Titanium Based Alloy Chemistry Optimization for Maximum Strength, Minimum Weight and Minimum Cost Using JMatPro and IOSO Software

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Key words: Alloy Design, Response Surfaces, Multi-objective Optimization, JMatPro, IOSO

Abstract

Chemical concentrations of new generations of Ti-base alloys containing Al, Cr and V were predicted computationally that simultaneously maximize Young's modulus of elasticity while minimizing alloy density and cost of its raw materials. A software JMatPro was used to calculate the desired properties and software IOSO was used to perform multi-objective evolutionary optimization by creating several Pareto optimal generations of new alloys. The method was applied over a wide range of temperature varying from 30 $^{\circ}$C to 1500 $^{\circ}$C.

Introduction

Titanium alloys parts are ideally suited for advanced aerospace systems[1] because of their unique combination of high specific strength at both room temperature and moderately elevated temperature, in addition to excellent corrosion resistance. Improvement in existing alloys and development new alloys continues with the object of obtaining further benefits in terms of overall performance, extended life and reduced cost. A number of researchers[2] have been working on the Ti-alloys suited for specific application. To find the best Ti-base alloy where alloying elements are Al, Cr and V would require finding optimum concentrations of each of the alloying elements (that is, to find optimum alloy chemistry[3-5]). Without a powerful new generation of multi-objective evolutionary optimization algorithms, this task would require evaluation of an exorbitant number of candidate alloys. Furthermore, to evaluate multiple properties of each of the candidate alloys experimentally would be unacceptably time consuming and expensive. Neural networks have been used[6] to relate the alloys' properties with their chemical concentrations, but a faster method is required to perform such correlations while utilizing as small experimental data sets as possible in order to minimize the time and cost involved in the alloy design optimization process. Use of response surfaces can be one such methodology and it has been implemented by the authors in the design optimization of high temperature superalloys[7-9].

This is why we are here demonstrating the possibility to use large existing experimental data sets in conjunction with a reliable software for data mining such as JMatPro to predict the multiple alloy properties purely computationally to arrive purely computationally at the superior performance alloy compositions.

Alloy Design Optimization Methodology

The initial chemical compositions of the Ti-base alloys are chosen from the search space created by the composition of Al, Cr and V. There are various methods to generate a set of points well spaced in the s-dimensional space[10]. Quasi-random number sequences are designed to have a high level of uniformity in multidimensional space. It is believed, though it has not been proven, that no s-dimensional sequence can have discrepancy an order of magnitude smaller than $\log^{s}N$ in generating a set of N points from rectangular s-dimensional space. Sobol's method for generating quasi random sequences was used as these sequences have low discrepancies[11]. In the present implementation, 4 elements constitute the alloys with the composition range varying for each element as stated above. Therefore Sobol's points are generated in a 3-dimensional space where each point represents a composition of the components of a Ti-base alloy (concentration of Al, Cr, and V).
To start with, 50 such points representing 50 alloy compositions were generated using Sobol's algorithm. Density and Young's modulus were then calculated for each composition using the software JMatPro. The cost of raw material was taken from the website of Alfa Aesar for powders of 99.5% (-325 mesh) purity[12].

These 50 concentrations and the corresponding Young's moduli, densities and costs were then fed into IOSO evolutionary optimization algorithm which was asked to generate concentrations of 20 new Ti-base alloys that will be Pareto optimal, that is, which will be better than any of the original 50 Ti-base alloys. Properties of each of these 20 new Pareto-optimal alloys were computed using JMatPro software. These 20 optimized alloys were then added to the original 50 alloys to create an enlarged set of 70 Ti-base alloys. The optimization process was then repeated by utilizing these 70 alloys as the initial data set for the second application of IOSO optimizer with the request to automatically generate compositions of 20 new Pareto optimal alloys (Table 1). This constitutes the generation process of the second Pareto front. These 20 Pareto optimal Ti-base alloys were then added to the already existing 70 alloys to create an initial data set having 90 Ti-base alloys that were then used for the next cycle of generation of 20 Pareto optimal alloys.

Table 1. Parameters for the IOSO iteration

Parameter	Value
Input parameters	3
Number of responses	3
Number of Pareto optimal points desired	20
Optimization accuracy	0.0001
Constraints assurance accuracy	0.00001
Maximum number of iterations to be used	2000

Results

The ranges of the design variables (that is, concentrations of alloying elements) used in this work are shown in Table 2. The optimization of properties of alloys with respect to chemical composition concentrations has been carried out at temperatures varying from 30 °C up to 1500 °C. Results at temperatures of interest are shown below in figures from 1 to 4.

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

↓Range\Components→	Al	Cr	V	Ti
Min	0	0	0	Remaining
Max	50 %	15 %	15 %	

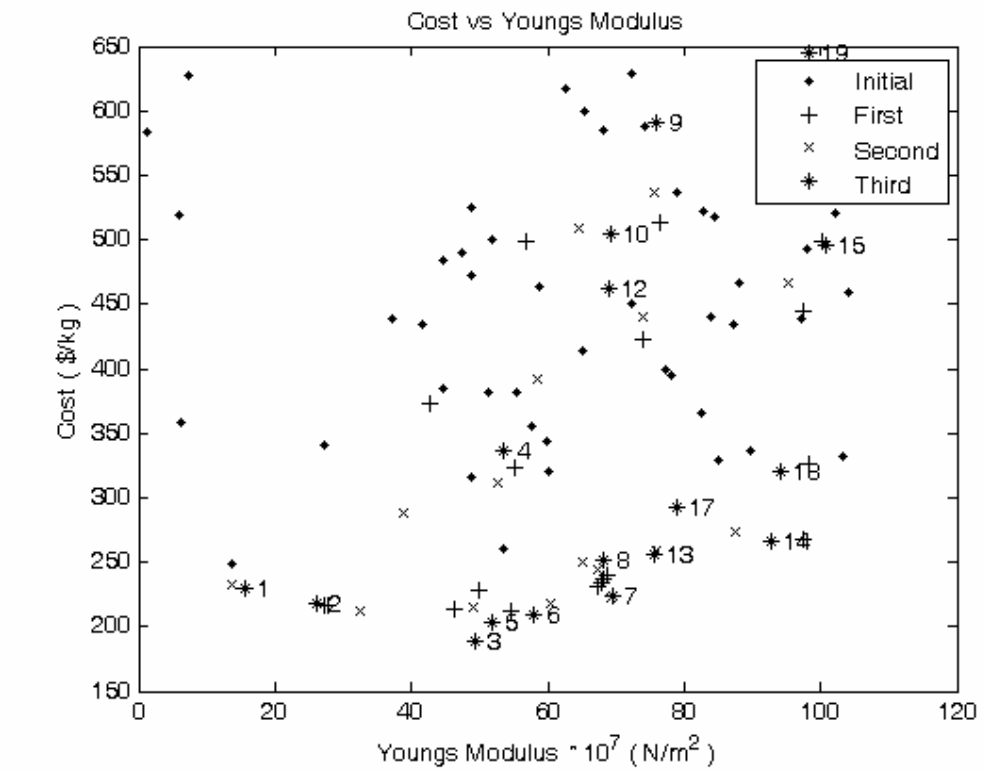

Fig 1 (i) Cost vs Young's modulus at 1200 °C

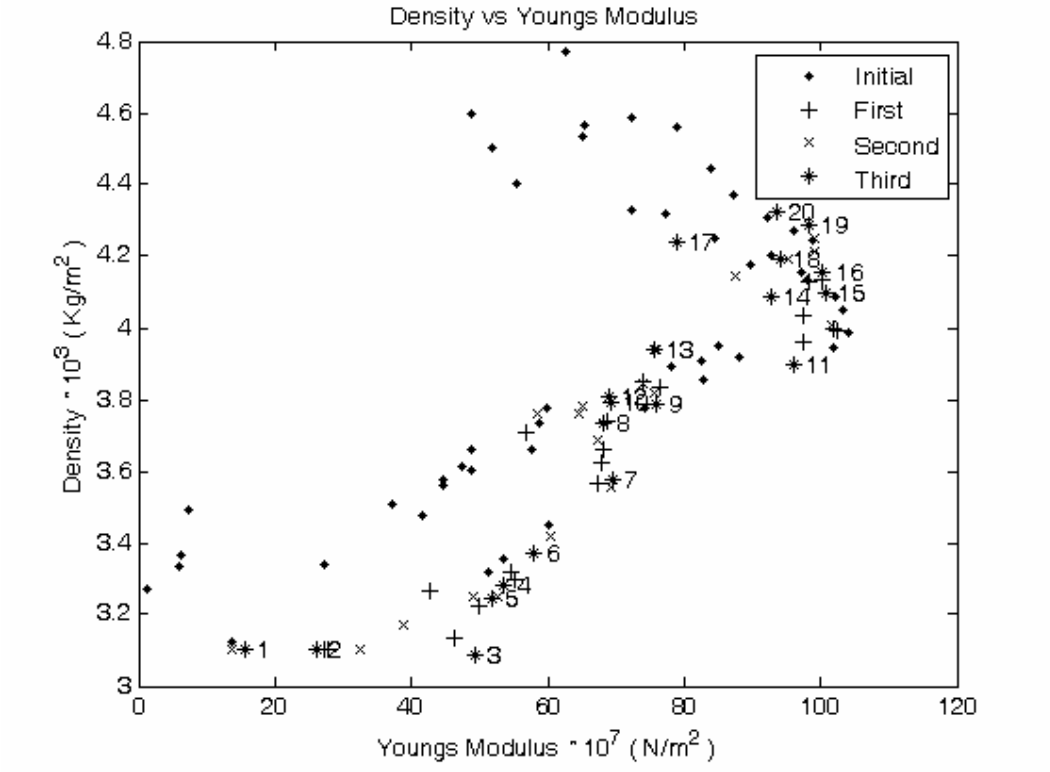

Fig 1 (ii) Density vs Young's modulus at 1200 °C

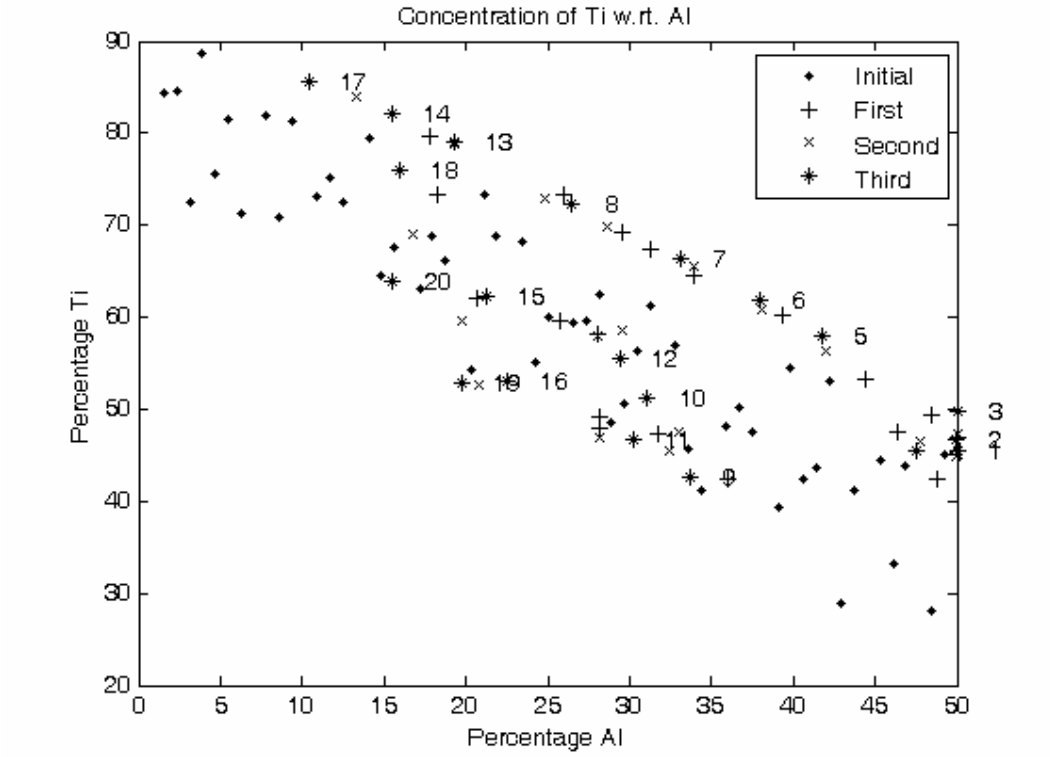

Fig 1 (iii) Concentration of Ti vs Al at 1200 °C

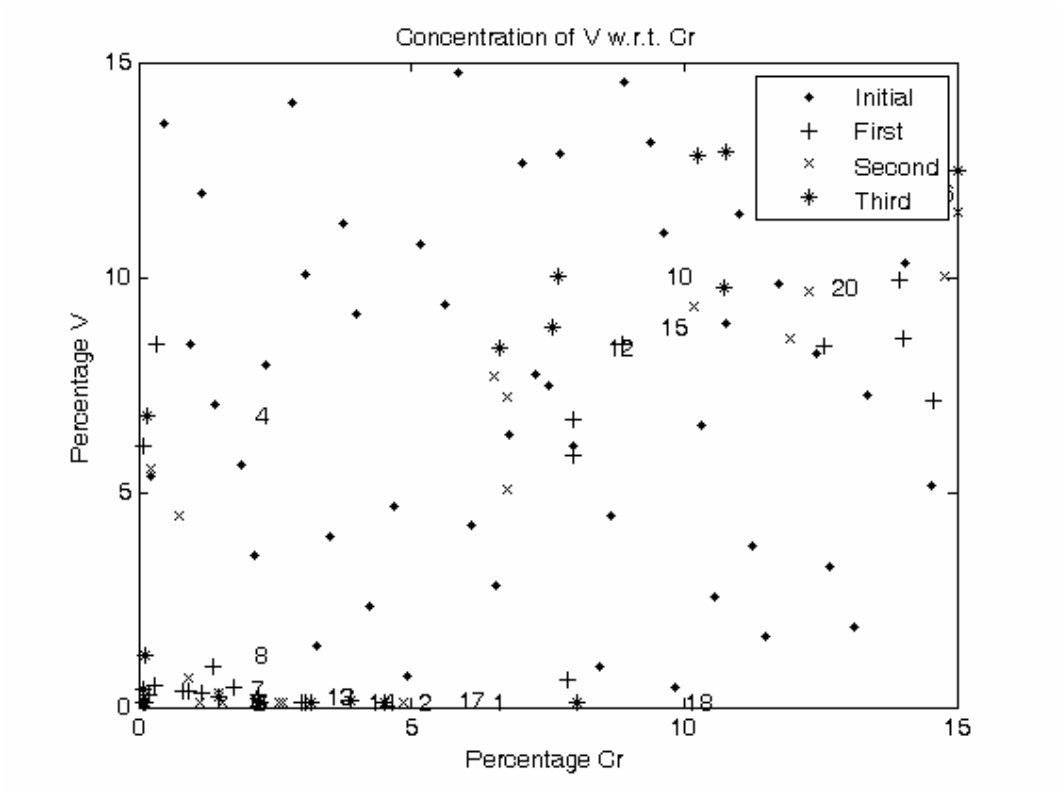

Fig 1 (iv) Concentration of V vs Cr at 1200 °C

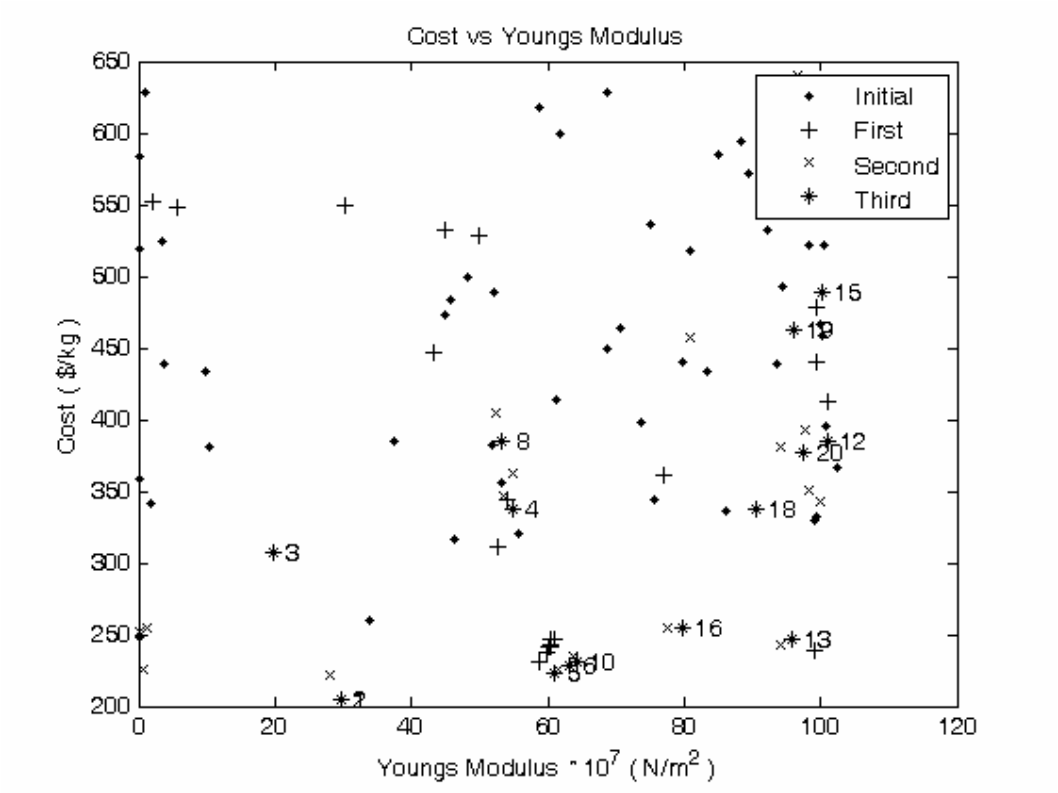

Fig 2 (i) Cost vs Young's modulus at 1300 °C

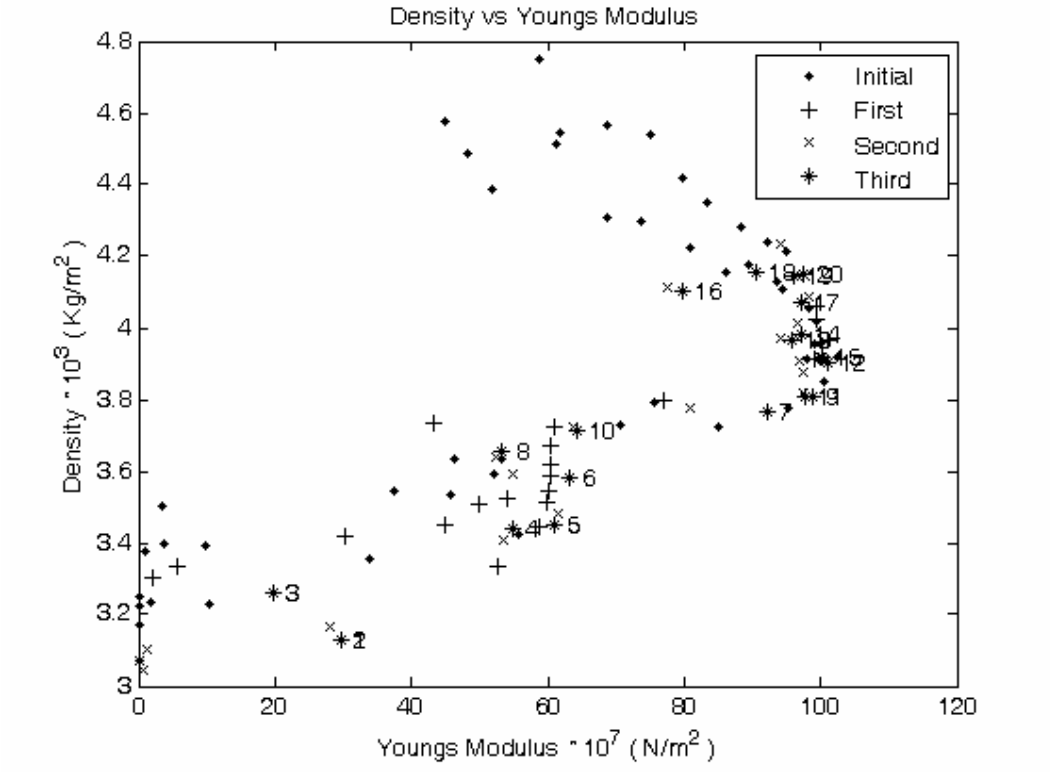

Fig 2 (ii) Density vs Young's modulus at 1300 °C

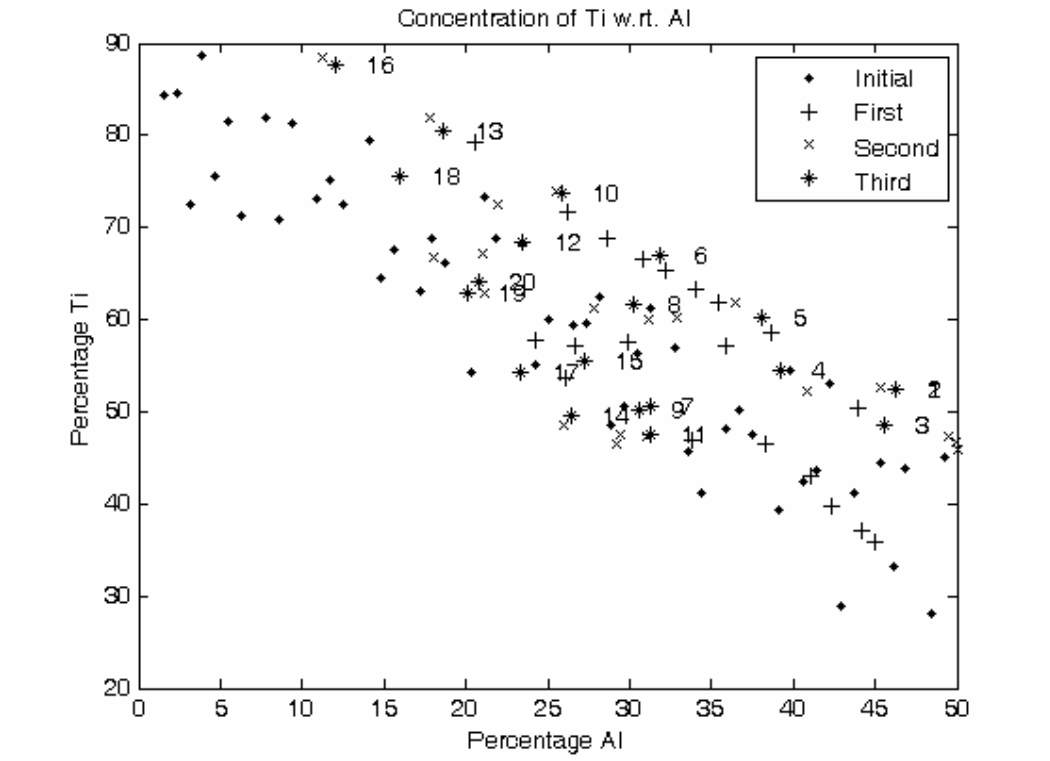

Fig 2 (iii) Concentration of Ti vs Al at 1300 °C

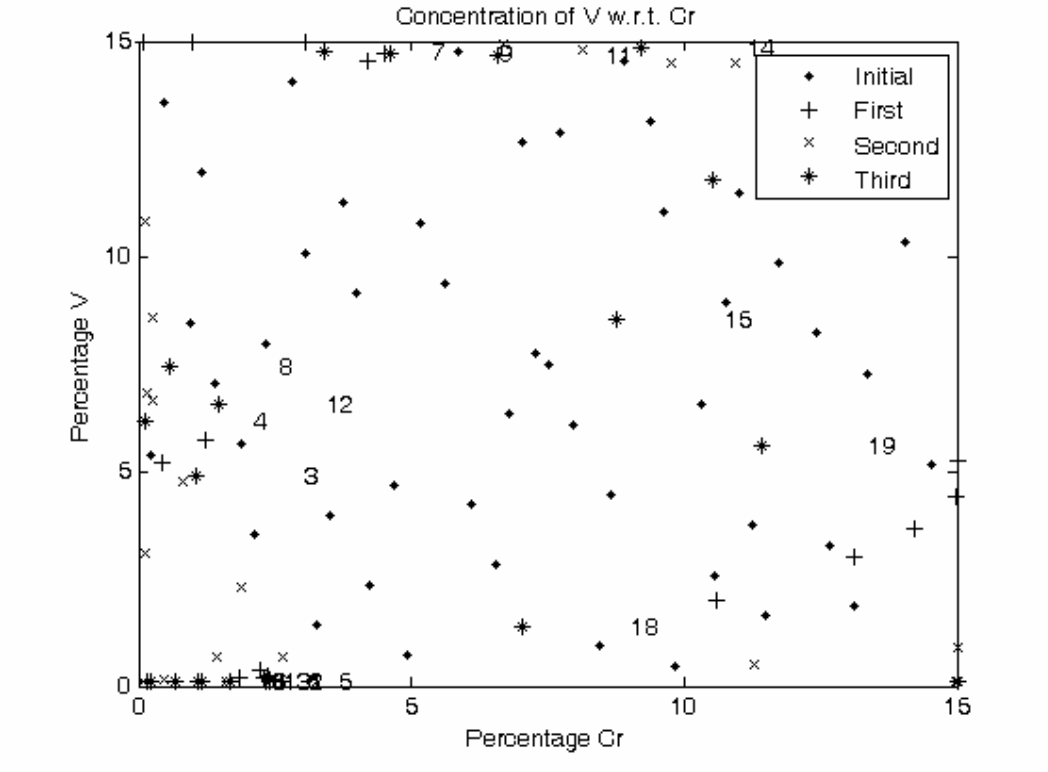

Fig 2 (iv) Concentration of V vs Cr at 1300 °C

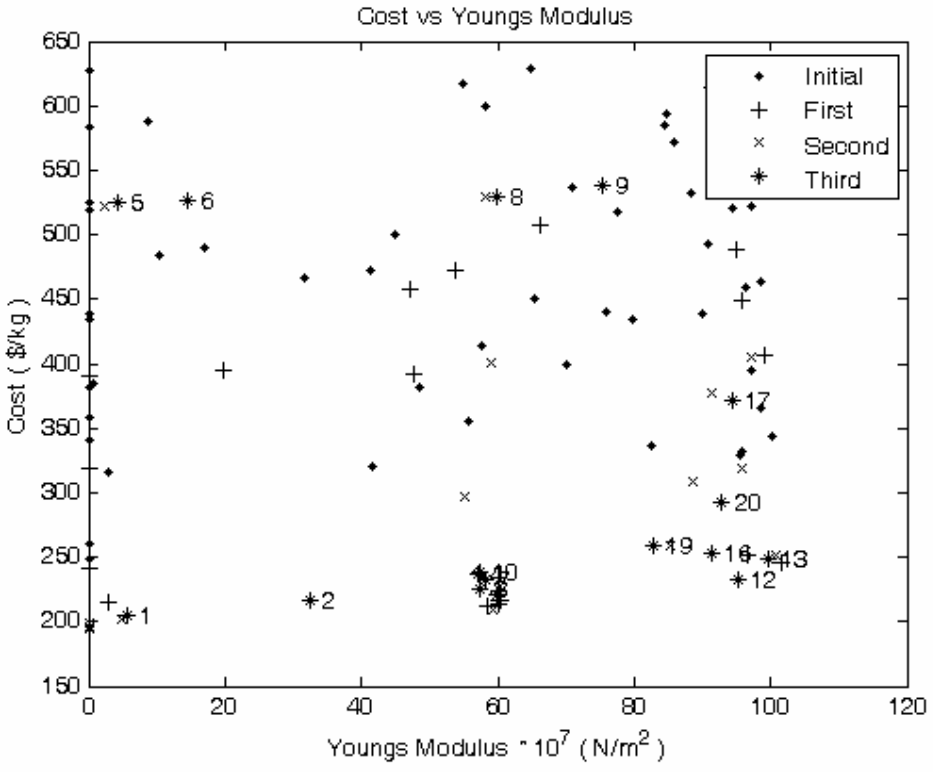

Fig 3 (i) Cost vs Young's modulus at 1400 °C

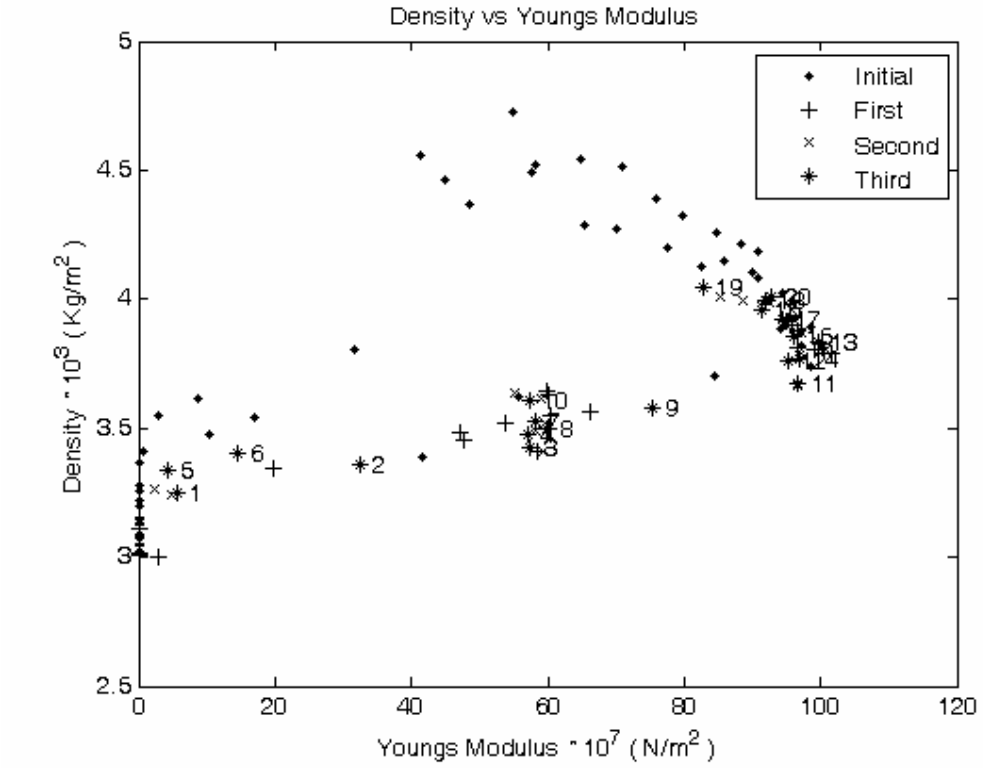

Fig 3 (ii) Density vs Young's modulus at 1400 °C

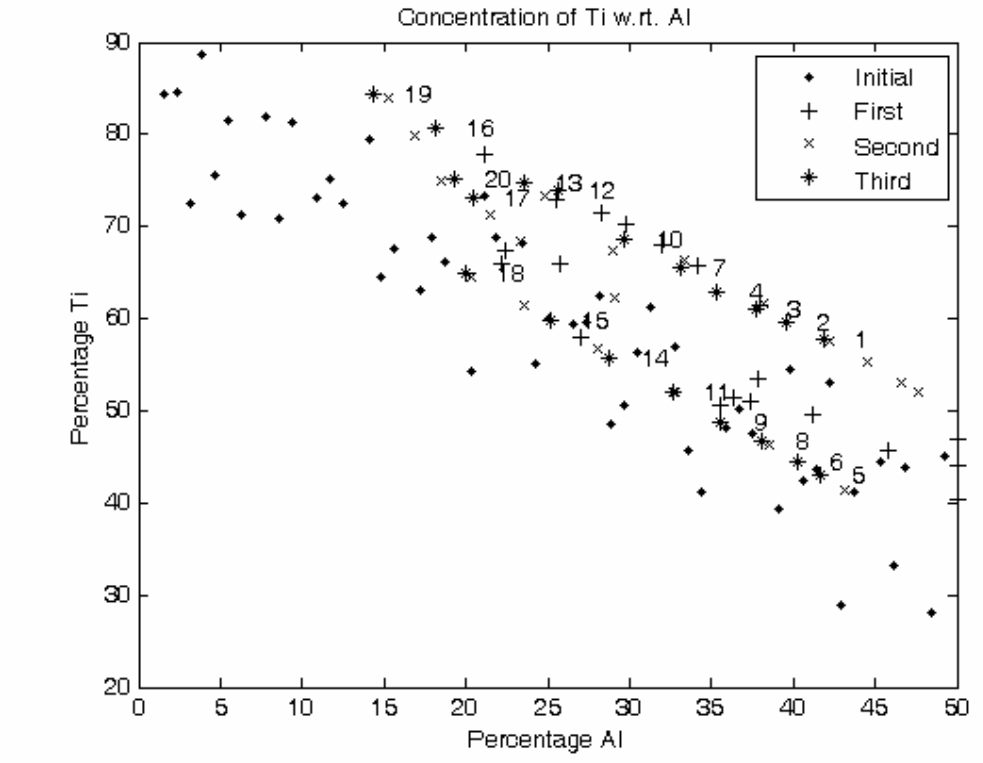

Fig 3 (iii) Concentration of Ti vs Al at 1400 °C

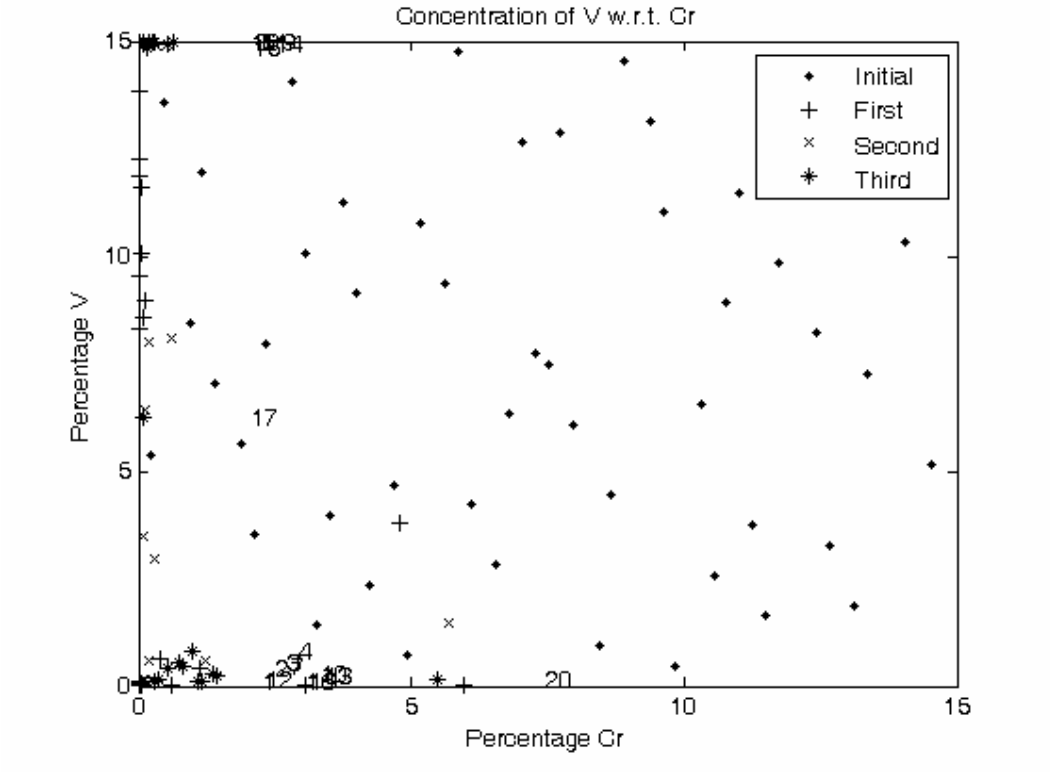

Fig 3 (iv) Concentration of V vs Cr at 1400 °C

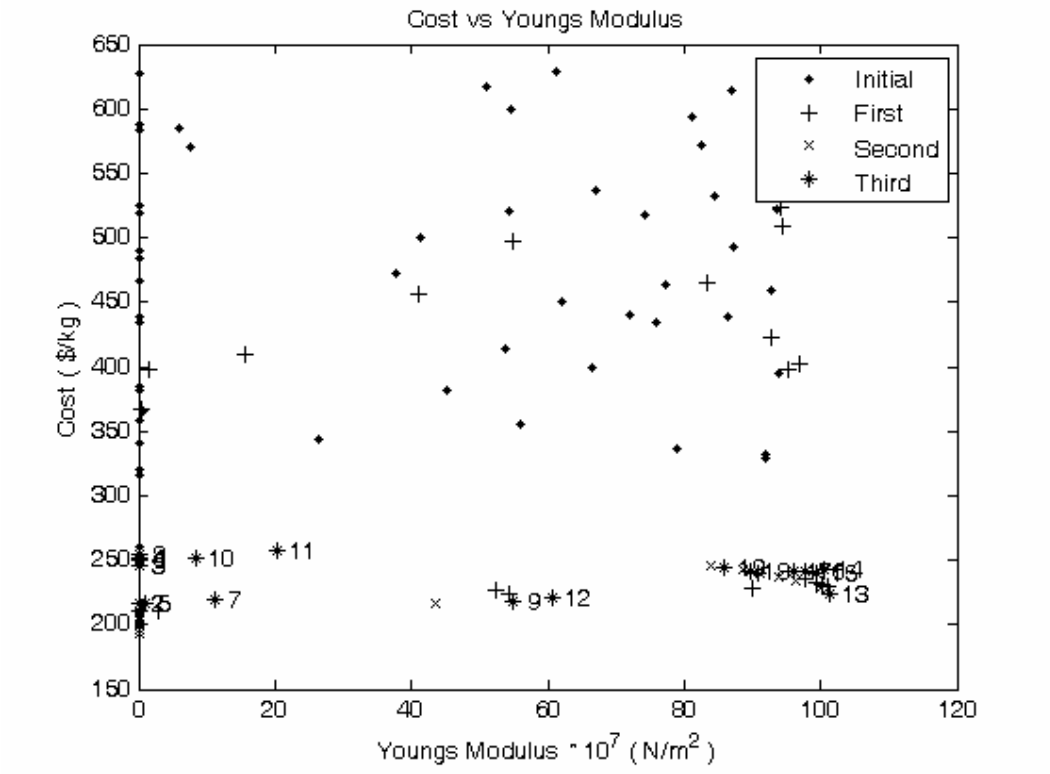

Fig 4 (i) Cost vs Young's modulus at 1500 °C

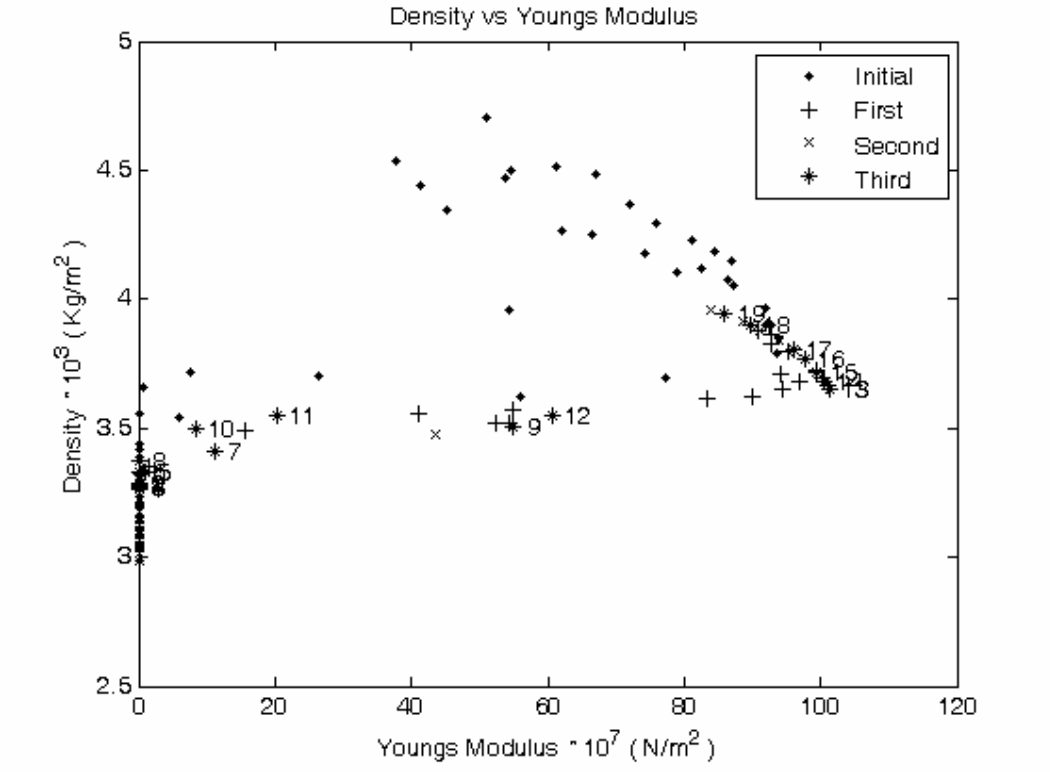

Fig 4 (ii) Density vs Young's modulus at 1500 °C

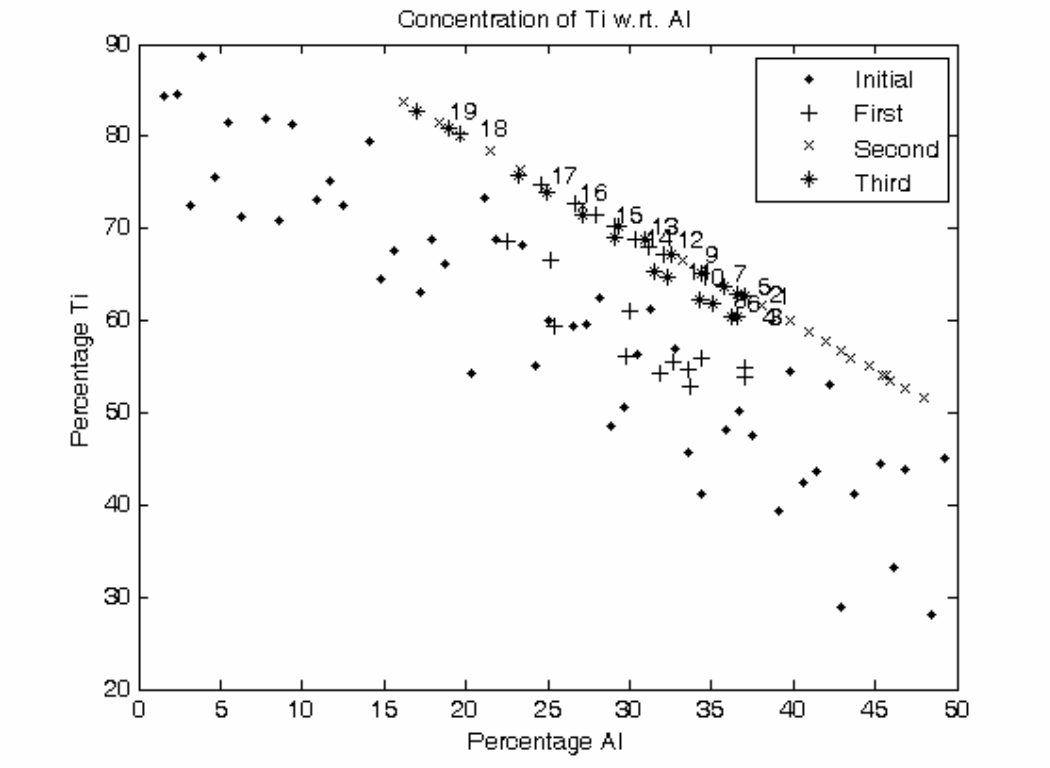

Fig 4 (iii) Concentration of Ti vs Al at 1500 °C

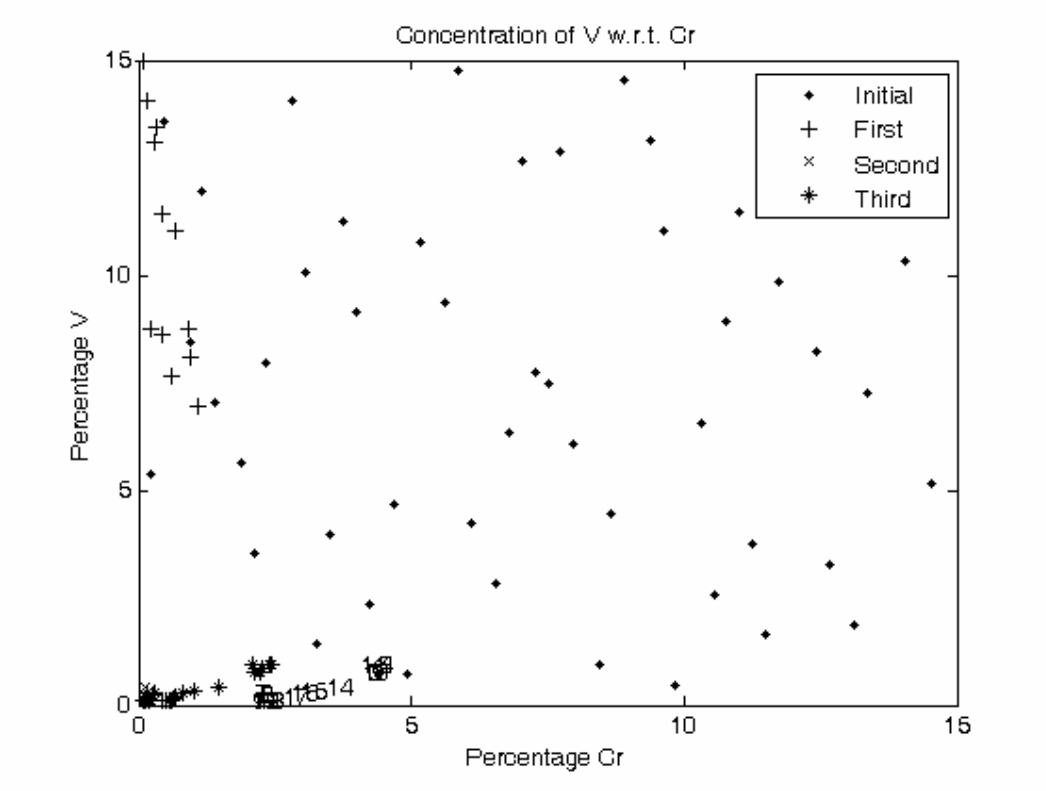

Fig 4 (iv) Concentration of V vs Cr at 1500 °C

The Pareto response set obtained at the 3rd iteration is shown for these temperatures. The Pareto front at 1200 °C is shown in table 3 below.

Table3 Pareto-response set obtained after third optimization iteration at 1200 °C

No.	Ti	Al	Cr	V	Density*10^3 (kg/m^3)	Y.M.*10^8 (N/m^2)	Cost ($/kg)
1	45.3853	50	4.5147	0.1	3.1035	1.5641	229.9365
2	46.7508	49.9793	3.1699	0.1	3.1017	2.6169	217.4651
3	49.8	50	0.1	0.1	3.0892	4.9269	188.88
4	45.5007	47.5693	0.1466	6.7834	3.2796	5.3638	337.0998
5	58.036	41.764	0.1	0.1	3.2427	5.1815	202.7497
6	61.8258	37.9593	0.1149	0.1	3.3717	5.7998	209.2955
7	66.3288	33.1437	0.1	0.4275	3.5755	6.9432	224.3064
8	72.2073	26.4799	0.1104	1.2024	3.7319	6.8074	252.2859
9	42.6508	33.674	10.764	12.9112	3.7853	7.5887	590.989
10	51.1791	31.1043	7.6789	10.0377	3.7898	6.9138	504.845
11	46.6739	30.2515	10.2344	12.8402	3.8984	9.6086	590.3007
12	55.5799	29.4464	6.6063	8.3674	3.8075	6.8968	461.7488
13	79.0544	19.2438	1.4783	0.2235	3.9374	7.56	256.1474
14	82.1972	15.4691	2.2337	0.1	4.088	9.27	266.8733
15	62.3614	21.2003	7.5843	8.854	4.1	10.0762	495.1943
16	53.0377	22.5759	12.4471	11.9393	4.1561	10.0319	604.4352
17	85.5768	10.3754	3.8914	0.1564	4.2375	7.8902	292.08
18	75.9629	15.9027	8.0344	0.1	4.1902	9.406	320.0902
19	52.7729	19.7277	15	12.4994	4.2886	9.8277	645.0157
20	63.9844	15.5293	10.743	9.7433	4.3226	9.3596	553.2395

The Pareto front obtained at 1300 °C is shown in table 4 below.

Table4 Pareto-response set obtained after third optimization iteration at 1300 °C

No.	Ti	Al	Cr	V	Density*10^3 (kg/m^3)	Y.M.*10^8 (N/m^2)	Cost ($/kg)
1	52.4346	46.3091	1.1563	0.1	3.1285	2.9695	204.9194

2	52.4351	46.3089	1.156	0.1	3.1285	2.9704	204.9163
3	48.5588	45.526	1.0426	4.8726	3.262	1.9691	307.7924
4	54.506	39.2151	0.1139	6.165	3.4406	5.4923	337.5684
5	60.1791	38.0481	1.6728	0.1	3.4485	6.0925	223.6341
6	66.9003	31.9095	1.0902	0.1	3.5825	6.3053	228.5535
7	50.5678	31.2519	3.4173	14.763	3.7655	9.2183	566.5573
8	61.7158	30.2798	0.5643	7.4401	3.6577	5.3304	384.2203
9	50.1179	30.5491	4.6287	14.7043	3.8059	9.8732	577.745
10	73.8171	25.8467	0.2178	0.1184	3.7157	6.4332	231.0445
11	47.4825	31.275	6.5788	14.6637	3.8094	9.7721	593.7857
12	68.4845	23.4696	1.4791	6.5668	3.9029	10.0962	385.419
13	80.5806	18.642	0.6774	0.1	3.9638	9.5869	247.0564
14	49.5206	26.4272	9.1952	14.857	3.9805	9.7123	630.4376
15	55.4898	27.2229	8.7726	8.5147	3.9203	10.0236	488.8069
16	87.6709	12.0096	0.2154	0.1041	4.1008	7.9762	254.018
17	54.3327	23.3684	10.5263	11.7726	4.0726	9.7159	581.6531
18	75.6221	15.9815	7.0357	1.3607	4.1532	9.0418	337.774
19	62.8984	20.085	11.4083	5.6083	4.1466	9.6115	462.8521
20	64.1042	20.7958	15	0.1	4.1524	9.7556	376.6299

The Pareto front obtained at 1400 °C is shown in table 5 below.

Table5: Pareto-response set obtained after third optimization iteration at 1400 °C

No.	Ti	Al	Cr	V	Density*10^3 (kg/m^3)	Y.M.*10^8 (N/m^2)	Cost ($/kg)
1	57.7453	41.8552	0.2995	0.1	3.2524	0.5655	204.4514
2	59.5329	39.5182	0.5412	0.4077	3.3578	3.2351	217.2495
3	61.0108	37.7075	0.7461	0.5356	3.4231	5.7457	224.955
4	62.8503	35.3507	0.9683	0.8307	3.479	5.7058	237.3347
5	43.1035	41.6322	0.2768	14.9875	3.3345	0.4249	524.6964
6	44.4698	40.281	0.2589	14.9903	3.4016	1.4418	526.8656
7	65.5275	33.1792	0.8221	0.4712	3.5258	5.808	231.9022
8	46.7081	38.1211	0.1757	14.9951	3.499	5.9747	529.8332
9	48.7826	35.5693	0.6481	15	3.5812	7.523	538.6284
10	68.6518	29.7042	1.369	0.275	3.6093	5.7324	238.6228
11	52.1174	32.6056	0.3101	14.9669	3.6711	9.6712	539.7648
12	73.9012	25.601	0.3509	0.1469	3.7623	9.521	233.3095
13	74.7669	23.5491	1.4345	0.2495	3.8328	9.9619	249.0488
14	55.7434	28.7916	0.5349	14.9301	3.7713	9.6904	547.4871
15	59.8738	25.1463	0.1385	14.8414	3.8596	9.6069	548.0322
16	80.6664	18.1092	1.0986	0.1258	3.9589	9.1369	252.4268
17	73.183	20.4639	0.1	6.2531	3.9254	9.4445	370.9098
18	64.9592	19.9408	0.1	15	3.9946	9.1969	559.8497
19	84.4319	14.3061	1.1613	0.1007	4.047	8.287	258.8727
20	75.0708	19.2918	5.4679	0.1695	4.0066	9.2889	292.0092

The Pareto front obtained at 1500 °C is shown in table 6 below.

Table6: Pareto-response set obtained after third optimization iteration at 1500 °C

No.	Ti	Al	Cr	V	Density*10^3 (kg/m^3)	Y.M.*10^8 (N/m^2)	Cost ($/kg)
1	62.7223	37.0717	0.1	0.106	3.2615	0.0013	210.7797
2	62.8378	36.5978	0.2777	0.2867	3.2858	0.0086	217.1164
3	60.4754	36.5212	2.2382	0.7652	3.272	0	245.7651
4	60.4082	36.2144	2.432	0.9454	3.2813	0	251.9583
5	63.6866	35.8248	0.2467	0.2419	3.328	0.0908	217.1671
6	61.786	35.1089	2.2577	0.8474	3.3314	0.0016	250.0919
7	65.1288	34.4381	0.158	0.2751	3.4094	1.132	219.3902
8	62.317	34.3298	2.405	0.9482	3.3744	0.021	254.9403
9	67.2059	32.5833	0.1063	0.1045	3.5041	5.5015	218.3654
10	64.7778	32.307	2.1394	0.7758	3.4954	0.8364	252.1708
11	65.4145	31.5289	2.0968	0.9598	3.5463	2.0192	257.041

12	68.7938	30.9842	0.122	0.1	3.5522	6.0594	221.1068
13	70.3415	29.3742	0.1843	0.1	3.6525	10.1338	224.3976
14	69.0371	29.0869	1.474	0.402	3.6773	10.0414	243.3688
15	71.4883	27.1802	1.0026	0.3289	3.7166	9.9525	240.6242
16	73.9412	24.9595	0.8084	0.2909	3.7668	9.7755	241.7413
17	75.8404	23.2652	0.6888	0.2056	3.8049	9.5992	241.6491
18	80.799	18.9195	0.1815	0.1	3.8984	8.9636	241.9773
19	82.7657	17.0343	0.1	0.1	3.9404	8.5937	244.3942
20							

At each temperature, four different alloy compositions were chosen from the Pareto response set and are shown in the Table 7 below.

Table7 Four most promising alloy compositions at each temperature from the third Pareto-response set

Temperature	Al	Cr	V	Density*10^3 (kg/m^3)	Y.M.*10^8 (N/m^2)	Cost ($/kg)
At 30 °C	11.1532	0.4007	0.1059	4.2127	10.76617	257.2211
	8.8518	0.4750	0.1000	4.2986	11.55225	261.6606
	5.9848	0.3820	0.1000	4.3834	12.00505	265.6241
	0.1000	0.1000	0.1000	4.5012	11.22163	272.9116
At 200 °C	7.0068	0.1000	0.1160	4.3371	11.25249	261.6238
	5.2768	0.5000	0.1000	4.3792	10.89794	267.9135
	1.6916	0.1000	0.1009	4.4475	10.49487	270.2498
	0.6573	2.4734	0.1042	4.5140	10.32714	294.1347
At 400 °C	50.0000	0.1000	0.1000	3.3011	8.81919	188.88
	8.7292	0.1195	0.1002	4.2476	9.63033	258.5649
	7.4309	0.1376	0.1000	4.3001	10.11433	260.9164
	6.0764	0.1185	0.1187	4.3301	9.98209	263.4206
At 600 °C	50.0000	4.1722	6.8242	3.3376	7.52423	371.3228
	50.0000	0.7502	0.1000	3.2598	7.68817	194.9264
	11.1532	0.4007	0.1059	4.1225	7.5934	257.2211
	8.8518	0.4750	0.1000	4.2158	8.3424	261.6606
At 800 °C	5.1083	7.0043	10.7116	4.6161	8.08971	556.8373
	7.8861	10.1294	2.7214	4.5268	8.45047	409.4336
	7.8552	11.8639	5.8778	4.6209	9.14469	493.4788
	7.3018	12.7498	6.9427	4.6686	9.06854	525.5443
At 1000 °C	23.8941	13.6337	4.7765	4.1142	9.96989	459.2509
	17.7553	2.7838	0.2588	4.1105	9.23391	271.5529
	4.1343	9.3590	0.4144	4.6726	9.29801	358.9867
	3.3077	15.0000	0.1000	4.4832	9.59231	406.0798
At 1200 °C	15.4691	2.2337	0.1000	4.0880	9.27	266.8733
	21.2003	7.5843	8.8540	4.1000	10.07617	495.1943
	15.9027	8.0344	0.1000	4.1902	9.40602	320.0902
	15.5293	10.7430	9.7433	4.3226	9.35961	553.2395
At 1300 °C	23.4696	1.4791	6.5668	3.9029	10.09623	385.419
	18.6420	0.6774	0.1000	3.9638	9.58687	247.0564
	15.9815	7.0357	1.3607	4.1532	9.0418	337.774
	20.7958	15.0000	0.1000	4.1524	9.75563	376.6299
At 1400 °C	25.6010	0.3509	0.1469	3.7623	9.52097	233.3095
	23.5491	1.4345	0.2495	3.8328	9.96185	249.0488
	18.1092	1.0986	0.1258	3.9589	9.13694	252.4268
	20.4639	0.1000	6.2531	3.9254	9.44449	370.9098
At 1500 °C	29.3742	0.1843	0.1000	3.6525	10.13382	224.3976
	29.0869	1.4740	0.4020	3.6773	10.04141	243.3688
	27.1802	1.0026	0.3289	3.7166	9.95253	240.6242
	24.9595	0.8084	0.2909	3.7668	9.7755	241.7413

The compositions listed in Table 3 are the ones which show good Young's modulus, low density and the material cost is also low. We found a considerable difference between the final properties and the properties in the initial data set. Table 8 lists the highest Young's modulus in the initial data set and that obtained in final (third) Pareto optimal set consisting of 20 optimized Ti-base alloys.

Table8. Comparison between the properties with highest Young's modulus from initial data set and final data set.

Temperature (°C)	Density*10^3 (kg/m^3)	Y.M. *10^8 (N/m^2)	Cost ($/kg)

30	Initial	4.7413	12.0265	414.3059
	Final	4.3834	12.00505	265.6241
200	Initial	4.7190	11.07423	414.3059
	Final	4.3371	11.25249	261.6238
400	Initial	4.6900	9.95387	414.3059
	Final	4.3001	10.11433	260.9164
600	Initial	4.6597	8.85692	599.6047
	Final	4.3062	8.74322	265.6241
800	Initial	4.6430	9.28128	535.9809
	Final	4.6209	9.14469	493.4788
1000	Initial	4.2981	10.69701	614.1703
	Final	4.1142	9.96989	459.2509
1200	Initial	4.0858	10.23026	521.1059
	Final	4.1902	9.40602	320.0902
1300	Initial	3.9053	10.08012	394.7797
	Final	3.9029	10.09623	385.419
1400	Initial	3.8090	10.01833	344.1375
	Final	3.8328	9.96185	249.0488
1500	Initial	3.8491	9.38491	394.7797
	Final	3.6525	10.13382	224.3976

Conclusions

Comparing the three simultaneous objectives (Young's modulus of elasticity, density and cost of raw material) for given chemical compositions from the initial data set and those obtained after three global optimization cycles with IOSO software and JMatPro software, we find that at each temperature, we have significantly reduced the cost and without affecting the Young's modulus and density of the alloy appreciably. At a higher temperature, 1500 °C, significant improvement in Young's modulus value is observed with lower density and at significantly lower cost of material. This method can be extended to arrive at composition which satisfies more than just three objectives.

Acknowledgements

The authors are grateful for the financial support provided by the ARO grant 50486-MS-H monitored by Dr. William M. Mullins.

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