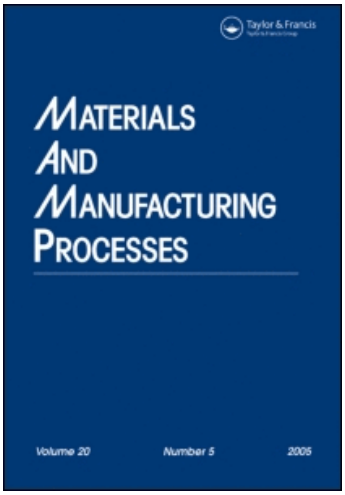

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Stress Corrosion Cracking Resistant Aluminum Alloys: Optimizing Concentrations of Alloying Elements and Tempering

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The objective of this study is to develop a new family of aluminum alloys with superior stress corrosion cracking resistance (SCCR) and mechanical properties. This approach uses experimentally obtained stress corrosion resistance, tensile strength, and yield strength data from the literature and then performs hybrid multiobjective evolutionary optimization combined with multidimensional response surfaces. This software has the proven capability to deal with various alloy design applications using minimal amount of experimental data. The selected objectives in this study are superior stress corrosion resistance, tensile strength, and yield strength. The design variables are concentrations of alloying elements and the individual alloy tempers as they are important parameters that directly affect macroscopic properties and microscopic details of the alloy such as grains, phases, precipitates, etc. The computational trials yield optimal alloys' chemical compositions and standard thermal treatment protocols for the best combination of superior stress corrosion resistance and mechanical properties. Single-objective optimization results confirm the known experimental observations that dilute Al alloys yield the best corrosion resistance at the expense of tensile strength. Optimizations with two simultaneous objectives and more alloying elements create better trade-off solutions. Quality and number of initially available experimentally evaluated alloys have decisive effects on accuracy of this alloy design method.

Keywords Alloy design; Alloy optimization; Alloy tempering; Aluminum alloys; Stress corrosion.

Introduction

The basic assumption in this work is that multiple thermomechanical properties of aluminum alloys depend strongly on the concentrations of each of the alloying elements and on the thermal treatment (tempering) of such alloys in an a posteriori mode. Thus, extreme thermomechanical properties of such alloys could be obtained if appropriate (optimized) values of concentrations of each of the alloying elements could be found simultaneously with an appropriate (optimized) thermal treatment. Obtaining the best trade-off (Pareto frontier) optimized alloys cannot be performed using a brute-force approach. It would take an exorbitant number of candidate alloys to be generated and experimentally evaluated. For example, if only three alloying elements are used in an alloy, the concentrations of each of the two alloys should be varied in increments of, say, 10%. This means that 1000 alloys would need to be manufactured and tested so that a meaningfully accurate search could be performed in this three-dimensional space of design variables (concentrations of the three alloys). This means that in the case of an alloy with six alloying elements, this "optimization" would require determining properties of $10^{**}6 = 1{,}000{,}000$ alloys, each having a different chemical composition. This approach is obviously unrealistic and should be replaced by a more economical mathematical optimization in order to reduce the number of alloy candidates by orders of magnitude.

In order to significantly reduce the number of experimentally evaluated alloys in the alloy design process, during the past decade, there has been an intense effort to develop and use several very complex mathematical models that are based on nonequilibrium thermodynamics of solids, thus minimizing the need for manufacturing and experimental evaluation of the actual alloy samples. However, the exclusive use of this strictly computational approach has been shown to have its own limitations concerning reliability and versatility, as demonstrated by Bhadeshia [1] and Bhadeshia and Sourmail [2]. For example, artificial neural networks (ANNs) are efficient interpolating ("data mining") algorithms for multiparameter functions, but they are not capable of performing reliable extrapolations outside of an initial data set. Therefore, ANNs cannot be used alone for designing truly new alloys with possibly significantly better multiple properties than any of the alloys that belong in the initial data set. Moreover, ANNs require a large number of alloys having different chemical concentrations to be manufactured and tested in order to provide a sufficiently reliable training set. An alternative to ANNs is using genetic algorithms [3] for designing new alloys. Even with this approach, the number

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of alloys that need to be manufactured and experimentally evaluated becomes too large, as the number of alloying elements in an alloy is increased.

The proposed methodology [4–13] for simultaneously extremizing the multiple properties of alloys, by accurately determining proper concentrations of each of the alloying elements, is based on combining: a) experimentally obtained multiple properties of the alloys and b) an advanced, stochastic, multiobjective, evolutionary optimization algorithm using multidimensional response surface as a metamodel. During the iterative computational design procedure, a relatively small number of new alloys need to be periodically manufactured and experimentally evaluated for their properties in order to continuously verify and improve the accuracy of the entire design methodology. The total number of alloys that needs to be manufactured and experimentally evaluated as a part of this optimization strategy is expected to be approximately at least $2^*A^*A^*(1 + P)$, where A is the number of design variables (concentrations of alloying elements) and P is the number of simultaneous objectives (properties of the alloy that need to be extremized simultaneously).

The proposed computational design optimization method was recently verified by Ni-based steel superalloys using strictly experimental data [6–8] and has already been applied to design optimization of H-class steels [4, 5], bulk metallic glasses [9–11], and titanium-based alloys [12]. The proposed optimization methodology is expected to perform equally well in the optimization of chemical concentrations and thermal treatment protocols of aluminum alloys.

Specifically, a novel methodology for predicting the concentration of each of the important alloying elements and the best standard thermal treatment protocol (temper) in aluminum-based alloys is being proposed here. The new alloys will have simultaneously increased stress corrosion cracking resistance (SCCR), increased tensile strength, and increased yield strength. It should be pointed out that this work uses strictly experimentally obtained values for these three objectives, thus avoiding explicit modeling of microstructure, grain, phases, precipitates, boundary films, etc., which is still insufficiently reliable for predicting multiple macroscopic properties of thermally treated alloys. Furthermore, the objective of this research was not to determine the degree of sensitivity (interdependence) of any of the three chosen objectives on any other possible objective, such as toughness, but to limit this study to the information that could be extracted from a very small set of experimental data available in the open literature linking chemistry and tempers to chosen macroscopic properties. The proposed optimization method is based on combining experimentally obtained multiple properties of the aluminum-based alloys and a sophisticated, multiobjective, hybrid, evolutionary optimization algorithm [14, 15] that utilizes a polynomial form of radial basis functions to construct multidimensional response surfaces [16]. This alloy design method is capable of exploring alloy concentrations that are outside of the initial data set, since response surfaces can be extended outside of the domain populated by the original data points because expressions for the response surfaces are analytical functions. Notice that such response surfaces are built from values of experimentally evaluated macroscopic properties of alloys, thus directly accounting for the influences of different concentrations of the alloying elements and influences of different tempers (which then influence the alloys' microstructures) that will be optimized.

Optimization algorithms: background

Classical gradient-based optimization algorithms can find the optimal value only in the case of a single-objective and only if the minimized function is smooth and convex [17]. In the case of multiobjective optimization, one is dealing with a problem of finding the best trade-off solutions among several objectives simultaneously. That is, for multiobjective optimization there is not a single optimal solution, but an entire set of Pareto-optimal (nondominated) solutions [18] for which it is not possible to improve further any individual objective without deteriorating the value of at least one of the remaining objectives. If using gradient-based optimization algorithms, the problem of finding the group of nondominated solutions (the Pareto front) is reduced to several single objective optimizations where the objective function becomes a weighted linear combination of the actual objectives called utility function. This approach is computationally very lengthy, and it can find only a few points on the Pareto front if such a front is continuous.

In this work, a true multiobjective hybrid optimization [14, 15] was used. This optimizer utilizes several multiobjective, evolutionary optimization algorithms and orchestrates the application of these algorithms to multiobjective 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 this code against a number of prominent multiobjective optimization algorithms and one hybrid optimizer confirmed that it performs reliably and accurately.

For problems where objective function evaluations are already expensive and where the number of design variables is large, thus requiring many such objective function evaluations, the only economically viable approach to optimization is to use a cheap and accurate surrogate model (a metamodel) instead of the actual high-fidelity evaluation method (experiments). Such low-fidelity surrogate models are known as response surfaces [14, 16, 18–20] which, in case of more than three dimensions, become high-dimensional hyper-surfaces that need to be fitted through the available, often small, original set of high-fidelity values of the objective function. Once the response surface (hyper-surface) is created using an appropriate analytic formulation, it is very easy and fast to search such a surface for its minima given a set of values of design variables (concentrations of alloying elements and tempers used) supporting such a response surface. Separate response surfaces were generated for each of the three objectives to be optimized: inverse of SCCR, inverse of tensile strength, and inverse of yield strength. The multidimensional response surfaces were fitted through the initial set of experimental data points by using polynomials of multidimensional Radial Basis Functions (RBFs), since they required low computing time

and performed accurate fitting of the provided data including the capability of dealing with scattered data [14, 16, 18, 21]. A convincing comparison [16] of a RFB-based-response surface method and a wavelet-based ANN method [19] demonstrated superiority of RBF-based methods, especially for high dimensionality response surfaces.

Aluminum alloys classification and properties

Aluminum alloys can be divided into nine groups [22–26]. In this study we have decided to focus on 2xxx, 6xxx and especially 7xxx series aluminum alloys. For clarity, definitions of these alloy groups are provided here:

2xxx Series: These alloys require solution heat treatment to obtain optimum properties; in the solution heat-treated condition, mechanical properties are similar to, and sometimes exceed, those of low-carbon steel. In some instances, precipitation heat treatment (aging) is employed to further increase mechanical properties. This treatment increases yield strength, with attendant loss in elongation; its effect on tensile strength is not as great. The alloys in the 2xxx series do not have as good corrosion resistance as most other aluminum alloys, and under certain conditions they may be subject to intergranular corrosion. Alloys in the 2xxx series are good for parts requiring good strength at temperatures up to 150°C (300°F). Except for alloy 2219, these alloys have limited weldability, but some alloys in this series have superior machinability.

6xxx Series: Alloys in the 6xxx series contain silicon and magnesium approximately in the proportions required for formation of magnesium silicide (Mg_2Si), thus making them heat treatable. Although not as strong as most 2xxx and 7xxx alloys, 6xxx series alloys have good formability, weldability, machinability, and relatively good corrosion resistance, with medium strength. Alloys in this heat-treatable group may be formed in the T4 temper (solution heat treated, but not precipitation heat treated) and strengthened after forming to full T6 properties by precipitation heat treatment.

7xxx Series: Zinc, in amounts of 1 to 8% is the major alloying element in 7xxx series alloys, and when coupled with a smaller percentage of magnesium results in heat-treatable alloys of moderate to very high strength. Usually other elements, such as copper and chromium, are also added in small quantities. 7xxx series alloys are used in airframe structures, mobile equipment, and other highly stressed parts. Higher strength 7xxx alloys exhibit reduced resistance to stress corrosion cracking and are often utilized in a slightly over aged temper to provide better combinations of strength, corrosion resistance, and fracture toughness.

Optimization of aluminum-based alloys using 41 alloys without temper

Although each of the three series of aluminum based alloys used in this study has more than four alloying elements (besides aluminum), only three or four alloying elements (besides aluminum) were taken into account when optimizing their respective concentrations by weight. From open literature resources [24–26], a table was compiled that contains chemical concentrations for 4 alloying elements (Cu, Mg, Zn, Mn) so that sum of their respective concentrations by weight and the concentration of aluminum in each such alloy amounts to 100 percent. In the same open sources, two additional experimentally evaluated properties (P1 = stress corrosion cracking resistance (given on a scale 1-100) and P2 = tensile strength [Ksi]) were also found (Fig. 1). Initially, design optimization was performed on a data set of 41 aluminum alloys. Notice that more than half of this space is not covered with the available experimental data.

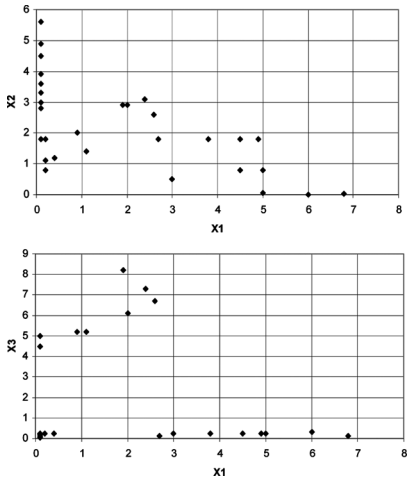

Figure 1.—Distribution of the initial 41 alloys in the space formed by the Cu concentrations (X1), Zn concentrations (X2), and Mg concentrations (X3).

Furthermore, notice (Fig. 2) that the objective P1 (SCCR) in this initial data set depends on the concentrations of each of the alloying elements in a manner which appears to form three distinct bands of dependencies, rather than being distributed uniformly over the entire range.

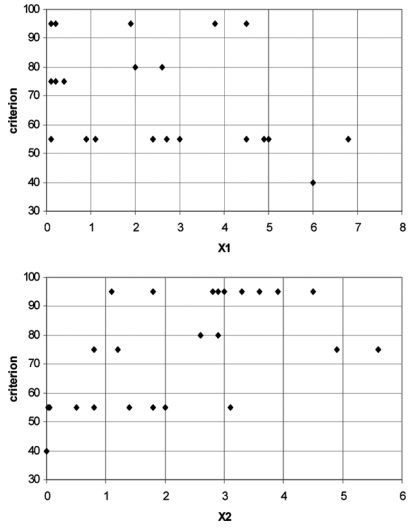

Figure 2.—SCCR criterion of the initial 41 alloys as a function of the Cu concentration alone (top figure) and Zn concentration alone (bottom figure).

When performing a simultaneous maximization of two objectives (SCCR and tensile strength), a Pareto-optimal front of superior alloys was generated (Fig. 3) using a multi-objective hybrid optimization software package [14] and polynomial radial basis functions based response surfaces. For comparison purposes, also shown are results obtained with a commercially available constrained Indirect Optimization based upon SelfOrganization (IOSO) algorithm [26]. IOSO is a semi-stochastic, multi-objective optimization algorithm incorporating certain aspects of a selective search on a continuously updated multi-dimensional response surface created using Ivanenko's selforganizing principle [27, 28] and graph theory.

In Fig. 3, for comparison, commercial optimization algorithm IOSO [26–28] predicted inferior properties (light diamond symbols). In the left figure, each optimized alloy was made with different concentrations of Cu, Mg and Zn in addition to Al base. In each right figure, each alloy was made with different concentrations of Cu, Mg, Zn and Mn in addition to Al base. No thermal treatment (temper) was involved in this optimization.

Although this initial data set was extremely small and the data was not distributed evenly over the concentration ranges, both optimization algorithms were able to solve the multi-objective optimization problem. With more initial experimental data and/or better distribution of their concentrations, it should be possible to obtain more accurate optimization results.

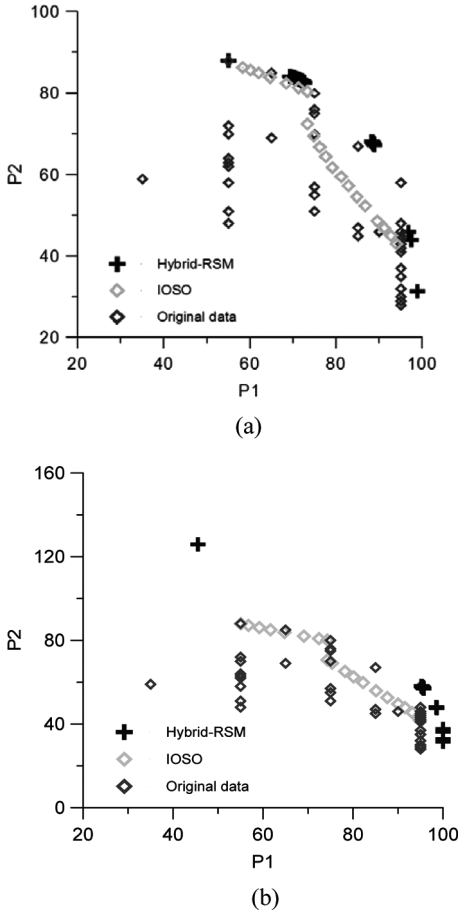

FIGURE 3.—Results of simultaneous hybrid optimization of 2 objectives (P1 = SCCR and P2 = tensile strength) by varying concentrations of 3 alloying elements (top figure) and 4 alloying elements (bottom figure). Initial data set had 41 alloys.

OPTIMIZATION OF ALUMINUM-BASED ALLOYS USING 57 ALLOYS INCLUDING TEMPER

For this reason, a few more experimentally evaluated aluminum alloys of 2xxx, 6xxx and 7xxx series were found in the open literature and added to the original data set of 41 alloys thus creating a data set that had 57 experimentally evaluated alloys. In addition, each of these 57 alloys was thermally treated using a particular standard thermal protocol. Table 1 shows for each of the 57 alloys the concentrations of the four leading alloying elements (X1 = Cu, X2 = Zn, X3 = Mg, X4 = Mn), thermal treatment code number (X12), experimentally evaluated SCCR factor (A = 100, B = 75, C = 50, D = 25), and their respective maximum tensile stress and maximum yield stress. There were 28 different thermal protocols used in this set of 57 alloys.

Since temper (thermal treatment protocols) in the open literature is specified with a letter and a number, they had to be converted into numerical values in order to treat temper as an additional variable that should be optimized. Table 2 depicts the numerical values that were assigned to each of the thermal treatment protocols used for 57 aluminum alloys depicted in Table 1.

Results of this multi-objective optimization of aluminum alloys that were based on an initial data set of experimental values for 57 such alloys that belong to 2xxx, 6xxx and 7xxx series (where each of these 57 alloys was also subjected to a standard temper out of a total of 28 different tempers – see Table 2) suggest that the best trade-off next generation Al-based alloys (those having simultaneously high stress corrosion cracking resistance (SCCR), high tensile strength, and high yield strength) will have to incorporate an unusually high concentration of Cu. From practical experience with Al-based alloys, it is known that high concentrations of Cu will make it harder to manufacture such alloys and will probably negatively affect SCCR.

So, the question is: Why did the powerful proven multi-objective design optimization software predict alloys with unusually high concentrations of Cu and/or Zn? The possible answers are:

Inadequate Size of the Initial Data Set

From open literature resources available, a data set of 57 Al-based alloys was compiled that contains chemical concentrations for four alloying elements (Cu, Mg, Zn, Mn) so that the sum of their respective concentrations by weight and the concentration of aluminum in such alloys amounts to 100 percent. This initial data set for the Al-based alloys of 2xxx, 6xxx and 7xxx series with tempers and the three properties (SCCR, tensile strength, yield strength) that were compiled from the open literature sources is extremely small. That is, when performing optimization where there are three simultaneous objectives and five design variables

TABLE 1.—Concentrations, tempers, and values of three objectives for the 57 experimentally evaluated aluminum alloys of 2xxx, 6xxx, and 7xxx series used for creating response surfaces.

No.	Alloy	X1 % Cu	X2 % Zn	X3 % Mg	X4 % Mn	X12 Temper Code	P1 SCCR Code	P2 Tensile strength [Mpa]	P3 Yield strength [Mpa]	Actual Temper	Actual SCCR
1	2011	5.5	0.3	0	0	3	25	380	295	T3	D
2	2011	5.5	0.3	0	0	20	25	405	310	T8	D
3	2014	4.45	0.25	0.6	0.8	7	50	425	290	T4	C
4	2014	4.45	0.25	0.6	0.8	11	50	485	415	T6	C
5	2024	4.35	0.25	1.5	0.6	2	50	485	345	T3	C
6	2024	4.35	0.25	1.5	0.6	11	25	475	395	T6	D
7	2024	4.35	0.25	1.5	0.6	4	50	470	325	T351	C
8	2024	4.35	0.25	1.5	0.6	7	50	470	325	T4	C
9	2024	4.35	0.25	1.5	0.6	5	50	495	395	T361	C
10	2124	4.35	0.25	1.5	0.6	25	75	490	440	T851	B
11	2218	4	0.25	1.5	0.2	12	50	405	305	T61	C
12	2218	4	0.25	1.5	0.2	15	50	330	255	T72	C
13	2219	6.3	0.1	0.02	0.3	3	50	360	250	T31	C
14	2219	6.3	0.1	0.02	0.3	4	50	360	250	T351	C
15	2219	6.3	0.1	0.02	0.3	6	50	395	315	T37	C
16	2219	6.3	0.1	0.02	0.3	21	75	455	350	T81	B
17	2219	6.3	0.1	0.02	0.3	25	75	455	350	T851	B
18	2219	6.3	0.1	0.02	0.3	11	100	470	345	T6	A
19	2219	6.3	0.1	0.02	0.3	28	75	475	395	T87	B
20	2618	2.3	0.1	1.55	0	12	50	440	370	T61	C
21	6005	0.1	0.1	0.5	0.1	9	100	260	240	T5	A
22	6009	0.375	0.25	0.6	0.5	7	100	235	130	T4	A
23	6010	0.375	0.25	0.8	0.5	7	100	255	170	T4	A
24	6061	0.275	0.25	1	0.15	7	75	240	145	T4	B
25	6061	0.275	0.25	1	0.15	8	75	240	145	T451	B
26	6061	0.275	0.25	1	0.15	11	100	310	275	T6	A
27	6061	0.275	0.25	1	0.15	14	100	310	275	T651	A
28	6063	0.1	0.1	0.675	0.1	1	100	150	90	T1	A
29	6063	0.1	0.1	0.675	0.1	7	100	170	90	T4	A
30	6063	0.1	0.1	0.675	0.1	9	100	185	145	T5	A
31	6063	0.1	0.1	0.675	0.1	11	100	240	215	T6	A
32	6063	0.1	0.1	0.675	0.1	22	100	255	240	T83	A
33	6063	0.1	0.1	0.675	0.1	23	100	205	185	T831	A
34	6063	0.1	0.1	0.675	0.1	24	100	290	270	T832	A
35	6066	0.95	0.25	1.1	0.85	7	75	360	205	T4	B
36	6066	0.95	0.25	1.1	0.85	8	75	360	205	T451	B
37	6066	0.95	0.25	1.1	0.85	11	75	395	360	T6	B
38	6066	0.95	0.25	1.1	0.85	14	75	395	360	T651	B
39	6070	0.275	0.25	0.85	0.7	7	75	315	170	T4	B
40	6070	0.275	0.25	0.85	0.7	11	75	380	350	T6	B
41	6201	0.1	0.1	0.75	0.03	21	100	330	310	T81	A
42	6351	0.1	0.2	0.6	0.6	11	100	310	285	T6	A
43	6463	0.2	0.05	0.675	0.05	1	100	150	90	T1	A
44	6463	0.2	0.05	0.675	0.05	9	100	185	145	T5	A
45	6463	0.2	0.05	0.675	0.05	11	100	240	215	T6	A
46	7005	0.1	4.5	1.4	0.45	10	75	393	345	T53	B
47	7039	0.1	4	2.8	0.1	13	25	450	380	T64	D
48	7049	1.55	7.7	2.45	0.2	16	25	517	448	T73	B
49	7050	2.3	6.2	2.25	0.1	19	50	550	490	T76	C
50	7050	2.3	6.2	2.25	0.1	18	75	510	450	T74	B
51	7075	1.6	5.6	2.5	0.3	11	25	570	505	T6	D
52	7075	1.6	5.6	2.5	0.3	16	100	505	435	T73	A
53	7075	1.6	5.6	2.5	0.3	18	75	505	435	T74	B
54	7075	1.6	5.6	2.5	0.3	19	50	511	442	T76	C
55	7075	1.6	5.6	2.5	0.3	14	50	570	505	T651	C
56	7175	1.6	5.6	2.5	0.1	18	75	524	455	T74	B
57	7178	2	6.8	2.75	0.3	19	50	570	505	T76	C

(four concentrations plus one temper), typically, an initial data set should have involved at least $2^*A^*A^*(1+P) = 2^*5^*5^*(1+2) = 150$ alloys instead of 57 alloys that were available in the open literature. In case of sparse data, one possible alternative would be to use some standard data mining techniques as it was done in a recent work that creatively attempted it in conjunction with evolutionary multi-objective optimization [30]. Genetic programming

TABLE 2.—Numerical values assigned to each of the 28 tempers used for any of the 57 aluminum alloys utilized in this alloy design optimization exercise.

Temper	T1	T3	T31	T351	T361	T37	T4	T451	T5	T53
Value	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
Temper	T6	T61	T64	T651	T72	T73	T736	T74	T76	
Value	11.0	12.0	13.0	14.0	15.0	16.0	17.0	18.0	19.0	
Temper	T8	T81	T83	T831	T832	T851	T8510	T8511	T87	
Value	20.0	21.0	22.0	23.0	24.0	25.0	26.0	27.0	28.0	

TABLE 3.—Results of optimization of a single objective (SCCR) by varying concentrations of 3 and 4 alloying elements and values of temper.

Cu %	Zn %	Mg %	Mn par %	Temper	SCCR	Tensile strength [MPa]	Yield Strength [MPa]
0.1	0.05	0.184	N/A	T31	100	N/A	N/A
0.1	4.543	0.0	0.771	T83	100	N/A	N/A

combined with ANNs could be another possible approach to deal with this challenge [30].

In addition, each of the 57 alloys has more than four alloying elements besides aluminum. However, we have chosen not to take more than three or four alloying elements (besides aluminum) into account when optimizing their respective concentrations by weight. This might have been a mistake as those alloying elements that have been neglected obviously have an influence on the three objectives: SCCR, tensile strength, and yield strength. The objective function spaces (the topologies of the response surfaces for the three objective functions) do not have to be smooth. Actually, yielding of Aluminum alloys often exhibits highly nonlinear behavior as discussed in a recent publication using an evolution criterion [31].

Inadequate Distribution of the Initial Data Set

However, probably the most serious insufficiency of this initial data set was the extreme non-uniformity of the distribution of concentrations of the alloying elements. This can be clearly seen from Fig. 6.

Fitting a multidimensional response surface over such unevenly distributed support data points represents a challenging task as such a response surface will almost definitely have significantly large errors, especially in the areas where there is no information from the initial data set.

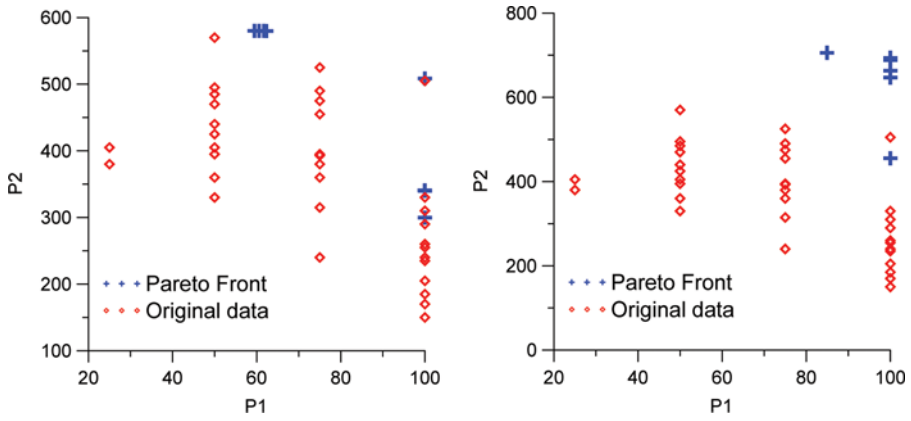

FIGURE 4.—Results of simultaneous optimization of 2 objectives (P1 = SCCR and P2 = tensile strength) by varying values of temper and concentrations of 3 alloying elements (left) and 4 alloying elements (right). Initial data set had 57 alloys.

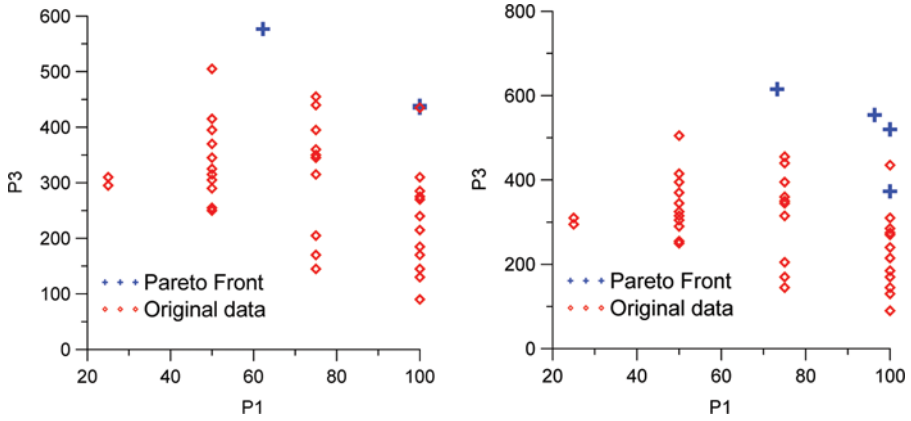

FIGURE 5.—Results of simultaneous optimization of 2 objectives (P1 = SCCR and P3 = yield strength) by varying values of temper and concentrations of 3 alloying elements (left) and 4 alloying elements (right).

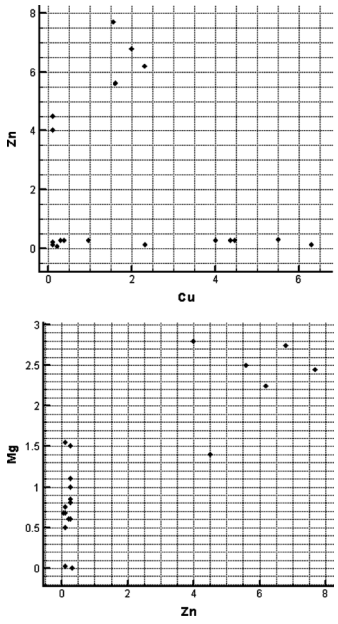

FIGURE 6.—Distributions of concentrations for Cu, Zn, and Mg in the initial set of 57 experimentally tested Al-based alloys. Units of concentration in all figures and tables are mass of the alloying element in the alloying mixture divided by the mass of the entire mixture.

There could also be a significant degree of interaction among variables in the decision space. A simple method to check this out was published very recently [32].

Oscillations in the Response Surface Due to Inadequate Distribution of the Initial Data Set

Multidimensional response surface is nothing more than a five-dimensional (because of the four alloying elements plus temper that are considered as design variables) interpolation of very sparse data (only 57 high fidelity or support points). It is well known that even when fitting a spline of the type $y = y(x)$ through a number of y-values will result in oscillations of the spline if the x-values are highly unevenly distributed. This same phenomenon (oscillatory behavior of the fitted hyper-surface) was observed in the Pareto optimized results for this set of Al-based alloys. That is, our algorithm for generating the multi-dimensional hyper-surfaces apparently makes these surfaces oscillatory just like other known algorithms are doing in cases when the distribution of the support points is extremely uneven, as is the case in our initial data set (Fig. 1).

TABLE 4.—Temper codes for 27 different tempers used among 57 initial alloys.

Temper	T1	T3	T31	T351	T361	T37	T4	T451	T5	T53
Value	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
Temper	T6	T61	T64	T651	T72	T73	T74	T76		
Value	11.0	12.0	13.0	14.0	15.0	16.0	17.0	18.0		
Temper	T8	T81	T83	T831	T832	T851	T8510	T8511	T87	
Value	19.0	20.0	21.0	22.0	23.0	24.0	25.0	26.0	27.0	

Mixture of Real Values and Integers as Design Variables

In this multiobjective optimization problem, the problem is that one has to deal with concentrations of either three or four alloying elements (treated as real numbers) and with code numbers assigned to different thermal treatment protocols (treated as integers). Most optimization algorithms treat all design variables as real numbers and then, at the end of the optimization cycle, round the optimized values to nearest integers. Other optimization algorithms work with a binary system which is an integer system to represent any real variables. This approach is beneficial in all evolutionary optimization algorithms where crossover of chromosomes is a required step since it is much easier to perform the crossover at prespecified values of the chromosome elements than at the prespecified values of the actual design variables. In our hybrid multiobjective optimization algorithm, currently all design variables are treated as real numbers. Thus, when incorporating thermal treatment protocols as an additional design variable, although they vary as assigned integers, they were treated as real numbers. Consequently, in the final optimized results, the optimized values of codes for the thermal treatment protocols turned out to be real numbers which then had to be rounded-off to the nearest integer code number. This can also influence the optimized values of other design variables (optimized concentration values of alloying elements).

Consequently, a few parameters in the response surface generation algorithm were adjusted to minimize oscillations of the response surface. In addition, the total number of tempers considered was reduced to 27 instead of 28 because T736 was now treated at T74. Thus, the new assignment of code numbers to different tempers used was as follows (see Tables 4 and 5 and Fig. 7).

Then, the same optimization tasks were repeated while accounting for these minor alterations.

When comparing these new results (Fig. 7) against the Pareto optimized results reported in Fig. 4, one can see that the new Pareto front envelopes the initial data more closely. However, notice that for high SCCR alloys the newly suggested concentrations of Cu and Zn are now in the widely accepted range (Tables 6 and 7).

When comparing these new results (Fig. 8) against the Pareto optimized results reported in Fig. 5, one can see

TABLE 5.—Results of a single-objective optimization for P1 = SCCR using 3 and 4 design variables (X1, X2, X3, X4) and one extra design variable (X12 = temper) which varied from 1 to 27.

X1 Cu	X2 Zn	X3 Mg	X4 Mn	X12 Temper	P1 SCCR	P2 Tensile	P3 Yield	X5 Al
0.74956	2.02219	N/A	0.325	27	100	257.916	238.76	96.9033
0.38206	1.49512	0.36315	0.20558	25	100	256.81	237.922	97.5541

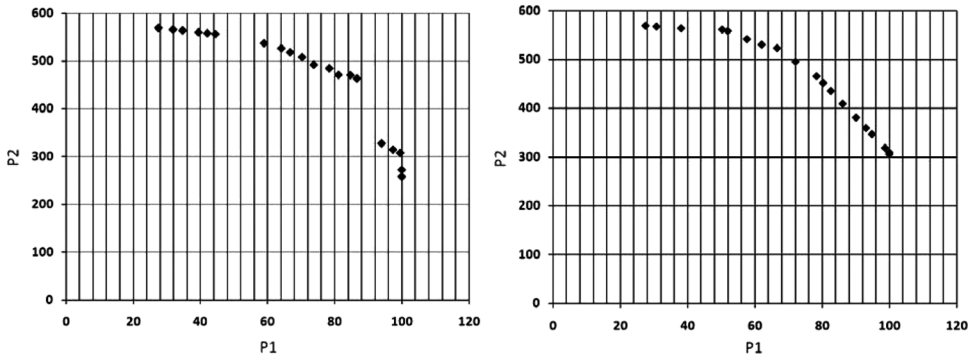

FIGURE 7.—Results of simultaneous optimization of two objectives (P1 = SCCR and P2 = tensile strength) by varying values of temper and concentrations of 3 alloying elements (left) and 4 alloying elements (right). These results (partial data shown in Tables 6 and 7) were obtained with a modified response surface method and 57 initial alloys. It should be compared to results in Fig. 4.

TABLE 6.—Results of simultaneous optimization of 2 objectives (P1 = SCCR and P2 = tensile strength) using 3 design variables (X1, X2, X3) and one extra design variable (X12 = temper).

X1 Cu	X2 Zn	X3 Mg	X4 Mn	X12 Temper	P1 SCCR	P2 Tensile	P3 Yield	X5 Al
1.10069	0.7902	0.25042	0.325	27	100	258.181	239.007	97.5337
1.06698	1.26882	1.01639	0.325	20	99.9888	272.28	248.507	96.3228
0.74485	1.47754	1.50297	0.325	17	99.537	307.726	272.274	95.9496
1.16716	2.34806	1.34523	0.325	18	97.4006	314.59	278.976	94.8145
1.06144	2.35756	1.44083	0.325	17	93.9808	327.674	289.31	94.8152

TABLE 7.—Results of simultaneous optimization of 2 objectives (P1 = SCCR and P2 = tensile strength) using 4 design variables (X1, X2, X3, X4) and one extra design variable (X12 = temper).

X1 Cu	X2 Zn	X3 Mg	X4 Mn	X12 Temper	P1 SCCR	P2 Tensile	P3 Yield	X5 Al
0.55826	2.37353	0.13541	0.45959	25	99.9984	305.476	280.973	96.4732
2.36293	2.31366	0	0.66913	27	98.7213	318.794	292.557	94.6543
2.61489	1.63181	0.09406	0.57119	26	94.8363	346.852	316.437	95.088
2.56317	1.8821	0.18641	0.67268	27	90.0923	380.694	345.848	94.6956
2.74757	2.53814	0.16946	0.65579	26	86.0949	409.126	370.25	93.889
2.69177	3.49744	0.29233	0.60034	27	80.2857	451.799	407.042	92.9181
2.55594	0.82201	0.58157	0.6504	26	78.3398	465.626	419.013	95.3901

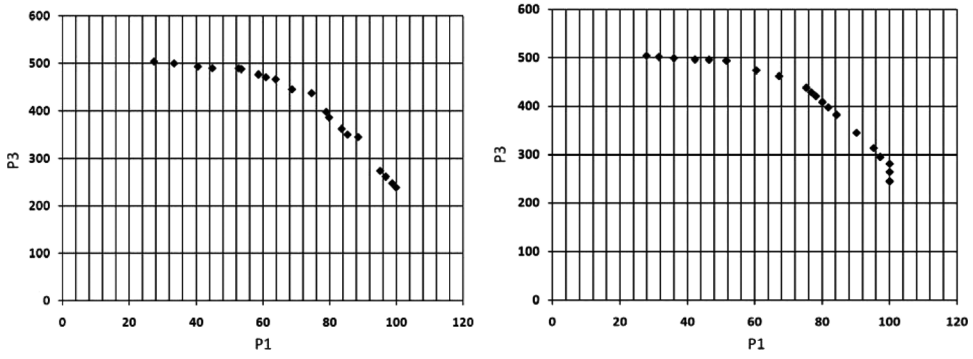

FIGURE 8.—Results of simultaneous optimization of 2 objectives (P1 = SCCR and P3 = yield strength) by varying values of temper and concentrations of 3 alloying elements (left) and 4 alloying elements (right). These results were obtained with a modified response surface method and 57 initial alloys. It should be compared to results in Fig. 5.

that the new Pareto front envelopes the initial data more closely. The resulting optimized concentrations of Cu and Zn for high SCCR alloys were now in the widely accepted range.

In conclusion, our minor modifications to the existing initial data set and to the response surface algorithm resulted in an overly conservative Pareto front estimate, although the predicted optimal values of Cu and Zn were now in

TABLE 8.—Initial set of 46 (series 2xxx, 6xxx, and 7xxx) Al-based alloys that do not use T8xx tempers.

Alloy	X1 Cu %	X2 Zn %	X3 Mg %	X4 Mn %	X12 Temper	P1 SCCR	P2 Tensile strength	P3 Yield strength	Actual temper
2011	5.5	0.3	0	0	2	25	380	295	T3
2014	4.45	0.25	0.6	0.8	7	50	425	290	T4
2014	4.45	0.25	0.6	0.8	11	50	485	415	T6
2024	4.35	0.25	1.5	0.6	2	50	485	345	T3
2024	4.35	0.25	1.5	0.6	11	25	475	395	T6
2024	4.35	0.25	1.5	0.6	4	50	470	325	T351
2024	4.35	0.25	1.5	0.6	7	50	470	325	T4
2024	4.35	0.25	1.5	0.6	5	50	495	395	T361
2218	4.0	0.25	1.5	0.2	12	50	405	305	T61
2218	4.0	0.25	1.5	0.2	15	50	330	255	T72
2219	6.3	0.1	0.02	0.3	3	50	360	250	T31
2219	6.3	0.1	0.02	0.3	4	50	360	250	T351
2219	6.3	0.1	0.02	0.3	6	50	395	315	T37
2219	6.3	0.1	0.02	0.3	11	100	470	345	T6
2618	2.3	0.1	1.55	0	12	50	440	370	T61
6005	0.1	0.1	0.5	0.1	9	100	260	240	T5
6009	0.375	0.25	0.6	0.5	7	100	235	130	T4
6010	0.375	0.25	0.8	0.5	7	100	255	170	T4
6061	0.275	0.25	1	0.15	7	75	240	145	T4
6061	0.275	0.25	1	0.15	8	75	240	145	T451
6061	0.275	0.25	1	0.15	11	100	310	275	T6
6061	0.275	0.25	1	0.15	14	100	310	275	T651
6063	0.1	0.1	0.675	0.1	1	100	150	90	T1
6063	0.1	0.1	0.675	0.1	7	100	170	90	T4
6063	0.1	0.1	0.675	0.1	9	100	185	145	T5
6063	0.1	0.1	0.675	0.1	11	100	240	215	T6
6066	0.95	0.25	1.1	0.85	7	75	360	205	T4
6066	0.95	0.25	1.1	0.85	8	75	360	205	T451
6066	0.95	0.25	1.1	0.85	11	75	395	360	T6
6066	0.95	0.25	1.1	0.85	14	75	395	360	T651
6070	0.275	0.25	0.85	0.7	7	75	315	170	T4
6070	0.275	0.25	0.85	0.7	11	75	380	350	T6
6351	0.1	0.2	0.6	0.6	11	100	310	285	T6
6463	0.2	0.05	0.675	0.05	1	100	150	90	T1
6463	0.2	0.05	0.675	0.05	9	100	185	145	T5
6463	0.2	0.05	0.675	0.05	11	100	240	215	T6
7005	0.1	4.5	1.4	0.45	10	75	393	345	T53
7039	0.1	4.0	2.8	0.1	13	25	450	380	T64
7049	1.55	7.7	2.45	0.2	16	75	517	448	T73
7075	1.6	5.6	2.5	0.3	11	50	570	505	T6
7075	1.6	5.6	2.5	0.3	16	100	505	435	T73
7075	1.6	5.6	2.5	0.3	14	50	570	505	T651
7075	1.6	5.6	2.5	0.3	16	100	505	435	T73
7175	1.6	5.6	2.5	0.1	17	75	525	455	T736
7175	1.6	5.6	2.5	0.1	18	50	550	505	T74
7178	2.0	6.8	2.75	0.3	19	50	570	505	T76

the widely accepted range. Similarities in Fig. 8 suggest that yielding of Al alloys follow some unique behavior. An excellent work was carried out recently [31] using evolution criteria to address this issue.

OPTIMIZATION RESULTS USING 46 ALLOYS THAT DID NOT HAVE T8XX CLASS TEMPERS

After eliminating all alloys that had thermal treatment protocols that belong to T8xx class of tempers (see yellow colored tempers in Table 1 of temper codes listed earlier), there were only 46 Al-based alloys left in the initial data set. They are given in Table 8.

Also note that there are now only 19 different tempers considered since T736 became temper 17, T74 became temper 18, and T76 became temper 19 in Table 4. It should be pointed out that now there are 4 design variables (X1, X2, X3, X4) that are real numbers and one design variable (X12 = temper code) that is integer. There is also the fifth design variable (X5 = concentration of aluminum), but it is treated as a constraint, that is, $X5 = 100 - (X1 + X2 + X3 + X4)$. It means that, for example, for the first point of data set X1 = 5.5, X2 = 0.3, X3 = 0, X4 = 0.

TABLE 9.—Results of optimization of a single objective (P1 = SCCR) by varying concentrations of 3 and 4 alloying elements and values of temper (X12), while excluding any alloys with T8xx tempers.

X1	X2	X3	X4av	X5	X12	P1
1.68005	7.241	0.51393	N/A	90.56502	8	100
0.23737	0.05	0.66061	0.35435	98.69767	11	100

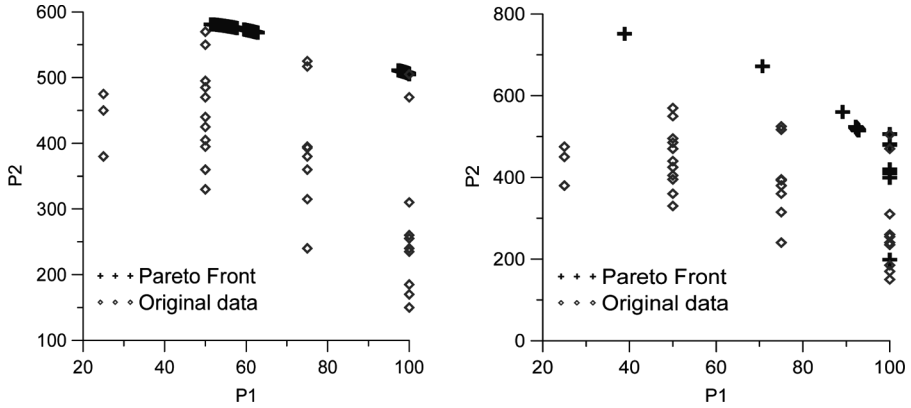

FIGURE 9.—Results of simultaneous optimization of 2 objectives (P1 = SCCR and P2 = tensile strength) by varying values of temper and concentrations of 3 alloying elements (left) and 4 alloying elements (right) using a data set with 46 alloys (none with T8xx class of tempers). These results (partial data shown in Tables 10 and 11) were obtained with a modified response surface method and should be compared to results in Fig. 7.

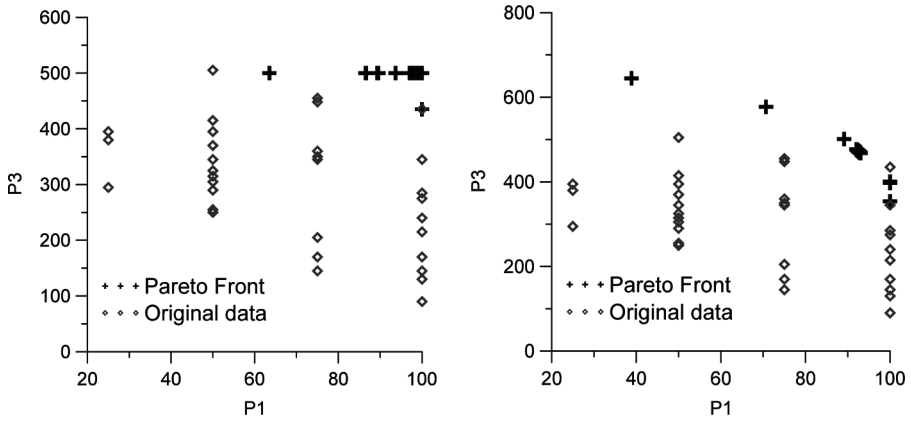

FIGURE 10.—Results of simultaneous optimization of 2 objectives (P1 = SCCR and P3 = yield strength) by varying values of temper and concentrations of 3 alloying elements (left) and 4 alloying elements (right) using a data set with only 46 alloys (none with T8xx class of tempers). These results (partial data shown in Tables 12 and 13) were obtained with a modified response surface method and should be compared to results in Fig. 8.

Hence, the remaining concentration will be this of the base metal (aluminum), which in this case is $X5 = 100 - (5.5 + 0.3 + 0 + 0) = 94.2$. This means that one can define X5 for current values of X1, X2, X3, and X4 including optimization procedure. Thus, in this formulation, there are 5 independent design variables (X1, X2, X3, X4, and X12) and one dependent variable (X5). As a result, approximation functions (response surfaces) were built using (X1, X2, X3, X4, and X12), optimization was performed using these functions, and then X5 was defined for current point. For the test cases with 3 alloying elements, $X5 = (100 - X4initial) - (X1 + X2 + X3)$ optimized was used. This means that each value X5 can be defined for each point of the data set (for example, for first point it is $X5 = 94.2$, which is the same value obtained for test cases when X4 is included as a design variable). Thus, X5 was not used for building approximation functions (response surfaces). Instead, X5 (concentration of aluminum) was defined for each current value (X1, X2, X3, X4) during optimization procedure.

Table 9 and Fig. 9 show the results of optimization runs based on an initial data set having only 46 alloys, where none of these alloys was subjected to T8xx class of temper.

From Figs. 9 and 10 (and Tables 10–13), it is again evident that by involving more alloying elements in the optimization process, better performing alloys can be developed.

TABLE 10.—Results of simultaneous optimization of 2 objectives (P1 = SCCR and P2 = tensile strength) using 3 design variables (X1, X2, X3) and one extra design variable (X12 = temper). Initial data had only 46 alloys, none of which used any of the T8xx class tempers.

X1	X2	X3	X4av	X5	X6	P1	P2
4.86052	7.7	2.8	0.354348	84.28513	14	52	580.807
4.309192	7.7	2.693342	0.354348	84.94312	15	55	578.659
2.768017	6.580344	2.477758	0.354348	87.81953	14	62	569.371
1.678668	5.680418	2.49579	0.354348	89.79078	16	97	511.196
1.674659	5.676813	2.495771	0.354348	89.79841	16	98	510.791
1.638711	5.645006	2.495338	0.354348	89.8666	16	99	507.488
1.626474	5.63446	2.495051	0.354348	89.88967	16	100	506.561

TABLE 11.—Results of simultaneous optimization of 2 objectives (P1 = SCCR and P2 = tensile strength) using 4 design variables (X1, X2, X3, X4) and one extra design variable (X12 = temper). Initial data had only 46 alloys, none of which used any of the T8xx class tempers.

X1	X2	X3	X4	X5	X12	P1	P2
6.3	7.7	0	0.85	85.15	19	71	671.902
0.1	7.7	0	0.85	91.35	19	89	560.097
0.1	7.7	0	0.59349	91.6065	19	92	519.098
0.1	7.7	0	0.55800	91.6419	19	93	514.824
0.1	4.4336881	0	0.40656	95.0597	19	100	419.644
0.53313	4.0262615	0	0.34763	95.0929	19	100	409.899
0.97974	2.9725843	0	0.41114	95.6365	19	100	398.993

TABLE 12.—Partial results of simultaneous optimization for two objectives (P1 = SCCR and P3 = yield strength) using 3 design variables (X1, X2, X3) and one extra design variable (X12 = temper). Initial data had only 46 alloys, none f which used any of the T8xx class tempers.

X1	X2	X3	X4av	X5	X12	P1	P3
0.10003	5.02348	0.25116	0.35435	94.2709	6	87	500
0.11300	4.13551	0	0.35435	95.3971	5	89	500
0.17428	0.95443	0	0.35435	98.5169	8	100	500
0.24298	1.25978	0.00578	0.35435	98.1371	17	100	500
0.35625	0.99193	0.02207	0.35435	98.2754	16	100	500
0.18075	1.28627	0.03790	0.35435	98.1407	17	100	500
0.40153	0.79242	0.05421	0.35435	98.3975	15	100	500
1.6	5.6	2.5	0.35435	89.9456	16	100	435

TABLE 13.—Partial results of simultaneous optimization for 2 objectives (P1 = SCCR and P3 = yield strength) using 4 design variables (X1, X2, X3, X4) and one extra design variable (X12 = temper). Initial data had only 46 alloys, none of which used any of the T8xx class tempers.

X1	X2	X3	X4	X5	X6	P1	P3
6.3	7.7	0	0.85	85.15	19	71	577.301
0.1	7.7	0	0.85	91.35	19	89	501.241
0.1	7.7	0	0.63671	91.5633	19	92	476.85
0.1	7.7	0	0.59025	91.6097	19	93	472.597
0.1	3.9261069	0	0.49766	95.4762	19	100	399.936

CONCLUSIONS

Based on these proof-of-concept optimization results shown above (using 41 alloys without accounting for temper, using 57 alloys accounting for all tempers actually used, and using only 46 alloys with tempers that do not include T8xx series), the following conclusions could be drawn:

1. Initial data set must be enlarged if more trustworthy numerical results are to be obtained. Specifically, at least 10 additional alloys need to be manufactured and tested experimentally (after appropriate tempers have been applied). Each of these new alloys should be made having concentrations of the alloying elements that cover the previously not covered domain of concentrations. Compositions (concentrations of each of the alloying elements) and temper for each of these 10 new alloys should be determined using the results of the Pareto optimization process presented in this work.
2. Multidimensional response surface generation of the three objective functions (SCCR, maximum tensile strength, and maximum yield strength) should be further improved in order to minimize oscillations of such hypersurfaces when utilizing non-uniformly distributed scarce data of experimentally tested alloys.
3. Some of the macroscopic properties of the alloys that were chosen to be extremized might be progressively similarly depended on more than one of the alloying element. In other words, there could be a linear dependency between two design variables thus making one of them redundant as the design variable. Although we have not included an algorithm for detecting such possibilities in this work, such algorithms exist and can be useful in reducing the overall computing time effort.
4. In case of sparse data one possible alternate would be to use some standard data mining techniques in conjunction with evolutionary multiobjective optimization. Genetic programming could be another possible approach to address this problem.

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