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Soft Computing Methods in Design of Superalloys

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SUMMARY

Soft computing techniques of neural networks and genetic algorithms are used in the design of superalloys. The cyclic oxidation attack parameter K_a, generated from tests at NASA Lewis Research Center, is modelled as a function of the superalloy chemistry and test temperature using a neural network. This model is then used in conjunction with a genetic algorithm to obtain an optimized superalloy composition resulting in low K_a values.

INTRODUCTION

In this report we show the results of research involving application of soft computing techniques to modelling and optimizing alloys. In the design and manufacturing of advanced materials such as superalloys, a material possessing desired output properties is a requirement. These properties can be expressed as a function of material composition and parameters of the fabrication process. Optimizing the composition of a material can be broken into two problems: finding the function between inputs, such as material composition and process parameters, and outputs such as strength and density, and then optimizing that function. Such functions are usually highly nonlinear and difficult to find. Moreover, the properties of the superalloys are very sensitive to the process fabrication parameters such as temperature, pressure, and so forth. For those reasons we have used neural networks to learn the mapping function between the inputs and outputs.

Optimization can be defined as a process that seeks to improve performance of a system toward some optimal point or a set of points. Local optimization techniques work well for problems that have relatively nice search spaces and when the user has a good feel for the space. If that is not the case, global optimization techniques of genetic algorithms are often used.

Barrett (ref. 1) used the data generated from tests at NASA Lewis Research Center to rank the Ni- and Co-based superalloys for their cyclic oxidation resistance. The test results were reduced to a single "attack parameter" K_a, and he used multiple linear regression analysis to derive an estimating equation for this parameter as a function of the alloy chemistry and test temperature. This equation was then used to predict the K_a values for similar alloys and also for the design of an optimal superalloy composition.

Soft computing methods of neural networks, genetic algorithms, and fuzzy sets have proven to be useful (ref. 2) where the conventional methods have limitations. In this work we use the techniques of neural networks and genetic algorithms for modelling and optimization, respectively. The backpropagation neural network is used for modelling and the GENOCOP genetic algorithm is used for optimization (see fig. 1). It will be shown that the neural network modelling of K_a gives as good, or better, a fit as the linear regression model (ref. 1). Optimization of the function learned by the neural network using the genetic algorithm (ref. 3) achieves low values for the K_a parameter.

Barrett's data (ref. 1) were used to train the backpropagation network to model the cyclic oxidation attack parameter K_a as a function of superalloy composition. This trained network was then used as an objective function (K_a) generator for an optimizer using a genetic algorithm (fig. 1).

In this report we shall briefly discuss the soft computing methods of neural networks for function approximation in the section FUNCTION APPROXIMATION and genetic algorithms for optimization in the section OPTIMIZATION.

FUNCTION APPROXIMATION

Artificial neural networks are composed of many simple nonlinear processors called neurons connected in parallel. Each neuron performs a computation of the following form:

$$o_i = f(s_i) \text{ and } s_i = W^T X$$

where $X = (x_1, x_2, ..., x_m)$ is the vector input to the neuron and W is the weight matrix with w_{ij} being the weight (connection strength) of the connection between jth element of the input vector and ith neuron. The f() is a nonlinear function (usually a sigmoid), o_i is the output of the ith neuron, and s_i is the weighted sum of the inputs.

Neural networks can learn from the input/output training data pairs. Once the training is completed, the network can be used as a function simulator. The learning capability is a result of the ability of the network to modify the weights through usage of a learning rule. The topology used here is the multilayer feed-forward network, and the learning rule is backpropagation. A neural network with one hidden layer was used to simulate $\log_{10}(K_a)$ as a function of the superalloy chemistry and test temperature. The network had 18 nodes in the input, 36 nodes in the hidden layer, and one in the output layer. The superalloys used in the test were Ni- and Co-based and their composition was described by weight percent (wt %) of the components Ni, Co, Cr, Al, Ti, Mo, W, Cb, Ta, C, B, Zr, and Hf. This data is shown in the Appendix.

Barrett's (ref. 1) fitting of the function using linear regression resulted in the value of R^2 equal 84.43 percent. We achieved an R^2 value of 86.56 percent on the same data. The Appendix shows the comparison of regression and backpropagation results for the average values of the K_a parameter for the superalloys used. Different results were obtained when multiple tests were conducted for some alloys (experiment repeated), and hence the average values for comparison were used. The trained network was used to predict the K_a value for an alloy, not included in the training data set, being exactly the same as used by Barrett. The results shown in table I are better than the ones obtained from regression at both temperatures (1150 and 1200 °C). All values are log to the base 10 of the K_a parameter.

OPTIMIZATION

Optimization can be defined as a search towards some optimal point. In most engineering systems attainment of the optimum at any cost is not required, but instead what usually suffices is a "good" solution. Genetic algorithms (ref. 4) have proved to be of considerable help towards achieving this goal. The genetic algorithms are global optimizers used to overcome the limitations of many conventional methods like Bayesian/sampling, Monte Carlo, Torn's, and simulated annealing (ref. 5).

The genetic algorithm (GA) is an evolutionary computation method useful in performing searches and optimization. A GA involves a set of elements $(x_1, ..., x_n)$, called the population X(t) at time t. Each element x_i represents a possible solution and is represented by a string of variables. The standard GA is described as the following sequence of steps (ref. 6):

Step 1: Randomly generate an initial population $X(0) = (x_1, x_2, ..., x_n)$
Step 2: Compute the fitness $f(x_i)$ of each individual x_i of the current population
Step 3: Generate an intermediate population $X_r(t)$ applying the reproduction operator
Step 4: Generate $X(t + 1)$ applying other operators to $X_r(t)$
Step 5: $t = t + 1$; if not (end_test) go to Step 2

where the most commonly used operators are reproduction, crossover, and mutation.

To improve the objective function value towards an optimum, the genetic algorithm only needs the function values at the population points, and not the function itself. In this sense the algorithm is said to be blind. The algorithm (ref. 3) uses probabilistic transition rules and random choice as a tool to guide the search towards a region of a search space with likely improvement. The GA's also have the advantage of being able to optimize while

avoiding local minima unlike gradient-descent methods. The GA method of optimization is very different from conventional methods and can be characterized by (refs. 3 and 5) the following differences:

- They directly use the code (i.e., the parameters)
- They search from a population of points instead of a single point
- They are blind to all auxiliary information
- They use randomized operators

The algorithm we have used for optimization is the GENOCOP (Genetic Algorithm for Numerical OPtimization) developed at the University of North Carolina by Zbigniew Michalewicz. The GENOCOP system aims at finding a global optimum (minimum or maximum) of a function subject to linear constraints (equations and inequalities). This algorithm had been demonstrated to successfully optimize both linear and nonlinear functions. Even though the algorithm is blind to the function, the functions were needed to generate the function values. We wanted the algorithm to optimize an unknown function, which was simulated on a neural network. The programs were modified so that the function values were generated by another program, developed at the University of Toledo, using the backpropagation network.

The problem of designing a superalloy was broken down into two tasks: function approximation and optimization. The backpropagation net was trained using available test data from the tests and thus functioned as a simulator of the K_a parameter. This generated K_a was then used as input to the genetic algorithm, which searched for points with minimum corresponding K_a values. This search led to the results shown in table II. The search was restricted to the temperature 1100 °C. The constraints used in finding an alloy composition were obtained from NASA Lewis Research Center and are listed in table III.

The obtained results (see table II) indicate that the desired alloy belongs to group-II alloys (ref. 1), that is, chromia/chromite formers. We think that this is a direct result of the given constraints. If a group-I alloy was to be designed, we should have used a much closer range for Aluminum (Al) percent weight. We have used the 0 to 6 range (percent weight), but it can be noticed from reference 1 that for group-I alloys the range is 5 to 6. Given the latter, the genetic algorithm optimization might have resulted in a group-I alloy.

The K_a value for these newly designed alloy composition is 0.90918058, which puts the superalloy in the category of fair according to Barrett's classification (ref. 1) in which the K_a values are ranked as

	K_a	<= 0.20	excellent
0.20 <=	K_a	<= 0.50	good
0.50 <=	K_a	<= 1.00	fair
1.00 <=	K_a	<= 5.0	poor
5.00 <=	K_a		catastrophic

The lowest value of K_a obtained in the actual tests at 1100 °C, for group-II alloys was 1.708 (U-700) (ref. 1). Thus the soft computing methods have resulted in a design that can meet the requirement of low K_a values.

CONCLUSIONS

We have applied the soft computing methods of neural networks and genetic algorithm to the design of advanced superalloys. The key feature of this approach is the use of the neural network for modelling the material properties as functions of alloy chemistry and process parameters and the use of a genetic algorithm for optimizing the function and thus obtaining a superalloy with low K_a values. The genetic algorithm used for optimization needs only the objective function values which are provided as the outputs of the neural network. To summarize, the following results were obtained:

1. The trained neural network (R^2 = 86.56 percent) gives a better fit than the regression (R^2 = 84.43 percent).
2. The predicted value for NASAIR-100 alloy is much better for the neural net model than the linear regression model.
3. A new superalloy, of group-II, was designed using the genetic algorithm, with a K_a value of 0.9091 at 1100 °C, which is classified as fair (ref. 1). In test results used for modelling, none of this group of superalloys had such a low K_a value.

Given different constraints these results could be most probably further improved.

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APPENDIX- NEURAL NETWORK TRAINING RESULTS

Alloy	Temperature, °C	K_a (Observed)	K_a (Neural Net)	K_a (Regression)
Alloy-625	1100	28.71441	33.12075	11.27800
Alloy-625	1150	36.42085	65.32808	17.99260
Alloy-718	1100	28.56603	30.54570	36.16710
Alloy-718	1150	43.39103	60.06204	69.82400
Astroloy	1100	3.23743	10.80936	9.13700
Astroloy	1150	61.72343	21.69202	21.93610
B-1900	1000	0.05310	0.05354	0.01870
B-1900	1100	0.19269	0.44463	0.31000
B-1900	1150	1.68384	1.66802	1.08980
B-1900-+-Hf	1100	0.72219	0.38940	0.32770
B-1900-+-Hf	1150	1.10053	1.87759	1.15220
IN-100	1093	28.49377	34.80566	1.86570
IN-100	1100	46.06277	39.31424	24.30670
IN-100	1150	97.48773	84.51817	76.63070
IN-713-LC	1100	0.71499	20.17901	0.94390
IN-713-LC	1150	1.67359	71.84557	2.66850
IN-738	1000	1.69805	5.20595	3.12460
IN-738	1100	29.32580	30.11619	19.59870
IN-738	1150	37.93149	59.08810	44.55700
IN-792	1100	22.54759	28.20979	19.20340
IN-792	1150	50.10717	66.91138	52.25930
IN-939	1100	32.58367	40.81313	30.14130
IN-939	1150	55.37961	64.90826	49.41480
MAR-M-200	1150	74.25060	53.29665	47.77800
MAR-M-200-+-Hf	1100	17.31210	26.54911	16.17680
MAR-M-200-+-Hf	1150	64.41692	74.50749	53.85680
MAR-M-211	1100	73.45983	17.29419	11.60070
MAR-M-211	1150	57.18736	44.17740	38.62180
MAR-M-246	1100	1.55292	3.21440	0.83760
MAR-M-246	1150	18.07799	11.27847	2.50060
MAR-M-247	1000	0.05250	0.06792	0.04770
MAR-M-247	1100	0.50699	0.91254	0.77430

Alloy	Temperature, °C	K_a (Observed)	K_a (Neural Net)	K_a (Regression)
MAR-M-247	1150	4.98482	4.22766	2.69280
MAR-M-421	1100	9.53126	16.23865	8.63530
MAR-M-421	1150	34.93413	34.81770	19.84710
NASA-TRW-VIA	1100	0.32934	0.43451	0.35330
NASA-TRW-VIA	1150	1.59019	1.86423	1.37760
Nimonic-115	1000	0.40851	0.80131	0.40710
Nimonic-115	1150	1.64002	15.90560	7.43090
NX-188	1100	3.44588	3.38532	2.28170
NX-188	1150	8.21391	14.63356	12.40500
Rene-41	1150	33.14362	49.25496	38.79820
Rene-80	1100	37.40245	33.01795	20.00150
Rene-80	1150	60.76452	67.99076	50.70860
Rene-120	1100	6.85409	12.29986	8.85880
Rene-120	1150	14.91077	30.55272	24.49300
Rene-125	1100	3.02273	2.86913	2.06020
Rene-125	1150	9.78363	12.35521	6.85800
R-150-SX	1000	6.00136	5.29724	2.84800
R-150-SX	1100	45.00908	66.84979	68.24000
R-150-SX	1150	314.84732	151.56540	282.51901
TAZ-8A	1000	0.09700	0.07279	0.02520
TAZ-8A	1100	0.56735	0.70713	0.52440
TAZ-8A	1150	4.64408	2.87144	2.05340
TRW-R	1000	0.05600	0.03252	0.03230
TRW-R	1100	0.10650	0.26918	0.53650
TRW-R	1150	0.91201	1.19591	1.88630
TRW-1800	1100	0.73097	1.24753	0.87460
TRW-1800	1150	3.69020	3.55140	2.34160
U-520	1100	31.64828	16.21437	17.25930
U-520	1150	55.97576	32.47507	33.32080
U-700	1000	1.30707	0.97578	0.76570
U-700	1100	6.96226	6.64431	5.42470
U-700	1150	29.63467	15.18273	13.02350
U-710	1100	33.75592	26.89057	20.20680
U-710	1150	48.91026	48.23917	41.19590

Alloy	Temperature, °C	K_a (Observed)	K_a (Neural Net)	K_a (Regression)
U-720	1000	6.38851	5.16179	3.92420
U-720	1100	32.33329	23.74652	19.29180
U-720	1150	41.57671	43.54115	39.33060
Waspaloy	1000	4.99862	3.30446	3.70670
Waspaloy	1100	9.62941	18.38443	15.17910
Waspaloy	1150	28.89349	36.43763	28.51700
WAZ-20	1100	21.14707	32.38919	15.08830
WAZ-20	1150	89.21751	91.72762	82.03130
MAR-M-509	1100	25.42729	37.99707	25.66680
MAR-M-509	1150	49.77372	62.82031	38.77640
W-152	1093	47.03811	16.46076	16.11080
W-152	1100	45.28975	20.17901	54.95520
W-152	1150	120.57302	71.84557	95.14120
X-40	1100	35.57131	25.85235	24.45800

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TABLE I.—RESULTS OF PREDICTING K_a VALUE FOR NASAIR-100 ALLOY

Temperature, °C	1150	1200
K_a (Observed)	0.7645	1.0865
K_a (Regression)	0.2684	0.7554
K_a (Neural Net)	0.8937	0.9347

TABLE II.-GENOCOP SOLUTION POINT AT 1100 °C

Element	Weight percent
Ni	70.0552444
Co	5.03954935
Cr	9.97962761
Al	3.30380297
Ti	1.36296296
Mo	0.84048849
W	2.05709577
Cb	2.99739814
Ta	3.91278195
C	0.13449860
B	0.00077937
Zr	0.30375364
Hf	0.00200379
V	0.00000000
Re	0.00000000
Cu	0.00000000

TABLE III.—CONSTRAINTS USED IN OPTIMIZATION

Lower limit	Element	Upper limit
1100 °C	Temperature	1100 °C
50	Ni	100.0
0	Co	10.0
0	Cr	15.0
0	Al	6.0
0	Ti	2.0
0	Mo	2.0
0	W	4.0
0	Cb	3.0
0	Ta	8.0
0	C	0.5
0	B	0.1
0	Zr	1.0
0	Hf	1.0
0	V	0.0
0	Re	0.0
0	Cu	0.0

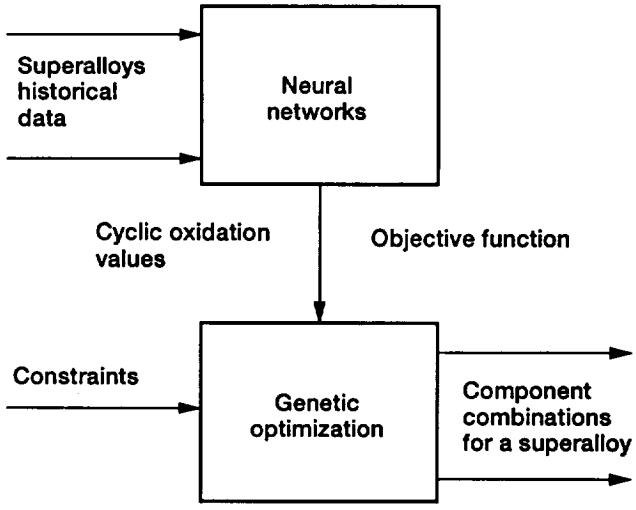

Figure 1.—Outline of neuro-genetic system.

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