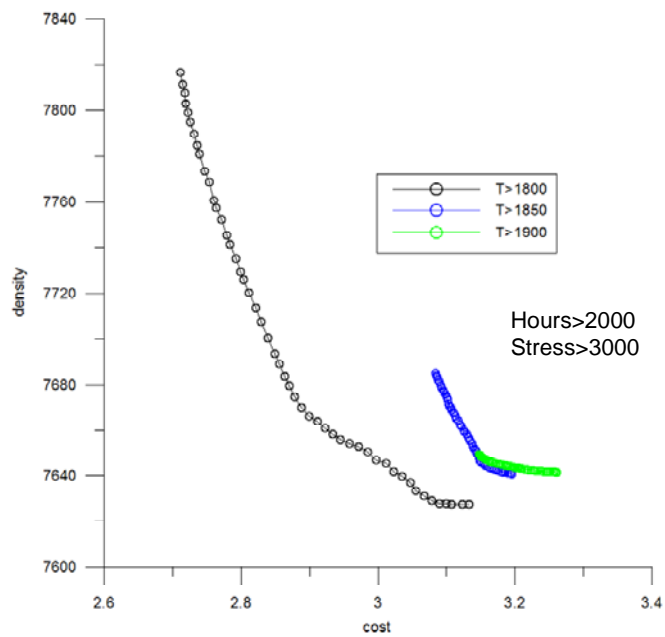


Figure 6: Pareto fronts for two primary constraints (time-to-rupture and maximum stress) and three secondary constraints (maximum temperature).

5 INVERSE DESIGN OF ALLOYS FOR SPECIFIED PROPERTIES

This is an entirely new concept in design of alloys. The inverse problem in this case is determination of chemical composition(s) of alloy(s) that will provide specified levels of, for example, stress at a specified temperature for the specified length of time. The inverse problem can be then formulated as, for example, a multi-objective optimization problem with a given set of equality constraints. We have used IOSO multi-objective optimization algorithm to achieve the solution of this type of inverse alloy design problem. The results (Fig. 7) demonstrate that it is possible to create a large number of alloy compositions that will satisfy the specified multiple properties. It should be pointed out that these are the visualizations of only two (Cr and Ni) of the 14 chemical elements whose concentrations were optimized in order to illustrate how the inverse design method works.

Notice that when the temperature and the life expectancy are introduced and progressively increased, the feasible domain for varying most of the alloying elements' concentrations will rapidly shrink. Similar general trend can be observed when the life expectancy is specified and progressively increased.

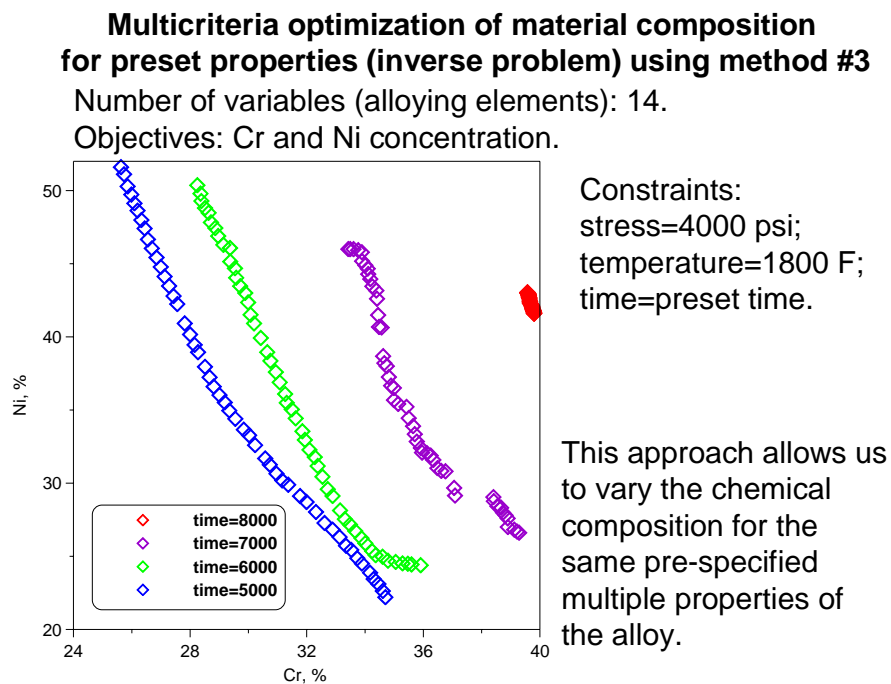


Figure 7: Inversely designed Pareto optimal concentrations of Ni and Cr as a function of time constraint.

CONCLUSIONS

The exposed alloy design methods use an evolutionary optimization algorithm that utilizes neural networks, radial basis functions, Sobol's algorithm, and self-adapting multi-dimensional response surface concepts based on graph theory. Evaluations of physical properties of all alloys (maximum stress at elevated temperature, maximum operating temperature, time-to-rupture at elevated temperature) were performed using classical experimental techniques thus automatically confirming the validity of the predictions of properties of the optimized alloys. Alloys were successfully designed for minimum weight and minimum cost of raw ingredients in addition to the multiple physical properties like maximum stress, time-to-rupture and operating temperature. These alloy design methods could also incorporate uncertainty of the alloy manufacturing and testing. These design methods are applicable to design of any type of alloys and could account for additional desired features of new alloys like corrosion resistance, microstructure features, thermal and mechanical treatment, manufacturing cost, etc.