Chapter 8

Inverse Design of Alloys' Chemistry for Specified Thermo-Mechanical Properties by using Multi-objective Optimization

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Abstract. Inversely designing new alloys for specific applications involves determining concentrations of alloying elements that will provide, for example, specified tensile strength at a specified temperature for a specified length of time. This represents an inverse problem which can be formulated as a multi-objective optimization problem with a given set of equality constraints. This chapter describes several such formulations for the multiple objective functions and comparatively evaluates these models when using optimization to solve this de facto inverse problem. This approach allows a materials design engineer to design a precise chemical composition of an alloy that is needed for building a particular object. This inverse method uses a multi-objective constrained evolutionary optimization algorithm to determine not one, but a number of alloys (Pareto front points), each of which will satisfy the specified properties while having different concentrations of each of the alloying elements. This provides the user of the alloy with additional flexibility when creating such an alloy, because he/she can use the chemical composition which is made of the most readily available and the most inexpensive elements. It should be pointed out that the inverse problem of determining alloy chemical composition is different from a direct optimization problem of designing alloys that will have extreme properties. This alloy design methodology does not require knowledge of metallurgy or crystallography and is directly applicable to alloys having an arbitrary number of alloying elements. Examples are presented for Ni-based steel alloys and bulk metallic glasses, although the method is applicable to inversely designing chemical concentrations of arbitrary alloys.

8.1 Introduction

It is well known that thermo-physical properties of alloys depend on the choice and number of the alloying elements, concentrations of each of the alloying elements, and thermal and/or mechanical treatment protocol that an alloy is typically submitted to in an a posteriori fashion. The microstructure of an alloy depends on these influencing factors. It represents an intermediate step in this cause-consequence relationship between chemistry and thermo/mechanical treatment on one side, and thermo-mechanical properties on another side. Mathematical modeling of the interdependency of various thermo-physical properties on each of the influencing factors is either non-existent or based on empiricism and heuristics. Thus, the general problem of designing new alloys is still an art, rather than a science. It involves the designer's experience with general metallurgy, personal intuition and an excessively long and expensive experimentation which makes the alloy design process very costly. It does not currently involve any aspects of chemistry.

Therefore, rather than attempting to develop a new fundamental science of alloys' chemistry based on nonlinear thermodynamics and atomistic modeling of basic structures, which is still restricted to relatively small number of atoms because of the excessive computing time and memory requirements, it is more prudent to utilize simple models that do not require detailed elaboration of microstructure and chemistry. Since such simple meta models linking causes and consequences can significantly reduce the overall time and cost of the alloy design process, it is of utmost importance to utilize such computational design tools that already exist and have been successfully applied in numerous other fields of science and engineering. Such proven design tools are various design optimization algorithms that can be used to create alloys with extreme thermo-physical properties [1–7] or can be used in conjunction with inverse design of alloys [8, 3, 7] having specified thermo-physical properties. For example, a designer of a crankshaft in an internal combustion engine needs to use an alloy that will sustain a very specific maximum stress, at a specific temperature, for a specific number of hours before it breaks. This would be a typical example of an inverse design of alloys [8]. The resulting alloys that will meet the desired specifications are typically considerably less expensive than the optimized alloys where the properties were extremized via an alloy design optimization process [1–7]. In this article, we will elaborate on a method that we created for inverse design of alloys that will have values of their thermo-physical properties as specified by the designer.

This inverse design method uses a variant of I. N. Egorov's optimization algorithm known as IOSO [9, 3] to determine not one, but a number of alloys, each of which is satisfying the specified properties while having different con-

centrations of each of the alloying elements. This provides the user of the alloy with increased flexibility when deciding to create such an alloy. In this way, the customer can choose the inversely determined alloy composition (the alloying elements to be used in a new alloy) and the inversely determined set of concentrations (of these alloying elements) that are the most available and the least expensive at the moment when it is ordered from the alloy manufacturer. It should be pointed out that the inverse problem of determining alloy chemical composition is different from a direct optimization problem [1–7] of designing alloys that will have extreme properties.

The inverse problem can then be formulated as, for example, a multi-objective optimization problem with a given set of equality constraints. We have used IOSO multi-objective optimization algorithm [9] to achieve the solution of this type of inverse alloy design problem [8, 3, 7].

We have developed eight mathematical formulations and corresponding software packages for different ways to achieve inverse determination of chemical concentrations of alloying elements that simultaneously satisfy several specified mechanical and cost/availability properties. These different formulations were then compared and analytically evaluated in an attempt to determine the most appropriate formulation.

8.2 Multi-Objective Constrained Optimization and Response Surfaces

The key to the success of the proposed inverse method for design of alloys is the robustness, accuracy, and efficiency of the multi-objective constrained optimization algorithm. This inverse problem solution methodology and results presented in this chapter are based on a special adaptation of IOSO [9], which is a robust stochastic multi-objective constrained optimization algorithm. The IOSO algorithm is of a semi-stochastic type incorporating certain aspects of a selective search on a continuously updated multi-dimensional response surface. IOSO can utilize either a weighted linear combination of several objectives or a true multi-objective formulation option for creating Pareto fronts. The main benefits of this algorithm are its outstanding reliability in avoiding local minima, its computational speed, and a significantly reduced number of required experimentally evaluated candidate alloys as compared to more traditional semi-stochastic optimizers such as genetic algorithms. Furthermore, the self-adapting response surface formulation [10] used in IOSO allows for incorporation of realistic non-smooth variations of experimentally obtained data and provides for accurate interpolation of such data.

One of the advantages of this approach is the possibility of ensuring good approximating capabilities using a minimum amount of available information.

This possibility is based on self-organization and evolutionary modeling concepts [10, 8, 3]. During the optimization process, the approximation function (multi-dimensional response surface) structure is being continuously improved, so that it allows successful approximation of the optimized functions and constraints having sufficiently complicated topology. The obtained analytical formulations for the response surface approximations can be used by multi-level optimization procedures with an adaptive change of approximation level accuracy for both a single and multiple objectives analysis, and also for the solution of their interaction problems.

With reference to a particular problem of the creation of alloys with desirable properties, there will inevitably arise a problem of constraints that need to be specified on the objective functions. These constraints are absent in a more general multi-objective optimization statement. Such objective constraints should be set by the user (expert) and could be allowed to vary during the solution process. For example, a minimum acceptable value for the Young's modulus of elasticity could be specified as an inequality constraint. Or, a maximum acceptable percentage for each of the most expensive chemical elements in the alloy could be specified as a cost objective constraint. Also, the maximum acceptable manufacturing cost of an alloy could be specified as an inequality constraint.

The problem of search for a Pareto-optimum solution set in the multi-objective optimization, while varying concentrations of alloying elements, would be an unacceptably labor-intensive process. This is because of an extremely large number of candidate alloys that would need to be created and because several of the properties of each of these alloys would have to be evaluated experimentally. In this case, we can speak only about the creation of some rather extensive database including the information on various properties of alloys for various combinations of a chemical structure. Such a database could be used for the solution of particular problems aimed at the creation of alloys with desirable properties. Unfortunately, inverse problems, as a rule, are difficult to formalize at the initial stage, since the user does not know initially what values of some objectives could be physically reached and how the remaining objectives will vary. That is, the user has very little if any a-priori knowledge of topology of the objective functions. Hence, it is very difficult to predict the number of experiments required in the optimization application proposed here.

Therefore, it appears that inverse design of alloys via use of optimization can be solved only in an interactive mode, when the user during the solution can modify both objective constraints and objective functions. Actually, in this case one can speak about optimally controlled experiments. Let us consider several different scenarios for the solution of optimization problems for these conditions.

The first approach is to perform a general multi-objective optimization of the material properties. Within the frame-work of this strategy, we are to solve the multi-objective optimization problem (to find the Pareto set) using the general IOSO algorithm. This strategy is the most accurate, but it requires a very large number of experiments.

The second approach is an interactive step-by-step optimization of the material properties. The first step of this strategy is to create an initial plan of experiments. This involves formulation of a single (hybrid) optimization objective by the user. This objective may be the convolution of particular objectives with different weight coefficients assigned to each of them. Then, one optimization step is needed to minimize this composite objective. The result of this strategy is the single solution that belongs to Pareto-set. However, during such relatively efficient quasi multi-objective optimization process we can accumulate the information about the particular objectives and construct progressively more accurate response surface models.

Thus, in order to develop and realize the most effective optimization strategies, both of the first and the second kind, we have to perform a thorough preliminary search for the classes of base functions that will be able to construct the most accurate multi-dimensional response surface models.

The number of experiments that is necessary for true multi-objective optimization problem solution depends not only on the dimensionality of the problem (the number of chemical elements in an alloy); it also depends to a considerable degree on the topologies of the objective functions. For example, for the solution of an actual problem in the car industry with 6 variables, we needed nearly 60 experiments when using a basic IOSO algorithm [11]. However, for finding the minimum of the classical Rosenbrock test function, having only 2 variables, it was necessary to perform almost 300 objective function evaluations.

8.3 Summary of IOSO Algorithm

An extremely important part of the optimization process is the creation and iterative improvements of a multidimensional response surface (an approximation of the objective function as an analytical expression relating it to the design variables-concentrations of different alloying elements). Each iteration of IOSO, therefore, consists of two steps. The first step is the creation of an approximation of the objective function(s). The response surface in IOSO is modeled analytically as a tree-structure or a multi-level graph, where each branch is a quadratic polynomial. Thus, the final analytic expression for a multidimensional response surface is a polynomial-of-a-polynomial-of-a-polynomial-..., where each polynomial is a simple quadratic function. Generally speaking,

the basic polynomial could be a linear function, a quadratic function, a cubic function, a quartic function, etc. [11, 12], but the best tradeoff between the accuracy of the fitting process and the computational cost appears to be the quadratic polynomial [11].

The second step in IOSO is the optimization of this approximation function. This approach allows for corrective updates of the structure and the parameters of the response surface approximation. The distinctive feature of this approach is an extremely low number of trial points needed to initialize the algorithm. The obtained response surface functions are used in the multi-level optimization, while adaptively utilizing various single and multiple discipline analysis tools that differ in their level of sophistication.

During each iteration of IOSO, the optimization of the response function is performed only within the current search area. This step is followed by a direct call to the mathematical analysis model or an actual experimental evaluation for the obtained point. During the IOSO operation, the information concerning the behavior of the objective function in the vicinity of the extremum is stored, and the response surface function is re-created locally and made more accurate only for this search area. Thus, during each iteration, a series of approximation functions for a particular objective of optimization is built. These functions differ from each other according to both structure and definition range. The subsequent optimization of these approximation functions allows us to determine a set of vectors of optimized variables.

During this work, algorithms of artificial neural networks (ANN) [13] were used that utilized radial-basis functions modified in order to build the response surfaces. The modifications consisted in the selection of ANN parameters at the stage of their training that are based on two criteria: minimal curvature of the response hyper-surface, and provision of the best predictive properties for a given subset of test points.

In summary, each iteration of IOSO multi-objective optimization applied to alloy design involves the following:

(1) Building and training ANN1 for a given set of test points.

(2) Conducting multi-objective optimization with the use of ANN1 and obtaining a specified number of Pareto optimal solutions P1.

(3) Determining a subset of test points that are maximally close to points P1 in the space of variable parameters.

(4) Training ANN2 proceeding from the requirement to provide the best predictive properties for obtained subset of test points.

(5) Conducting multi-objective optimization with the use of ANN2 and obtaining a set of Pareto-optimal solutions P2.

In general, the database contains information on experimentally obtained alloy properties compiled from different sources and obtained under different ex-

perimental conditions. As a result, alloys with the same chemical compositions can have considerable differences between their measured properties. These differences can be explained as errors due to the particular conditions existing during the experiments (measurement errors), and by the effect of certain operating conditions (for example, thermal condition of alloy making). Unless operating conditions are quantified numerically, their influence is regarded as an additional chance factor. Therefore, in its simplified form, the alloy design methodology that takes into account these uncertainties can be presented as the following set of actions:

(1) Formulation of optimization task, that is, selection of variable parameters, definition of optimization objectives and constraints, and setting initial (preliminary) ranges of variable parameters' variations.

(2) Preliminary reduction of the experimental database. At this stage, the alloys meeting optimization task statement are picked up from the database so that alloys having chemical composition outside the chosen set of chemical elements are rejected. Alloys for which there is no data for at least one optimization objective are rejected. In addition, alloys with chemical concentrations outside the set range of variable concentrations are also rejected.

(3) Final reduction of the experimental database. Since accuracy of the building of response surfaces substantially depends on uniformity of distribution of variable parameters in the surveyed area, rejection of experimental data values appearing significantly outside of the universal set is performed. At the end of this stage, a final range of variable parameters for optimization is set.

(4) Execution of multi-objective optimization resulting in a specified number of Pareto optimal solutions.

(5) Analysis of optimization results.

(6) Manufacturing and experimental evaluation of the obtained Pareto optimal alloys to obtain high fidelity values of the optimized objectives and analysis of the results obtained.

(7) Change of the optimization problem statement (number of simultaneous objectives and constraints, the set and range of variable parameters), and returning to step 2.

(8) Modification of database and returning to step 4.

(9) Stop.

8.4 Mathematical Formulations of Objectives and Constraints

In particular, the objective of this inverse alloy design task was to determine concentrations (by weight) of each of the 14 alloying elements (C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti) in high temperature steel alloys that

will have specified (desired) physical properties. No mathematical analysis was used to evaluate the physical properties of candidate alloys. The evaluations of properties were performed using classical experiments on candidate alloys. In other words, we used an existing experimental database [1, 2, 3, 4, 5, 8]. The ranges of concentrations of these elements were set by finding the minimum and the maximum values of concentrations for each alloying element in the existing set of experimental data (Expmin_i, Expmax_i, where $i = 1, \ldots, 14$). Then, new minimum and maximum values for concentrations of each of the 14 alloying elements were specified according to the following simple dependencies: ($\mathsf{Min}_i = 0.9\mathsf{Expmin}_i$, $\mathsf{Max}_i = 1.1\mathsf{Expmax}_i$, where $i = 1, \ldots, 14$). These ranges are given in Table 8.1.

Table 8.1. Ranges of variation of design variables (concentrations of alloying elements).

	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

The inverse problem can be then formulated as, for example, a multi-objective optimization problem with a given set of equality constraints. This optimization was formulated as a multi-objective statement with three simultaneous objectives: minimize the difference between the specified and the actual stress, minimize the difference between the specified and actual maximum temperature, and minimize the difference between the specified and actual time to rupture at the specified temperature and stress. One additional objective (minimizing the cost of the raw material used in the alloy) was also considered. Eight different mathematical formulations of this constrained optimization problem were created (Table 8.2) and implemented using IOSO algorithm.

In the case of inversely determining concentrations of each of the 14 alloying elements in steel alloys when using the eight mathematical formulations for the objective function(s) and constraints on the range of design variables (Table 8.1), IOSO optimization algorithm offered consistently high accuracy in satisfying the specified stress (Figure 8.1), operating temperature (Figure 8.2), time-until-rupture (Figure 8.3) and an overall combined accuracy (Figure 8.4).

Overall performance evaluation of the various inverse alloy design formulations was then developed that was based on an ad hoc analytical formulation summarized in equations (8.4.1) through (8.4.8).

Table 8.2. 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	$(\sigma - \sigma_{spec})^2$	$(T - T_{spec})^2$	$(H - H_{spec})^2$		
2	1	$(\sigma - \sigma_{spec})^2 + (T - T_{spec})^2 + (H - H_{spec})^2$				
3	3	$(\sigma - \sigma_{spec})^2$	$(T - T_{spec})^2$	$(H - H_{spec})^2$		$(\sigma - \sigma_{spec}) < \epsilon$ $(\sigma - \sigma_{spec}) < \epsilon$ $(T - T_{spec}) < \epsilon$ $(H - H_{spec}) < \epsilon$
4	1	$(\sigma - \sigma_{spec})^2 + (T - T_{spec})^2 + (H - H_{spec})^2$				$(\sigma - \sigma_{spec}) < \epsilon$ $(T - T_{spec}) < \epsilon$ $(H - H_{spec}) < \epsilon$
5	1	$(\sigma - \sigma_{spec})^2$				$(T - T_{spec}) < \epsilon$ $(H - H_{spec}) < \epsilon$
6	1		$(T - T_{spec})^2$			$(\sigma - \sigma_{spec}) < \epsilon$ $(H - H_{spec}) < \epsilon$
7	1			$(H - H_{spec})^2$		$(\sigma - \sigma_{spec}) < \epsilon$ $(T - T_{spec}) < \epsilon$
8	10	$(\sigma - \sigma_{spec})^2$	$(T - T_{spec})^2$	$(H - H_{spec})^2$	Ni, Cr, Nb, Co, Cb, W, Ti	

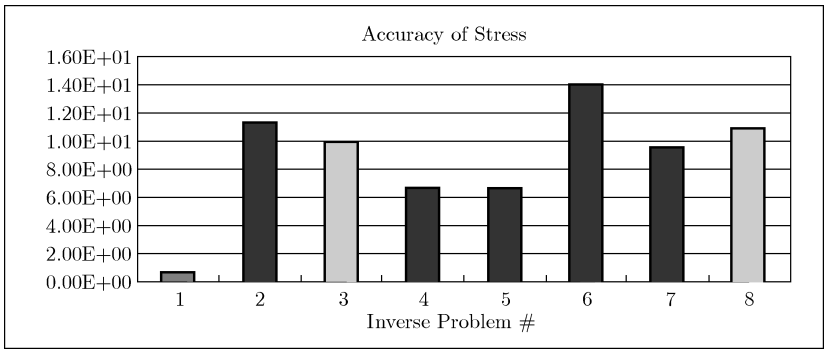


Figure 8.1. Comparison of accuracy of satisfying the specified stress for eight inverse design formulations.

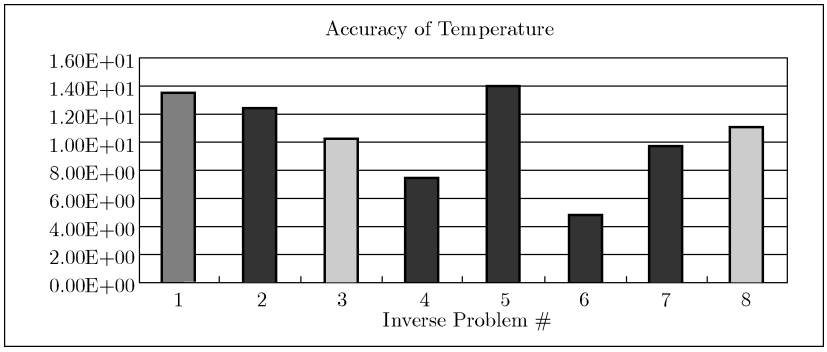


Figure 8.2. Comparison of accuracy of satisfying the specified temperature for eight inverse design formulations.

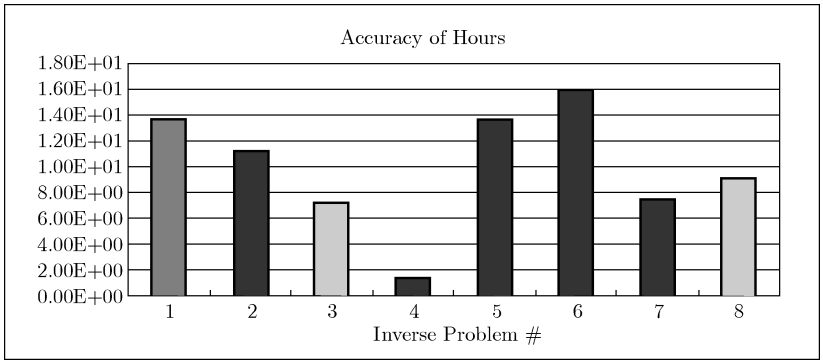


Figure 8.3. Comparison of accuracy of satisfying the specified time-to-rupture for eight inverse design formulations.

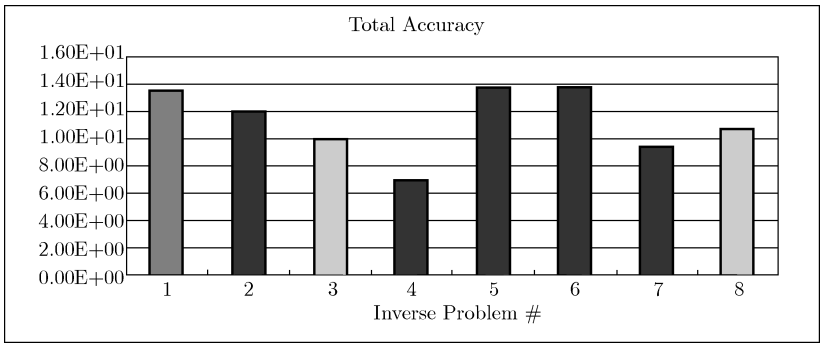


Figure 8.4. Comparison of combined accuracies of satisfying the specified values for eight inverse formulations.

$$\Delta\sigma = (\sigma - \sigma_{spec})/\sigma_{spec}, \tag{8.4.1}$$

$$\Delta T = (T - T_{spec})/T_{spec}, \tag{8.4.2}$$

$$\Delta H = (H - H_{spec})/H_{spec}, \tag{8.4.3}$$

$$EPS = \sum \left[(\Delta\sigma)^2 + (\Delta T)^2 + (\Delta H)^2\right]^{-1}, \tag{8.4.4}$$

$$K_1 = 10\ N_{objectives} + N_{constraints} + N_{variables}, \tag{8.4.5}$$

$$K_2 = 100\ (1 - \Delta\sigma) + (1 - \Delta T) + (1 - \Delta H), \tag{8.4.6}$$

$$K_3 = N_{calls}/N_{Pareto}, \tag{8.4.7}$$

$$\text{Maximize: } SCORE = \frac{K_1 K_2}{K_3} \exp(EPS). \tag{8.4.8}$$

When the suggested eight formulations were evaluated using this ad hoc evaluation procedure, only a few formulations appear to offer an overall superior performance (Figure 8.5).

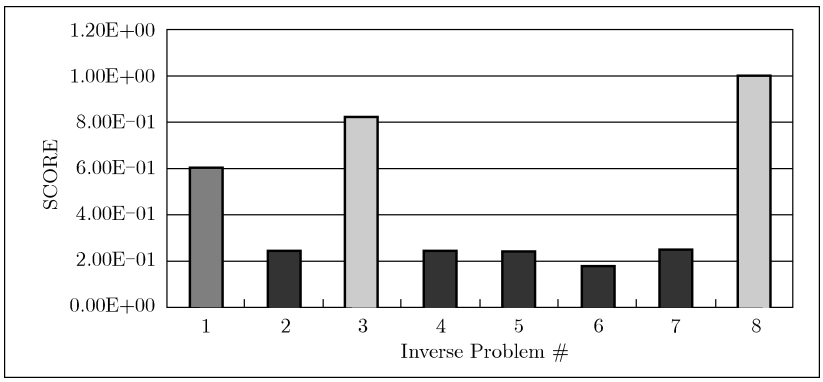


Figure 8.5. The values of overall performance (SCORE) for eight formulations for inverse design of alloys.

Table 8.3 presents a summary of accuracies in satisfying each of the constraints, number of the constraints, number of simultaneous objectives, number of Pareto points generated, number of optimization algorithm calls required, and the final performance scores of the eight design formulations with formulation number 8 being the best.

It is also highly educational to visualize the fact that the inverse design of alloys gives results that are not unique. That is, the same objectives and constraints can be met by using different concentrations of alloying elements. For example, if the designer specifies the desired stress level of $230\,\mathrm{N\,mm^{-2}}$ at the desired temperature of 975 C for the desired time of 5000 hours until rupture, the optimization algorithm can be asked to generate 50 possible combinations of Ni and Cr concentrations that will all provide life expectancy of 5000 hours at the desired stress level and the desired temperature. If the life expectancy is specified by the designer to be 6000 hours for the same stress and temperature levels, the allowable range of possible combinations of Ni and Cr concentrations will decrease. This becomes more noticeable as the specified time until the rupture is increased to 7000 hours and eventually to 8000 hours (Figure 8.6). Notice the reduction in the range of the acceptable variations of concentrations of the alloying elements as the specified alloy life expectancy increases.

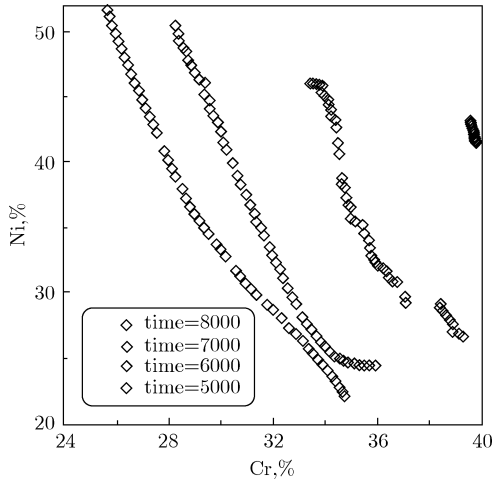


Figure 8.6. Allowable ranges of Ni and Cr concentrations for a specified level of stress at a specified temperature for different specified times until rupture.

Thus, the presented methodology for inversely designing chemical compositions of alloys offers a significant freedom to the designer to choose from a relatively large number of possible chemical concentration sets that satisfy the same specified physical properties. This is very attractive in cases when certain

Table 8.3. Summary of accuracies for each of the eight inverse design formulations for alloys.

	EPS_σ	EPS_T	EPS_H	EPS_{sum}	N_{constr}	N_{Obj}	N_{Pareto}	N_{calls}	$Score$
Prob. 1	$.408e{-}19$	$.356e{-}06$	$.536e{-}06$	$.297e{-}06$	0	3	50	417	0.590
Prob. 2	$.269e{-}08$	$.267e{-}07$	$.172e{-}08$	$.104e{-}07$	3	1	1	703	0.246
Prob. 3	$.897e{-}10$	$.143e{-}09$	$.134e{-}12$	$.777e{-}10$	3	3	50	445	0.817
Prob. 4	$.434e{-}13$	$.289e{-}12$	$.244e{-}18$	$.111e{-}12$	3	1	1	1020	0.246
Prob. 5	$.413e{-}13$	$.139e{-}05$	$.549e{-}06$	$.646e{-}06$	2	1	1	601	0.239
Prob. 6	$.954e{-}06$	$.576e{-}15$	$.980e{-}04$	$.646e{-}06$	2	1	1	774	0.180
Prob. 7	$.408e{-}10$	$.515e{-}10$	$.299e{-}12$	$.309e{-}10$	2	1	1	776	0.256
Prob. 8	$.714e{-}09$	$.928e{-}09$	$.127e{-}10$	$.552e{-}09$	3	10	46	834	1.000

alloying elements are becoming hard to obtain or too expensive in which case the optimized alloys with the lowest concentrations of such alloys can be used.

It is also highly educational to visualize the intrinsic nonlinearities of the unknown relationships between the concentrations of the alloying elements and the multiple properties of the alloys. Figure 8.7 shows that although concentrations of Ni and Cr in the 50 inversely designed alloys vary smoothly (Figure 8.6), concentrations of other alloying elements in these alloys have highly non-smooth variations, suggesting that even small variations of concentrations of certain alloying elements can cause significant variations in properties of alloys. Figure 8.7 was obtained using inverse design formulation number 3 with the following prescribed alloy properties: maximum stress = 4000 kpsi, temperature at which this stress is applied = 1800 F, time-until-rupture at the prescribed stress and the prescribed temperature = 5000 hours.

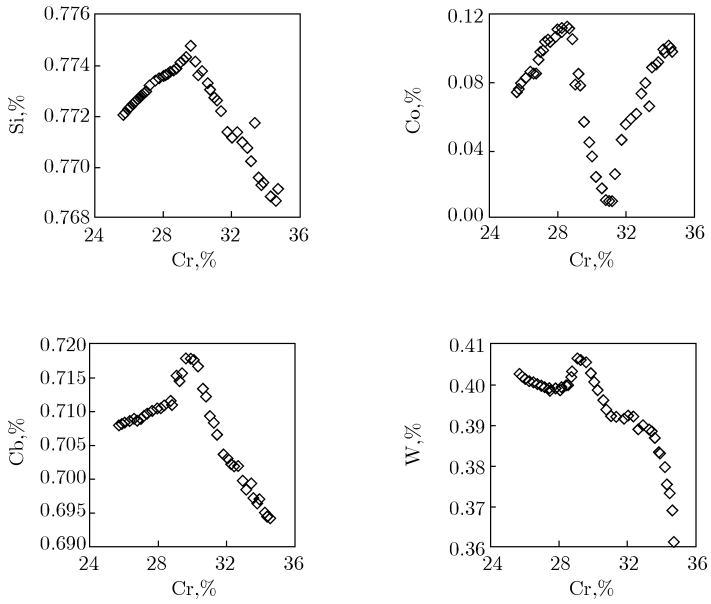


Figure 8.7. Variations of concentrations of several alloying elements corresponding to inversely designed alloys.

The results of this multiple simultaneous least-squares constrained minimization problem cannot be visualized for more than two alloying elements at a time. For example, when concentrations of only two alloying elements such as Ni and Cr are visualized, and temperature and life expectancy are unconstrained (unspecified), the optimization will result in a fairly large domain of acceptable variations of the concentrations of Cr and Ni [8]. However, as the constraints on temperature level are introduced and progressively increased, the feasible

domain for varying Cr and Ni will start to shrink (Figure 8.8). Similar general trends can be observed when the time until rupture is specified and progressively increased (Figure 8.9). The iso-contours in these plots depict the constant stress levels as functions of concentrations of Cr and Ni in these alloys.

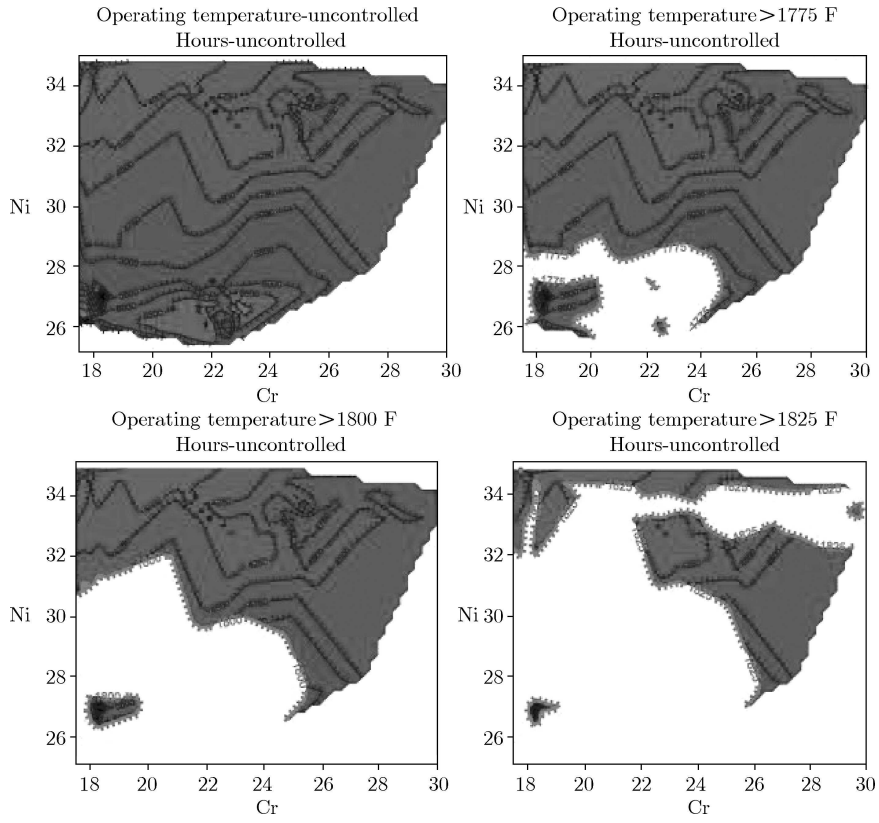


Figure 8.8. Effect of increasing specified temperature alone on allowable concentrations of Ni and Cr.

Finally, when temperature level and time until rupture are specified simultaneously and then progressively increased simultaneously, the feasible domain for concentrations of Cr and Ni reduces rapidly (Figure 8.10). Similar trends could be observed when looking at any other pair of alloying elements.

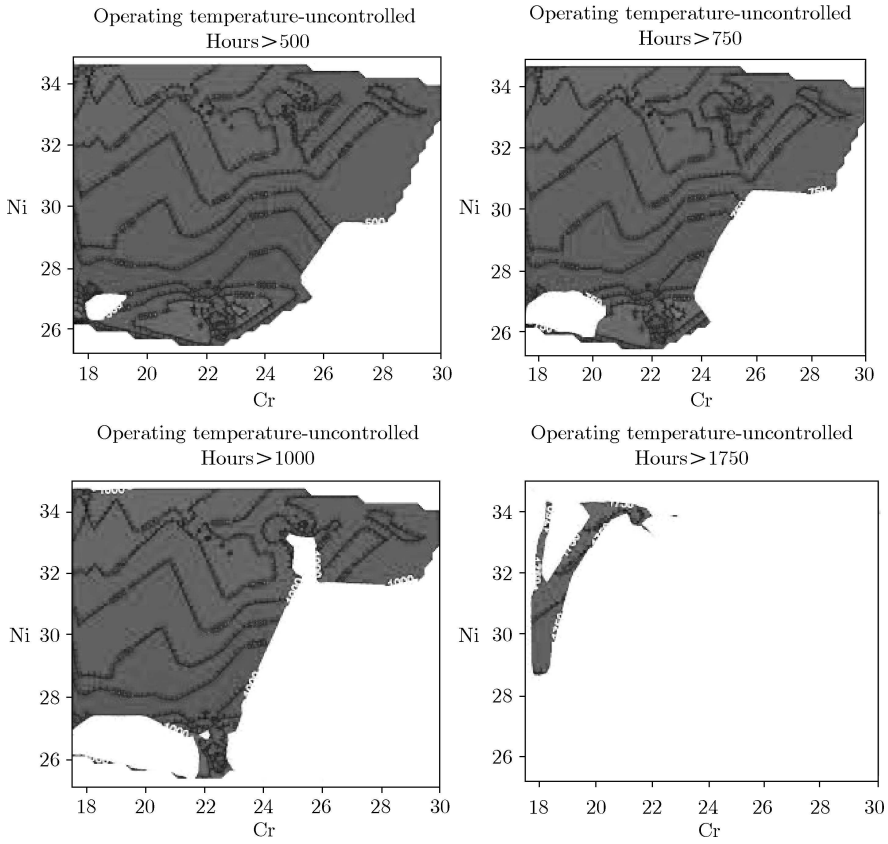


Figure 8.9. Effect of increasing specified time until rupture alone on allowable concentrations of Ni and Cr.

8.5 Determining Names of Alloying Elements and Their Concentrations for Specified Properties of Alloys

A more realistic (and considerably more complex) problem of inverse design of alloys is to actually determine which chemical elements to use in an alloy, while simultaneously determining the appropriate concentrations for each of the candidate elements. It is best to illustrate this inverse alloy design process by analyzing details presented in Figure 8.11. In this example, a maximum of 17 candidate alloying elements were considered (Cr, Ni, C, S, P, Mn, Si, Cu, Mo, Pb, Co, Cb, W, Sn, Al, Zn, Ti). The following three desired properties of the alloys were specified: stress = 4000 kpsi, temperature = 1800 F, time

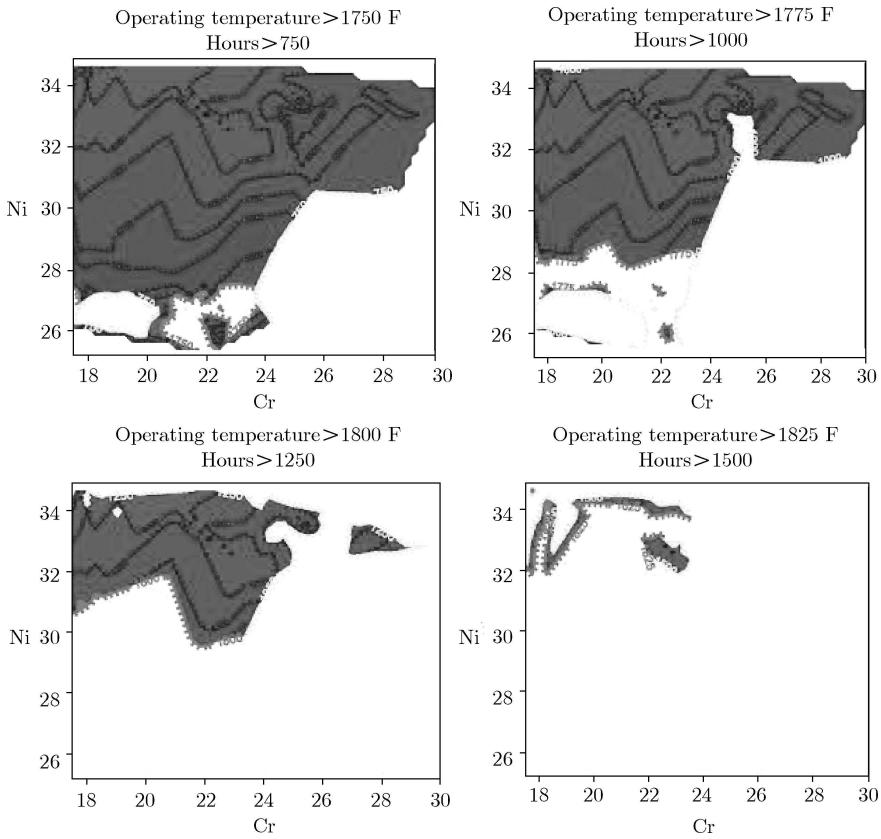
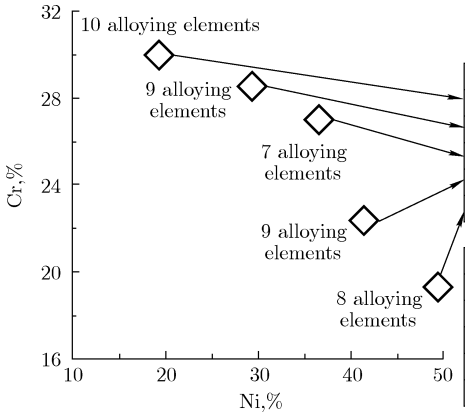


Figure 8.10. Effect of simultaneously increasing specified temperature and specified time until rupture on allowable concentrations of Ni and Cr.

until rupture = 6000 hours. These specified alloy properties were then treated as three equality constraints (satisfy accuracy of the three specified properties to within one percent) and the entire alloy design problem was formulated as a constrained multi-objective minimization problem (minimize Cr and Ni concentrations simultaneously in order to minimize cost of the raw material).

Results of this multi-objective constrained optimization task are given in Figure 8.11 by presenting five Pareto optimized alloys on the left hand side in terms of their concentrations of Ni and Cr, and the concentrations of the remaining 15 candidate alloying elements for each of the five Pareto optimized alloys given on the right hand side. Each of the five Pareto optimized alloys satisfies the three specified alloy properties while providing Pareto-optimized minimum use of Ni and Cr. It is fascinating to realize that optimized concentrations of some of the remaining 15 candidate alloying elements were found to be negligible although they are currently widely used in such alloys, thus



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

Figure 8.11. An example of simultaneously determining alloying elements and their concentrations for alloys with specified properties.

eliminating these elements as potential candidates for forming these types of steel alloys. Consequently, the number of alloying elements that actually needs to be used to create an alloy with the three specified properties could be as low as 7 instead of 15 (in addition to Ni and Cr). This is highly attractive for practical applications where regular supply, storage, and application of a large number of different pure elements are considered impractical, costly and financially risky.

This methodology of inversely designing chemical compositions of alloys offers a significant freedom to the designer to choose from a relatively large number of possible chemical compositions that satisfy the same specified physical properties. This is very attractive in cases when certain alloying elements are becoming hard to obtain or too expensive in which case the optimized alloys with the lowest concentrations of such alloys can be used.

8.6 Inverse Design of Bulk Metallic Glasses

Besides inverse design of Ni-based steel alloys, this alloy inverse design methodology can readily be used when designing arbitrary alloys including bulk metallic glasses (BMGs). For example, this inverse design method utilizing an optimization algorithm offers a capability to design a number of BMG alloys [7] with the same multiple properties, but having different chemistries that will make their availability, cost and utility more affordable. To demonstrate this, we created an initial data set of properties of 53 published experimentally evaluated Zr-based BMGs (Table 8.4) and then used IOSO optimization algorithm to determine chemical concentrations of 7 alloying elements (Zr, Cu, Al, La, (Cu, Ni), Pd, Si) in such BMGs that will all have glass transition temperature

Tg = 680 K for several prescribed values of BMGs' liquidus temperature, Tl (1000 K, 1100 K, 1200 K, 1240 K). Results of such inverse design procedures utilizing optimization are depicted in Figures 8.12–8.15 in the form of concentrations of the alloying elements.

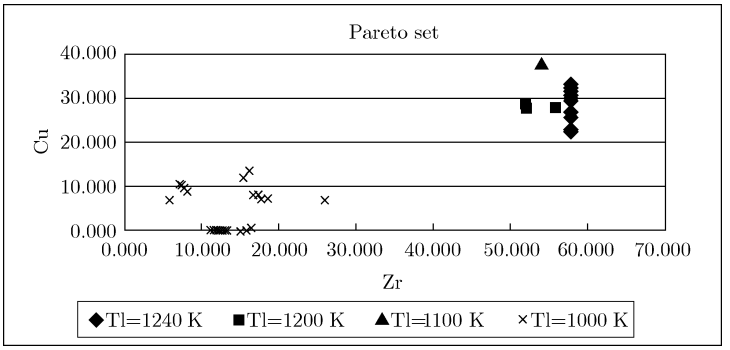


Figure 8.12. Results of an inverse design problem for Zr-based BMGs (specified Tg = 680 K and several specified values of Tl [7]) showing inversely determined concentrations of Cu and Zr for these conditions.

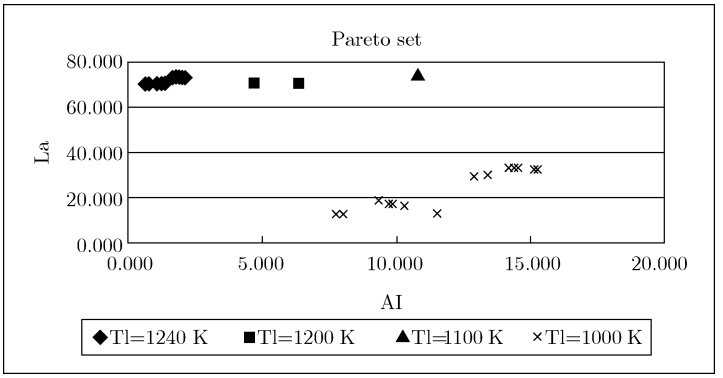


Figure 8.13. Results of an inverse design problem for Zr-based BMGs (specified Tg = 680 K and several specified values of Tl [7]) showing inversely determined concentrations of La and Al for these conditions.

8.7 Open Problems

The entire concept of inverse design of alloys is new and no other attempts to achieve the same have been found in the open literature. Since mathematical models linking the design variables (names and concentrations of the alloying elements) and the objectives (the specified multiple thermo-physical properties

Table 8.4. Experimental data for 53 Zr-based BMGs collected from open literature [7].

#	Tl(K)	Tg(K)	Tg/Tl	Zr%	Cu%	Al%	La%	(Cu,Ni)%	Pd%	Si%
1	1188	724	0.609428	50	36	14	0	0	0	0
2	1170	722	0.617094	50	38	12	0	0	0	0
3	1176	714	0.607143	50	40	10	0	0	0	0
4	1181	703	0.595258	50	43	7	0	0	0	0
5	1184	704	0.594595	49	44	7	0	0	0	0
6	1186	708	0.596965	48	45	7	0	0	0	0
7	1187	704	0.593092	49	45	6	0	0	0	0
8	1192	706	0.592282	48	46	6	0	0	0	0
9	1195	701	0.586611	49	46	5	0	0	0	0
10	1208	697	0.576987	49	47	4	0	0	0	0
11	1178	717	0.608659	45	49	6	0	0	0	0
12	1185	714	0.602532	45	50	5	0	0	0	0
13	1189	719	0.604710	44	51	5	0	0	0	0
14	1188	720	0.606061	45	48	7	0	0	0	0
15	1195	722	0.604184	45	47	8	0	0	0	0
16	1193	711	0.595977	46	49	5	0	0	0	0
17	1204	704	0.584718	47	49	4	0	0	0	0
18	1190	692	0.581513	54	38	8	0	0	0	0
19	1212	685	0.565182	56	36	8	0	0	0	0
20	1163	705	0.606191	52	38	10	0	0	0	0
21	1176	698	0.593537	54	36	10	0	0	0	0
22	1216	684	0.562500	54	40	6	0	0	0	0
23	759	403	0.530962	0	0	12.4	70	17.6	0	0
24	742	407	0.548518	0	0	13.2	68	18.8	0	0
25	674	405	0.600890	0	0	14	66	20	0	0
26	696	414	0.594828	0	0	14.6	64.6	20.8	0	0
27	699	420	0.600858	0	0	15.2	63.1	21.7	0	0
28	722	422	0.584488	0	0	15.7	62	22.3	0	0
29	729	426	0.584362	0	0	15.9	61.4	22.7	0	0
30	727	423	0.581843	0	0	16.3	60.5	23.2	0	0
31	743	426	0.573351	0	0	16.6	59.6	23.8	0	0
32	764	431	0.564136	0	0	17	58.6	24.4	0	0
33	783	435	0.555556	0	0	17.5	57.6	24.9	0	0
34	813	440	0.541205	0	0	17.9	56.5	25.6	0	0
35	844	436	0.516588	0	0	18.4	55.4	26.2	0	0
36	930	435	0.467742	0	0	20.5	50.2	29.3	0	0
37	763	404	0.529489	0	0	14	70	16	0	0
38	724	405	0.559392	0	0	14	68	18	0	0
39	674	405	0.600890	0	0	14	66	20	0	0
40	715	411	0.574825	0	0	14	64	22	0	0
41	738	417	0.565041	0	0	14	62	24	0	0
42	773	422	0.545925	0	0	14	59	27	0	0

(Continued)

#	Tl(K)	Tg(K)	Tg/Tl	Zr%	Cu%	Al%	La%	(Cu,Ni)%	Pd%	Si%
43	815	427	0.523926	0	0	14	57	29	0	0
44	1097.3	633	0.576871	0	2	0	0	0	81.5	16.5
45	1086	635	0.584715	0	4	0	0	0	79.5	16.5
46	1058.1	637	0.602022	0	6	0	0	0	77.5	16.5
47	1135.9	645	0.567832	0	8.2	0	0	0	75	16.8
48	1153.6	652	0.565187	0	10.2	0	0	0	73	16.8
49	862.7	428	0.496117	0	36	14	50	0	0	0
50	785.6	404	0.514257	0	26	14	60	0	0	0
51	731	395	0.540356	0	20	14	66	0	0	0
52	792.7	391	0.493251	0	14	14	72	0	0	0
53	825.5	361	0.437311	0	10	14	76	0	0	0

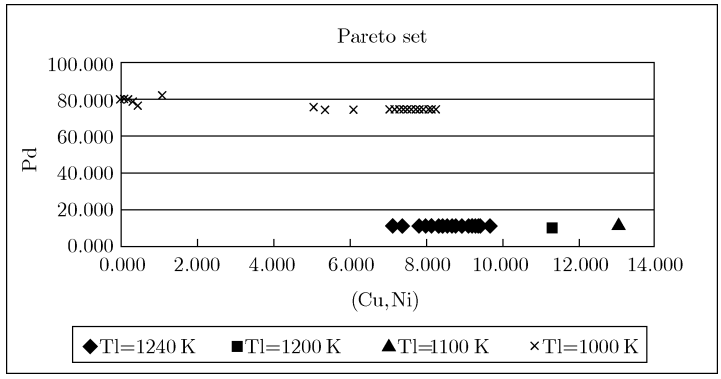


Figure 8.14. Results of an inverse design problem for Zr-based BMGs (specified Tg = 680 K for several specified values of Tl [7]) showing inversely determined concentrations of Pd and (Cu, Ni) for these conditions.

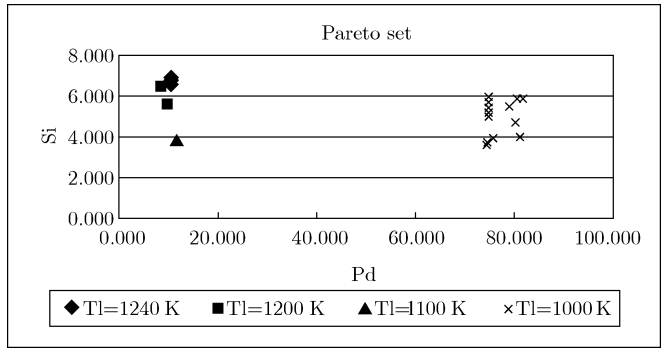


Figure 8.15. Results of an inverse design problem for Zr-based BMGs (specified Tg = 680 K and several specified values of Tl [7]) showing inversely determined concentrations of Si and Pd for these conditions.

of alloys) are non-existent, one might be inclined to use a heuristic interpolation algorithm (such as artificial neural networks (ANNs) [13]) to search an existing large data set of a similar class of alloys and try to interpolate these data in order to obtain a set of concentrations that will most closely provide for a specified set of alloy's properties. However, ANNs require an unacceptably large "training" data set of experimentally obtained multiple thermo-physical properties for each class of alloys studied. In addition, ANNs are strictly interpolation algorithms that cannot themselves perform constrained optimization nor can they extrapolate outside the initial data set with any confidence.

When testing samples of actual alloys, there is always a certain level of measurement error due to the finite accuracy of the testing equipment. This level of expected accuracy can now be specified and the results of the alloy composition optimization will automatically be modified to reflect this degree of uncertainty. Furthermore, during the manufacturing (melting and casting/solidification) of each new alloy, there is always a degree of uncertainty if the resulting alloy will have precisely the chemical composition that was expected when preparing and measuring the alloying components' masses. The level of this uncertainty depends on the level of sophistication of the alloy manufacturing process. Now, we have incorporated this feature in our alloy optimization software, whereby the materials designer can specify the accuracy level of the manufacturing process and the optimizer will automatically and appropriately modify the predicted quantities.

8.8 Conclusions

A new concept has been developed for designing alloys having specified multiple physical properties. The design variables are concentrations of the alloying elements and the names of the alloying elements themselves. This inverse method was formulated as a constrained multi-objective optimization problem and solved using a robust evolutionary optimizer of IOSO type. As a result, multiple choices are obtained for combinations of concentrations of alloying elements whereby each of the combinations corresponds to another Pareto front point and satisfies the specified physical properties. This inverse alloy design methodology does not require knowledge of metallurgy or crystallography and is directly applicable to alloys having an arbitrary number of alloying elements.

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