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EVOLUTIONARY OPTIMIZATION OF CHEMISTRY OF BULK METALLIC GLASSES

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Abstract. *Metallic glass is basically an alloy whose metallic species are "frozen" in amorphous glassy state rather than forming a standard crystalline structure. Metallic glasses have no grain boundaries and no dislocations and stacking faults. They are several times stronger than steel and considerably harder and more elastic. Formation of metallic glasses by extremely high cooling (~10^5 K/sec) of the melt was first accomplished in 1960s. The resulting metallic glass thickness was limited to extremely thin ribbons. In the 1990s, researchers formed new classes of metallic glasses in bulk. The bulk metallic glasses (BMGs) are composed of three or more metals in the alloy melt and a few diatomatous earth ingredients in order to lower the cooling rate. Cooling rates of the new alloys are from 100 K/s to 1 K/s. The possible thickness of these newer metallic glasses increased from micrometers to centimeters. One of the keys to lowering the cooling speed and creating larger specimens is that bulk metallic glasses should have ingredients with atomic species having large size and chemical differences. Thus, multiple thermo-mechanical properties and the cooling speed of bulk metallic glass alloys depend strongly on the concentrations of each of the chemical elements in a given alloy. The proposed methodology for accurately determining concentration of each of the important alloying elements is based on the use of a combination of a robust multi-objective optimization algorithm and on traditional experimentation. Specifically, the proposed alloy design method combines an advanced stochastic multi-objective evolutionary optimization algorithm based on self-adapting response surface methodology and a relatively very small data set of thermo-mechanical properties and the corresponding concentrations of alloying elements. During the iterative computational design procedure, new metallic glass alloys need to be manufactured and experimentally evaluated for their properties in order to continuously verify the accuracy of the entire design methodology. This metallic glass alloy design optimization method thus minimizes the need for costly and time-consuming experimental evaluations of new metallic glass alloys to fewer than 200 new alloys.*

1 INTRODUCTION

Metallic glasses were discovered in 1960 by Pol Duwez and co-workers [1], when they were working on rapid solidification of Au-Si alloys. But, the minimum cooling rate, R_c, required for their formation was of the order of 10^5 K/s. Achieving such high cooling rates necessitates that one of the dimensions of the product be very small, which is the case with melt-spun ribbons of thickness around 50-100 microns. Processes like planar low casting give rise to uniform ribbons which can be used for magnetic applications. The challenge was to make these materials in bulk form which necessitated a lower critical cooling rate. Drehman *et al*. [2] in 1982 found that almost 5mm thick castings can be made from the metallic glass of composition $Pd_{40}Ni_{40}P_{20}$. By using a suitable cooling, Kui *et al*. [3] were able to increase the thickness of the glass to more than 10mm. That gave rise to the possibility that metallic glasses can be manufactured in bulk form. Due to the pioneering and systematic work of Inoue *et al*. [3, 4] since 1988, a large number of compositions have been discovered in the La, Zr, Pd, Mg, Fe based systems. Based on these results Inoue had proposed three criteria for bulk glass formation.

1. Multi-component systems with more than three components – As the number of components increases, the number of possible phases that can nucleate from the melt increases. So, there is confusion in the melt as to which phase will nucleate first and the melt transforms into glass. This is known as the *confusion principle*.
2. Heat of mixing between the components should be negative – This would lead to intermetallic compound formation rather than cluster formation.
3. Difference between the radii of the atoms of the components should be more than 15% - This would ensure that solid solutions do not form.

The glass forming ability (GFA) of a system can be judged by the difficulty to measure parameter R_c. If critical cooling rates are lower, this means that thicker sections can be cast into glass, which implies a higher GFA. Turnbull [2] suggested that a high reduced glass transition temperature $T_{rg} = T_g/T_m$, where T_m is the melting (i.e., liquidus) temperature, is a good measure of GFA.

When a BMG is heated, it first undergoes structural relaxation where there is some rearrangement in atomic positions. Then, it undergoes a glass transition at temperature T_g, where its viscosity reduces drastically and it enters the supercooled liquid region. Then, at temperature T_x crystallization occurs by nucleation and growth of crystals. Inoue *et al*. have shown that the width of the super-cooled liquid region given by $\Delta T_x = T_x - T_g$ is a measure of glass forming ability. The larger the length of the super-cooled liquid region, the higher the GFA. Figure 1 shows the relation between R_c and the two GFA parameters. It can be seen that systems having lower R_c have larger values for T_{rg} and ΔT_x, but the scatter is less for ΔT_x. Inoue's criterion is widely accepted. Lu and Liu [5] have proposed yet another criterion for GFA defined as

$$\gamma = \frac{T_x}{T_g + T_{liq}} \tag{1}$$

where T_{liq} is the liquidus temperature. Figure 2 shows the variation of R_c with γ. It can be seen that by increasing the value of γ, a lower cooling rate, R_c, is possible and consequently larger critical section thickness can be cast [6].

There is also a growing need to minimize the amount of highly expensive components or their complete elimination by introducing some other components [7] offering comparable multiple thermo-physical properties of the resulting BMGs.

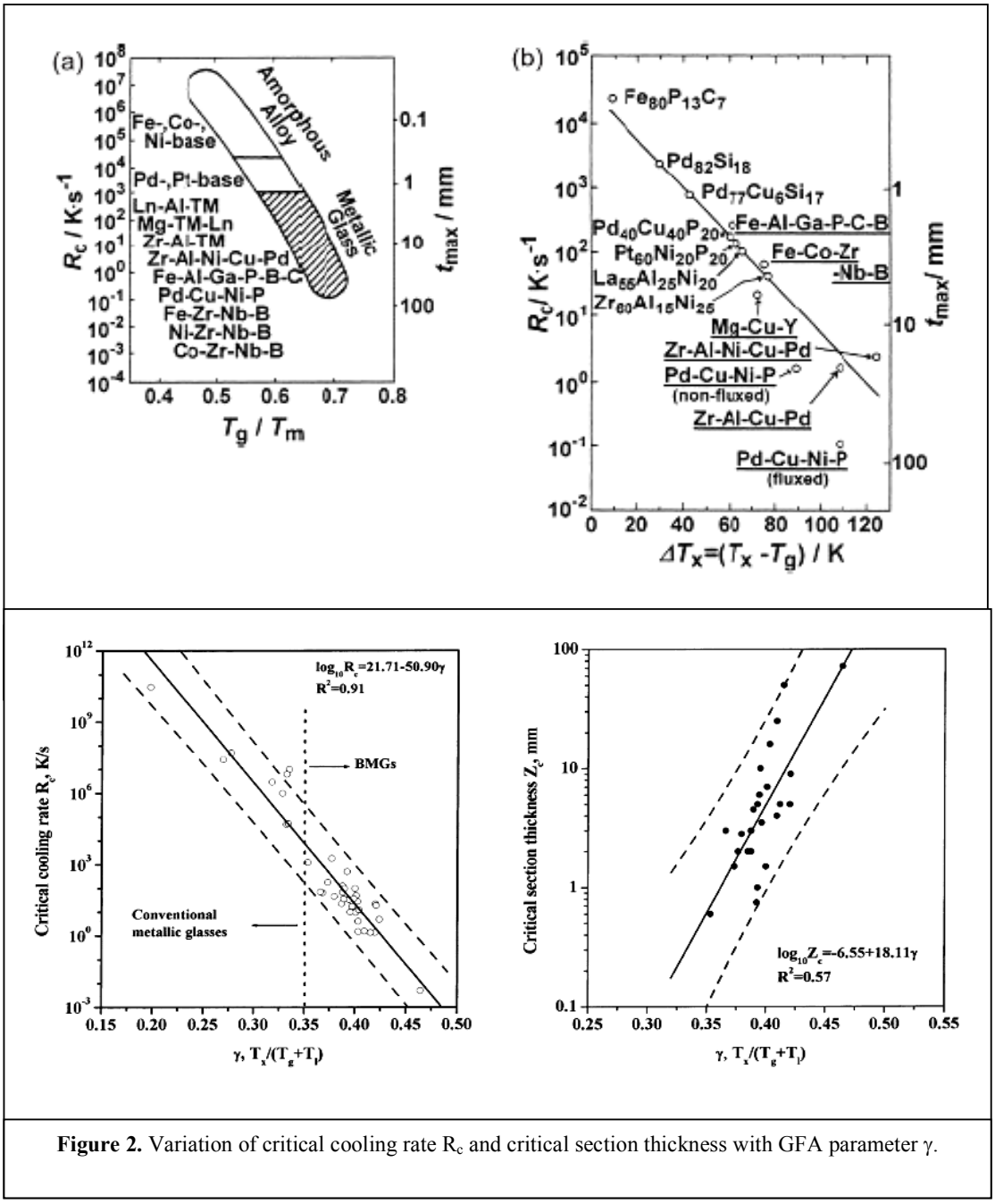

Figure 2. Variation of critical cooling rate R_c and critical section thickness with GFA parameter γ.

This BMG design method could have several simultaneous objectives. For example: maximize glass transition temperature T_g, maximize reduced glass transition temperature $T_{rg} = T_g/T_{liq}$, maximize the width of the super-cooled liquid region $\Delta T_x = T_x - T_g$, minimize liquidus temperature, T_{liq}, maximize hardness, H, maximize Young's modulus, E, and maximize density of the BMG [6-12] thus achieving high glass forming ability and its stability through computational means and verification of the results by rigorous experimentation. The key innovation lies in computationally arriving at the glass compositions which will have the high-

est glass forming ability while performing experimental verification of the predicted performance of the selected compositions.

Multiple thermo-mechanical properties and critical cooling rates of BMG alloys depend strongly on the concentrations of each of the alloying elements. A brute-force optimization of thermo-mechanical properties of BMGs by varying chemical concentrations of N alloying elements would involve creating an N-dimensional matrix of BMG compositions and then interpolating and searching for the extreme points in such a matrix. If concentration of each alloying element is varied within a specified range, this variation could be approximated by, for instance, ten parameters. This means that in the case of a BMG with six alloying elements, this "optimization" would require determining properties of 10^6 = 1,000,000 BMGs each having a different chemical composition. This is obviously impossible and should be replaced by a more economical mathematical optimization.

During the past decade, there has been a strong effort in the advanced metallurgy community to develop and use several very complex mathematical models that are based on non-equilibrium thermodynamics of solids, with the objective of minimizing the need for manufacturing and experimental evaluation of the actual alloy samples. However, the exclusive use of this strictly computational approach that utilizes artificial neural networks (ANNs) [13] and more recently on genetic algorithms [14] has been shown to possess dubious reliability and versatility as recently frankly demonstrated by Bhadeshia and Sourmail [15]. Furthermore, ANNs are efficient and relatively accurate interpolating algorithms for any multi-parameter function, but they are not efficient and accurate search algorithms and they are not extrapolation algorithms. Thus, the use of ANNs alone is not reliable for "getting out of the box" search outside the given data set.

Therefore, it is important to understand a need for mathematically sound multi-objective optimization algorithms capable of finding the global minimum and confidently search outside a given initial data base while accounting for uncertainties in the BMG manufacturing and testing.

We propose here a novel methodology for predicting the concentration of each of the important alloying elements in BMGs so that the new BMGs will have improved glass forming ability and thermal stability. The proposed optimization method is based on combining experimentally obtained multiple properties of the BMGs and a computational optimization algorithm [16-20] rather than on traditional experimentation alone, expert experience, and intuition. Specifically, the proposed BMG design method combines an advanced stochastic multi-objective evolutionary optimization algorithm based on self-organizing graph theory and a self-adapting response surface methodology [21-23]. During the iterative computational design procedure, a small set of new BMG alloys is periodically predicted, manufactured, and experimentally evaluated for their properties in order to continuously verify the accuracy of the entire design methodology [16-20]. The proposed BMG alloy design optimization method is thus experimentally verified and minimizes the need for costly and time-consuming experimental evaluations of new BMG alloys.

2 MULTI-OBJECTIVE OPTIMIZATION

With the continuing growth of computing resources available, the attention of design engineers has been rapidly shifting from the use of classical experimentation, repetitive computational analysis, personal experience, and intuition towards a reliable and economical mathematically based optimization algorithms. This trend has exposed the practical limitations of traditional gradient based optimization approaches that easily terminate in a local

minimum, can usually produce only single-objective optimized solutions, and require that the objective function satisfies continuity and derivability conditions [24]. These facts, together with the growing need for the multi-disciplinary and multi-objective approach to design with a large number of design variables and often conflicting simultaneous objectives, resulted in an increased interest in the use of various versions of hybrid [25, 26], semi-stochastic [27], and stochastic [20-23] optimization algorithms.

The *multi*-objective optimization problem maximizes a vector of n objective functions

$$max \;\; F_i(\overline{X}) \qquad \text{for } i = 1, \ldots n \tag{2}$$

subject to a vector of inequality constraints

$$g_j(\overline{X}) \leq 0 \qquad \text{for } j = 1, \ldots m \tag{3}$$

and a vector of equality constraints

$$h_q(\overline{X}) = 0 \qquad \text{for } q = 1, \ldots k \tag{4}$$

In general, the solution of this problem is not unique. With the introduction of the Pareto dominance concept [28] the possible solutions are divided in two subgroups: the *dominated* and the *non-dominated*. The solutions belonging to the second group are the "efficient" solutions, that is, the ones for which it is not possible to improve any individual objective without deteriorating the values of at least some of the remaining objectives. In formal terms, in case of a maximization problem, it is possible to write that the solution $\overline{X}$ dominates the solution $\overline{Y}$ if the following relation is true.

$$\overline{X} >_P \overline{Y} \Leftrightarrow (\forall i F_i(\overline{X}) \geq F_i(\overline{Y})) \cap (\exists j : F_j(\overline{X}) > F_j(\overline{Y})) \tag{5}$$

Classical gradient-based optimization algorithms are capable, under strict continuity and derivability hypotheses, of finding the optimal value only in the case of a single objective. For these algorithms, the problem of finding the group of non-dominated solutions (the Pareto front) is reduced to several single objective optimizations where the objective becomes a weighted combination of the objectives called utility function. However, this approach is computationally very intensive and fails in situations where Pareto front has discontinuities.

2.1 Response surface and self-organization concepts

Our approach to the proposed concept is based on the application of response surface technique, based upon the original approximation concept, within the frameworks of which we adaptively use global and middle-range multi-point approximations. One of the advantages of the proposed approach is the possibility of ensuring good approximating capabilities using a minimum amount of available information. This advantage results from self-organization and evolutionary modeling concepts [21-23].

The problem of search for a Pareto - optimum solution set in the multi-objective optimization while varying chemical composition of a BMG would be an unacceptably labor-intensive process. This is because of an extremely large number of BMG compositions that would need to be created and because several of the properties of each of these BMGs 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 BMGs for various com-

binations of a chemical structure. Such a database could be used for the solution of particular problems aimed at the creation of BMGs with desirable properties.

Instead, we propose to use IOSO multi-objective optimization [21-23] to determine BMG chemical compositions offering optimum properties of BMGs. Unfortunately, such 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 reached and how the remaining objectives will vary. That is, the user has very little if any *a priori* knowledge of objective function space topology.

The first approach is to perform a general multi-objective optimization of the material properties. Within the framework 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, not Pareto-set, solution. However, during such a 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, we have to perform a thorough preliminary search for the classes of base functions that will be able to construct the most accurate response surface models. However, the number of experiments that is necessary for true multi-objective optimization problem solutions depends not only on the dimensionality of the problem (the number of species in a BMG); it also depends to a considerable degree on the topologies of the object functions. This is why any predictions concerning the necessary number of trial points in the initial plan of experiment have a rather relative nature.

2.2 Summary of IOSO algorithm

Each iteration of IOSO consists of two steps. The first step is the creation of an approximation of the objective function(s). Each iteration in this step represents a decomposition of the initial approximation function into a set of simple approximation functions so that the final response function is a multi-level graph. The second step 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 to initialize the algorithm. The obtained response 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. In the process of 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 function is made more accurate only for this search area. While proceeding from one iteration to the next, the following steps are carried out: modification of the experiment plan; adaptive selection of current extremum search area; choice of the response function type (global or middle-range); transformation of the response function; modification of both parameters and structure of the optimization algorithms; and, if necessary, selection of new promising points.

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, while accounting for uncertainties, allows us to determine a set of vectors of optimized variables.

2.3 Examples of materials optimization results using IOSO algorithm

The algorithms and approaches that we propose have a universal nature and are applicable to any complex engineering system. An example of the recently published application of IOSO optimization to design of steel superalloys [16-20] is depicted in Figure 3. It demonstrates the ability of the proposed methodology to immediately in the first iteration create the superalloys with properties that are superior to any of the alloys in the original experimental data set.

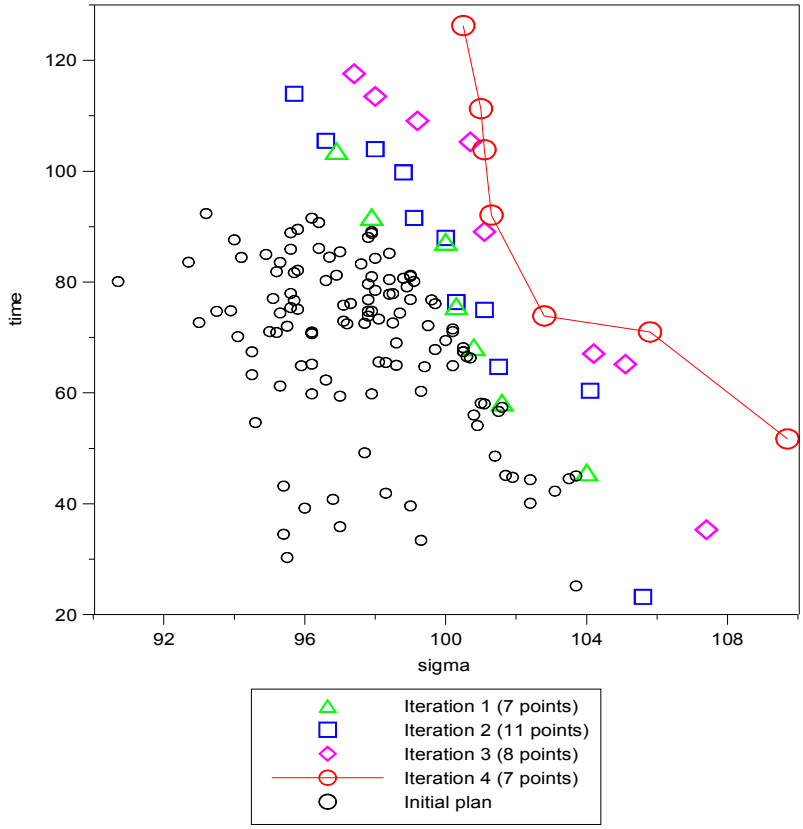

Figure 3. Experimental confirmation of the maximum stress at 20 C and time-to-rupture at 975 C for original 120 Ni-base steel superalloys (small circles) and four generations of 20 optimized Ni-base steel superalloys (other symbols) [19,20].

Our recent publication [30] gives a preliminary attempt to create a new generation of BMGs with improved multiple properties. Because of the unavailability of a large experimental data set for BMGs manufactured in a consistent manner, for the purpose of this study, we have decided to create such an experimental data set by combining data from several tables in the works of Prof. Y. Li [31,32]. Those BMGs for which experimental data were incomplete or inconsistent in these publications were not taken into account.

We then specified [30] that concentrations of all seven alloying elements (Zr, Cu, Al, La, (Cu,Ni), Pd, Si) should be optimized in each of the 46 new Pareto optimal BMGs to be cre-

ated by the IOSO algorithm while simultaneously maximizing T_g, T_{liq}.and T_g/T_{liq} and minimizing weight of the new BMGs. Results of this first iteration with IOSO are T_g, T_{liq} and T_{rg} values shown in Table 1 and Figures 4 - 6. Notice that the resulting Pareto optimized BMGs have properties that are better than the original BMGs. This is very encouraging since the initial data set was very small (only 46 BMGs) while optimizing concentrations of 6 alloying elements for 3 simultaneous objectives.

Table 1. Experimental data for BMGs collected from Works of Prof. Y. Li [31,32] and the values predicted by IOSO optimizer after its first application [30]

	Original experimental data [31,32]			Predicted by IOSO [30]		
#	Tg(K)	Tl(K)	Trg	Tg(K)	Tl(K)	Trg
1	724	1188	0.609	671.7	1243.3	0.540
2	722	1170	0.617	672.0	1242.7	0.541
3	714	1176	0.607	672.1	1242.4	0.541
4	703	1181	0.595	672.4	1241.8	0.541
5	726	1223	0.594	672.6	1241.3	0.542
6	714	1218	0.586	672.8	1240.7	0.542
7	704	1184	0.595	673.1	1240.2	0.543
8	708	1186	0.597	673.2	1239.7	0.543
9	704	1187	0.593	673.5	1239.0	0.543
10	706	1192	0.592	673.8	1238.4	0.544
11	701	1195	0.587	674.3	1238.0	0.544
12	697	1208	0.577	674.7	1237.2	0.545
13	717	1178	0.609	675.3	1236.1	0.546
14	714	1185	0.603	675.6	1235.5	0.547
15	719	1189	0.605	676.0	1234.8	0.547
16	720	1188	0.606	676.3	1234.1	0.548
17	722	1195	0.604	676.7	1233.6	0.548
18	711	1193	0.596	677.0	1232.9	0.549
19	704	1204	0.585	677.4	1232.3	0.550
20	692	1190	0.581	677.7	1231.7	0.550
21	685	1212	0.565	678.3	1230.8	0.551
22	705	1163	0.606	678.7	1230.3	0.551
23	698	1176	0.594	679.1	1229.5	0.552
24	684	1216	0.56	679.7	1228.6	0.553
25	671	1245	0.539	680.0	1228.1	0.553
26	403	759	0.53	680.4	1227.5	0.554
27	407	742	0.55	681.2	1226.4	0.555
28	405	674	0.6	681.6	1225.8	0.556
29	414	696	0.59	682.0	1225.1	0.556
30	420	699	0.6	682.4	1224.4	0.557
31	422	722	0.58	682.9	1223.7	0.558
32	426	729	0.58	683.3	1223.1	0.558
33	423	727	0.58	683.7	1222.5	0.559

34	426	743	0.57	684.0	1222.0	0.560
35	431	764	0.56	684.5	1221.3	0.560
36	435	783	0.56	684.9	1220.7	0.561
37	440	813	0.54	685.3	1220.2	0.561
38	436	844	0.52	685.8	1219.5	0.562
39	435	930	0.47	686.3	1218.6	0.563
40	404	763	0.53	686.6	1218.2	0.563
41	405	724	0.56	687.0	1217.7	0.564
42	405	674	0.6	687.4	1217.2	0.565
43	411	715	0.57	688.0	1216.6	0.565
44	417	738	0.57	688.2	1216.1	0.566
45	422	773	0.55	688.7	1215.5	0.566
46	427	815	0.52	724.8	1215.5	0.596

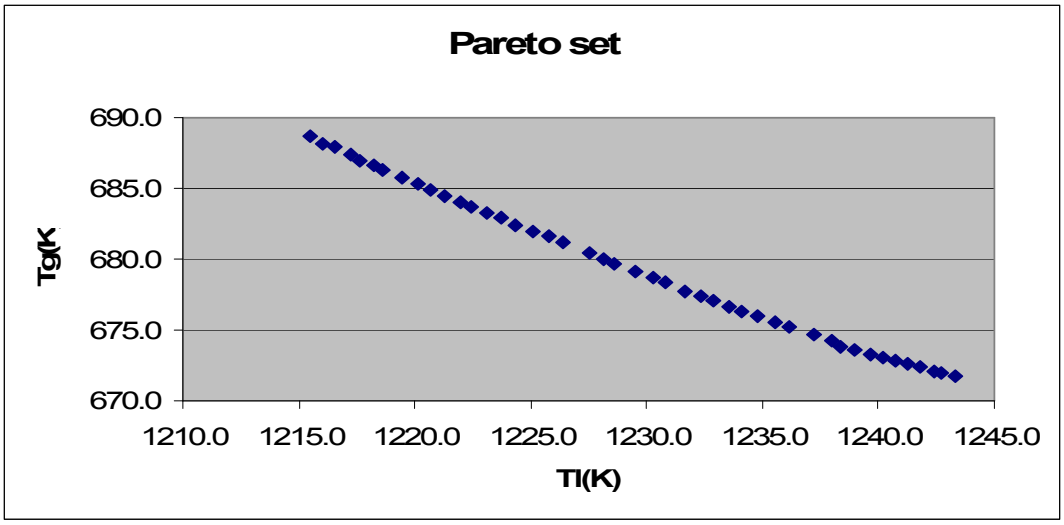

Figure 4. Pareto optimized BMGs when simultaneously maximizing T_g and T_{liq} [30].

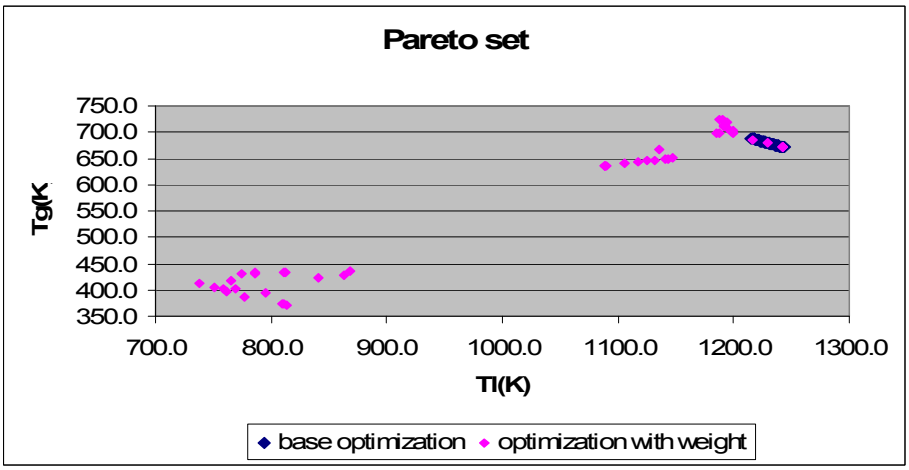

Figure 5. Pareto optimized BMGs when simultaneously maximizing T_g and T_{liq} and minimizing concentrations of each element (Zr, Cu, Al, La, (Cu,Ni), Pd, Si) in each new BMG [30].

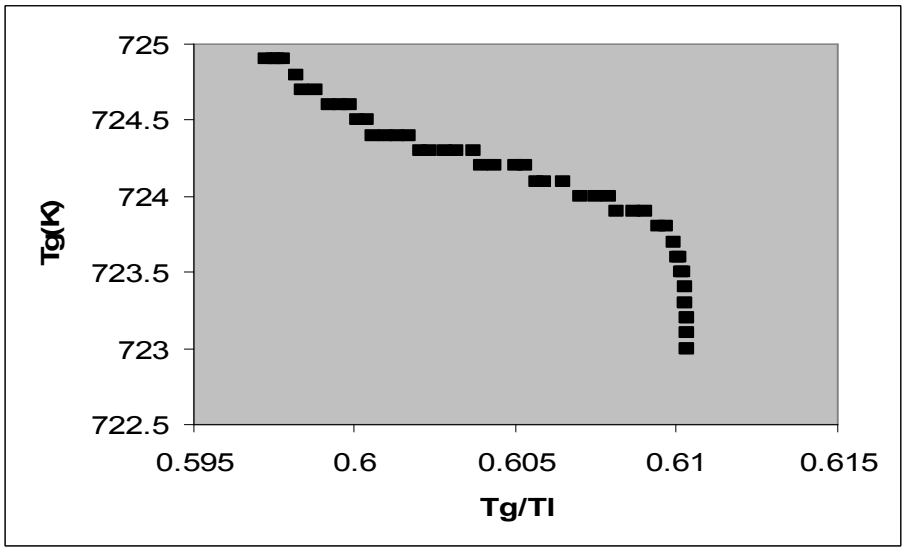

Figure 6. Pareto optimized BMGs when simultaneously maximizing T_g and T_g/T_{liq}.

2.4 Inverse design of BMGs

Conversely, an inverse design option [33] of this computational design optimization methodology can offer a capability to design a number of BMG alloys with the same multiple properties, but having different chemistries. This will make their availability, cost and utility more affordable. To this end, we utilized the original experimental data set and IOSO optimization algorithm to determine chemical concentrations of Zr, Cu, Al, La, (Cu,Ni), Pd, Si for a number of new BMGs that will all have T_g = 680 K and variable T_{liq} (1000 K, 1100 K, 1200 K, 1240 K). Results of such inverse design optimization of BMGs are depicted in Figures 7-13.

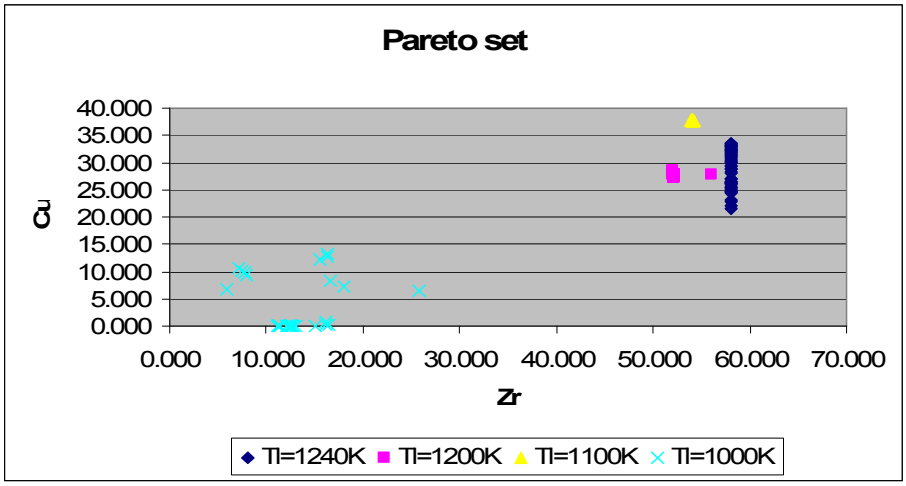

Figure 7. Results of an inverse design optimization problem: T_g = 680 K, T_{liq} = variable [30].

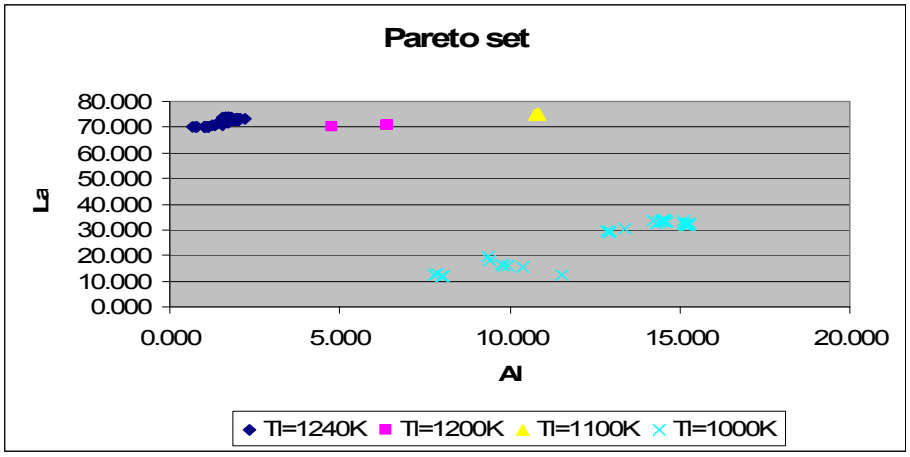

Figure 8. Results of an inverse design optimization problem: T_g = 680 K, T_{liq} = variable [30].

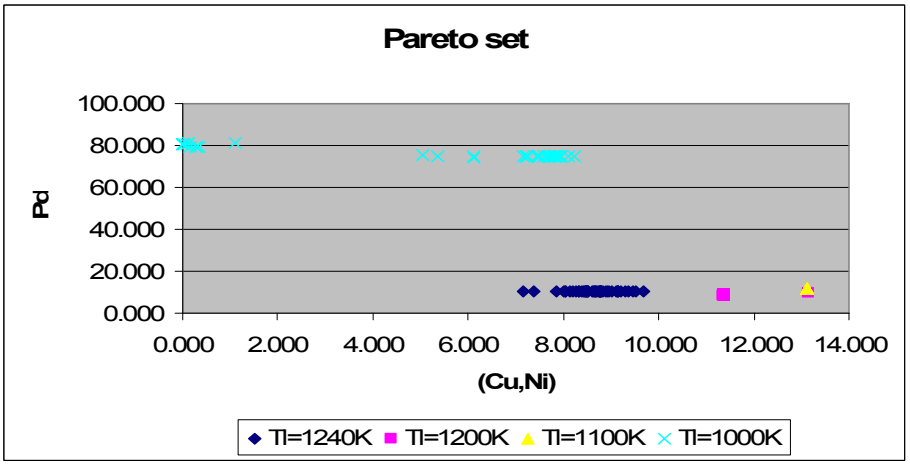

Figure 9. Results of an inverse design optimization problem: T_g = 680 K, T_{liq} = variable [30].

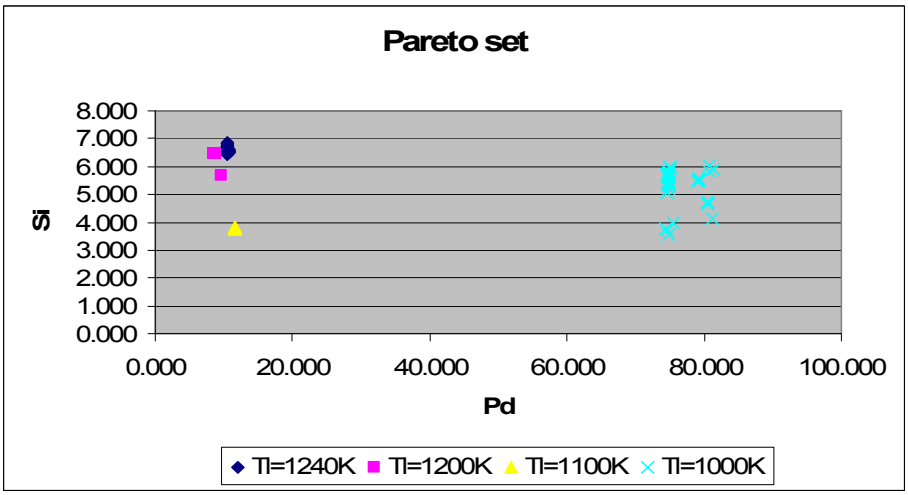

Figure 10. Results of an inverse design optimization problem: T_g = 680 K, T_{liq} = variable [30].

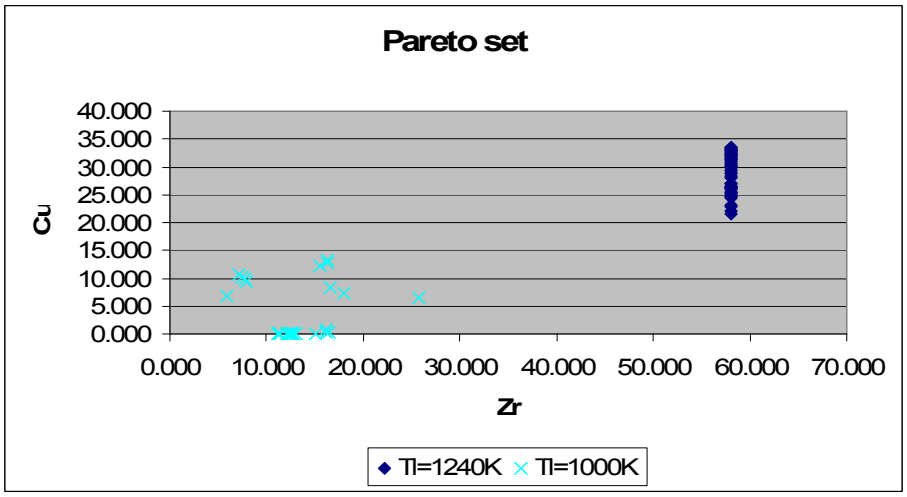

Figure 11. Results of an inverse design optimization problem: T_g = 680 K, T_{liq} = variable [30].

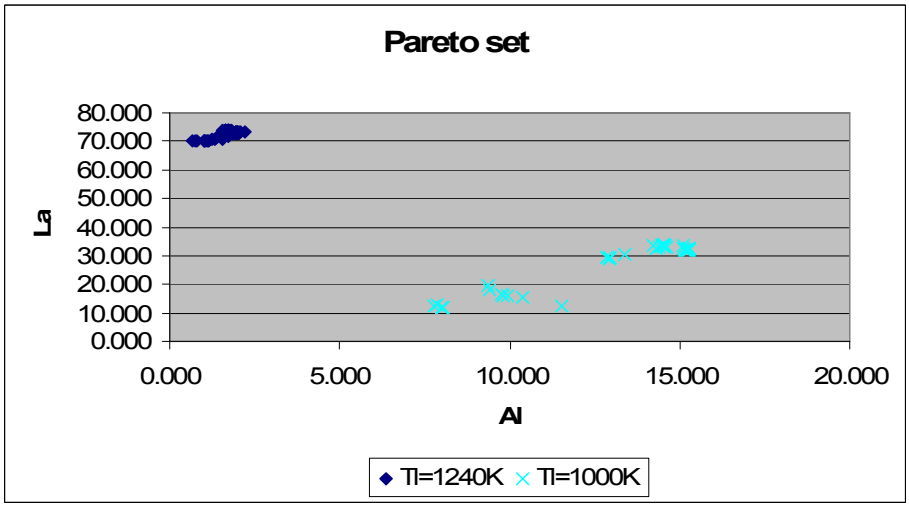

Figure 12. Results of an inverse design optimization problem: T_g = 680 K, T_{liq} = variable [30].

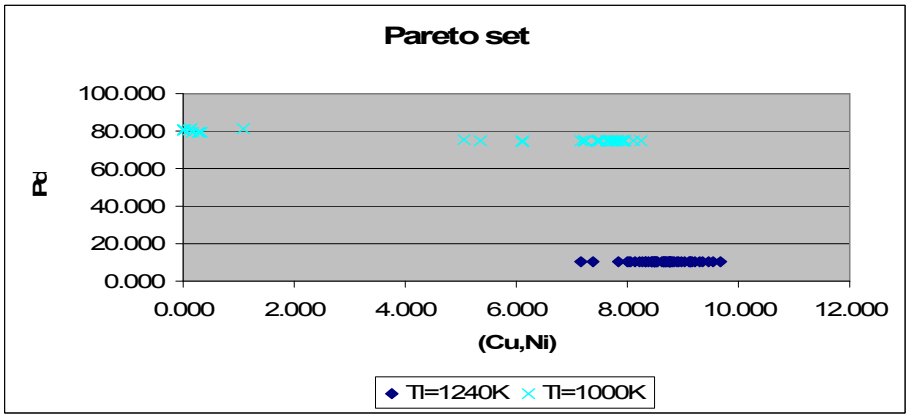

Figure 13. Results of an inverse design optimization problem: T_g = 680 K, T_{liq} = variable [30].

3 PROPOSED BMG DESIGN OPTIMIZATION METHODOLOGY

First, a finite number of simultaneous objectives should be defined despite the fact that several of these objectives might be mutually conflicting. For example: maximize glass transition at temperature T_g, maximize reduced glass transition temperature $T_{rg} = T_g/T_{liq}$, maximize length of the super-cooled liquid region $\Delta T_x = T_x - T_g$, minimize liquidus temperature, T_{liq}, maximize hardness, H, maximize Young's modulus, E, and maximize density of the BMG.

Based on the literature survey [6-12], Zr, Ti, Cu, Ni, Mg, Al, Fe, Nb, Si and Sn are the most commonly used elements and should be considered for the computational analysis and experimental testing to achieve the best BMG compositions. In the proposed design optimization methodology it is necessary that the user specifies the minimum and the maximum expected concentrations of a finite number of the most important BMG alloying elements. If the number of such elements is approximately five or six and the number of simultaneous objectives is two or three, from our experience with optimizing Ni-base superalloys [16-20] we expect that an initial data base of approximately 100 BMGs has to be developed by utilizing Sobol's algorithm [34] to prescribe chemical concentrations of these BMGs. The use of Sobol's algorithm is very helpful in distributing the initial concentrations in the best possible way so that the consequent multi-dimensional response surface fitting will be maximally accurate with the minimum number of available experimentally evaluated BMGs. These 100 initial BMGs then must be manufactured by casting them in an identical manner. These casts should be then experimentally tested for the specified number of simultaneous objectives. This information is then used for building approximation functions (multi-dimensional response surfaces) which will further be enriched by the IOSO optimizer using modified radial basis functions and multiple artificial neural networks. These approximation functions are then optimized using a non-gradient-based robust multi-objective optimization algorithm IOSO [21]. At each optimization iteration, a multi-criterion optimization task with a specified number of Pareto [28] optimal points (most likely 15) needs to be solved. The results of this complex numerical optimization process will be chemical concentrations of 5-6 specified alloying elements in these 15 new BMGs which the optimization algorithm predicted as belonging to the non-dominated Pareto optimal set, while accounting for specified level of uncertainty of BMG casting and testing.

Since the multi-dimensional response surfaces are fitted using a large number of points created by the artificial neural networks and the radial basis functions, instead of exclusively experimental data, the accuracy of the fit of the response surface will be relatively low. Consequently, it could be expected that not all of the 15 new optimized BMGs are actually superior to all of the initial 100 BMGs. To clarify this point, these 15 optimized BMGs then need to be manufactured and experimentally evaluated for the multiple properties. This concludes the first design iteration. The second iteration starts by using all (100 + 15 = 115) experimentally evaluated BMGs. The response surface building, enrichment, and optimization process is then repeated using these 115 data points with the same multiple objectives. The 15 newly optimized BMGs then need to be manufactured and experimentally tested to confirm that most of them are better than any of the 115 BMGs used in the second iteration of the design optimization process. The third iteration then starts with all accumulated experimentally tested BMGs (100 + 15 + 15 = 130), repeats all optimization steps, and results in 15 new optimized BMGs. The entire iterative process continues typically 4-5 cycles until a Pareto front sufficiently converges.

CONCLUSIONS

A multi-objective semi-stochastic optimization algorithm of IOSO family was used to demonstrate possibilities to determine optimum concentrations of the most important alloying elements forming a melt from which bulk metallic glasses are manufactured. This novel amorphous alloy design optimization method is expected to create entirely new generations of bulk metallic glass alloys with superior multiple thermo-mechanical properties that also cost less and weigh less. Conversely, an inverse design option of this computational methodology will offer a capability to design a number of alloys with the same multiple properties, but having different chemistries which will make their availability, cost and utility more affordable.

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