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Materials & Design. Vol. 17, No. 1, pp. 23–26, 1996

0261–3069/96 $15.00 + 0.00

PII: S0261-3069(96)00025-8

Superalloy design — a Monte Carlo constrained optimization method

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Received 14 March 1996; accepted 24 June 1996

A method, based on Monte Carlo constrained optimization, has been devised for designing superalloys. The Larson–Miller parameter at 100 MPa is maximized subject to M_d (total) < 0.99, $M_d(\gamma)$ < 0.94 and, for superalloys with at.%Mo + at.%W > 4.32, Mo/(Mo + W) < 0.27. The maximum density of the alloy can be specified as well as the composition range of any constituent element. The design of a patented alloy is illustrated and the possibility of designing new low density, corrosion resistant superalloys is discussed. Copyright © 1996 Elsevier Science Ltd.

Keywords: superalloys; optimization; creep strength

Introduction

The design and modelling of a material having specific properties, one or more of which must be optimized, can be formulated as a constrained optimization problem. For this type of problem the property that needs to be optimized, i.e. either maximized or minimized, is written as a function, the so-called objective function, of the material composition and any other relevant independent variables. Constraints, determined by the specifications, are also set as functions of the composition and other necessary independent variables. The dependent variable of the objective function is then optimized subject to the defined constraints. As an example, the density of a superalloy, which is a function of the composition, may be minimized subject to constraints such as a specified minimum creep strength and specified maximum corrosion rate. If the creep strength and the corrosion rate can be written as functions of the composition this problem can be treated as a constrained optimization problem.

When the objective function as well as the constraint functions are linear functions of the composition, the well-known technique of linear programming (simplex method)[1–4] can be used to obtain a solution. If the functions are non-linear, then for certain special cases[1,4] it is still possible to find solutions. When the cited methods are not applicable other approaches must be investigated. In industrial gas turbines increased inlet temperature gives rise to higher thermal efficiency but can adversely affect construction material properties. Larger blades improve overall efficiency but result in higher stresses. The creep of superalloy blades at high temperatures and stresses is therefore of major concern. In this paper a method for maximizing the design creep strength of a superalloy, based on Monte Carlo simulation and applicable to both the linear and the non-linear cases, is described.

Formulation of the problem

Objective function

The Larson–Miller parameter[5] at an applied stress of 100 MPa was used as a measure of the creep strength of superalloys. This parameter, LMP_{100}, is given by the expression $LMP_{100} = 10^{-3}T\,(20 + \log_{10}t)$, where T is the temperature in Kelvin and t the creep life in hours. This property can be expressed as the following function of composition:

$$LMP_{100} = \sum_{i=1}^{n} \alpha_i f_i(X_i) \qquad (1)$$

The X_i represent the atomic percentages (at.%) of the i elements in the superalloy, and the functions, $f_i(X_i)$, can be linear, quadratic or logarithmic functions of X_i. The coefficients α_i were calculated using non-linear multiple regression[3] of experimental data. In *Figure 1* the calculated results according to equation (1) versus the ex-

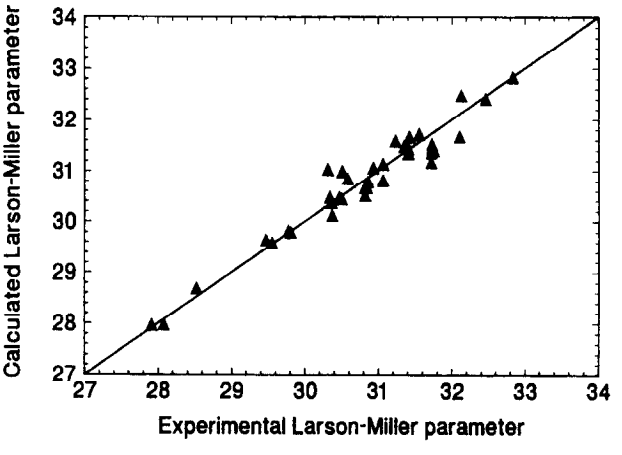

Figure 1 Plot of calculated versus experimental Larson–Miller parameters

perimental results are shown. The solid line represents equality of calculated and experimental results, and it is clear that equation (1) represents LMP_{100} sufficiently well for modelling purposes. LMP_{100} must be maximized subject to the constraints.

Formulation of constraints
For alloy design the constraints may be subdivided into two categories, i.e. compositional constraints (e.g. 4.5 < wt% Al < 8.5) and property constraints (e.g. density < 8.9 g cm^3).

Compositional constraints. Lower and upper limits for the content of each of the n elements that constitute the alloy need to be set as inequality constraints:

$$X_i > C_{il} \tag{2}$$

$$X_i < C_{ih} \tag{3}$$

X_i represents the at.% of element i in the alloy and C_{il} and C_{ih} the respective lower and upper at at.% limits. One or more but not all of these constraints can be m equality constraints, e.g. for constant chromium content one can state

$$X_j = X_{Cr} = C_{Cr} \tag{4}$$

An essential compositional constraint is the requirement that

$$\sum_{i=1}^{n} X_i = 100 \tag{5}$$

The total number of compositional constraints is therefore $2n - m + 1$.

Property constraints. For superalloys, the essential property constraints are the constrained values of the M_d parameters described by Morinaga *et al.*[6]. The values of these parameters are an indication of the propensity to form deleterious σ-phase. Two of these parameters are defined, M_{dt} for the total alloy, and $M_{d\gamma}$ for the γ-phase that is normally present in the alloy. To prevent the possible formation of σ-phase these constraints are set as follows[7,8]:

$$M_{dt} = \sum_{i=1}^{n} f_{it} M_{di} < 0.99 \tag{6}$$

$$M_{d\gamma} = \sum_{i=1}^{n} f_{i\gamma} M_{di} < 0.94 \tag{7}$$

where f_{it} and $f_{i\gamma}$ are the atomic fractions of the components in the alloy and in the γ-phase respectively, and the M_{di} are constants given by Morinaga *et al.*[6] for each element. Values for the atomic fractions of the components in the γ-phase as a function of the total composition were obtained by performing multiple regressions using literature values of the composition of the γ-phase[9]. In addition, the following expression for the volume percentage of the γ'-phase[10] was used:

$$V_{\gamma'} = 225\ M_{dt} - 187$$

A further essential property constraint that needs to be defined is the critical molybdenum to tungsten ratio, rMoW. The value of this constraint is an indication of the alloy's propensity to form possibly deleterious m-phase11. If fMo + fW > 0.0432 then

$$r_{MoW} = \frac{f_{Mo}}{f_{Mo} + f_W} < 0.27 \tag{8}$$

Optimization technique

The algorithm for maximizing LMP_{100} comprises the following steps:

1. Set fixed compositional constraints (equations (2)–(4)), C_{il} and C_{ih}, for each of the constituents.
2. Set an arbitrary low value, L^{low}, for LMP_{100} so that there is a very high probability that the calculated value of LMP_{100} (equation (1)) will be larger than L^{low}. Likewise set an arbitrary high value, L^{high}, so that there is a very high probability that the calculated LMP_{100} will be lower than L^{high}.
3. Set arbitrary low values, P_k^{low}, for each of the property constraints, e.g. set $P_{Mdt}^{low} = 0.0$. Set high values, P_k^{high}, for each of the property constraints equal to the maximum allowable values (equations (6)–(8)), e.g. set $P_{Mdt}^{high} = 0.99$ (equation (6)). These low and high values, together with those defined in step 2, define a region of acceptance (ROA) in the property parameter space. Initially the ROA is defined as large as possible.
4. For each constituent, i, except the major constituent (e.g. nickel in the case of nickel-based superalloys), j, generate a random at.%, X_i, so that $C_{il} < X_i < C_{ih}$.

   If $\sum_{\substack{i=1 \\ i \neq j}}^{n} X_i < 100$ then calculate $X_j = 100 - \sum_{\substack{i=1 \\ i \neq j}}^{n} X_i$.

   If $\sum_{\substack{i=1 \\ i \neq j}}^{n} X_i \geq 100$ repeat step 4. This technique ensures that the constraint given in equation (5) is attained.
5. Use the random composition generated in step 4 to calculate values for LMP_{100} (equation (1)). Also calculate values, P_k, for the properties given by equations (6)–(8). Repeat steps 4 and 5 until a composition is found which results in a successful hit, i.e. when $L^{low} < LMP_{100} < L^{high}$, and for all the properties, $P_k^{low} < P_k < P_k^{high}$. If successful this hit falls within the ROA.
6. Repeat steps 4 and 5 to find at least ten (or more) successful hits with values of LMP_{100} and P_k that fall within the ROA.
7. Determine which is the largest, L^L, of the ten or more values of LMP_{100} found in step 6. Also, for each property, determine which is the smallest, P_k^S, of the ten or more values of P_k, found in step 6. Substitute $L^{low} = L^L$, and for all the properties, $P_k^{low} = P_k^S$. These substitutions shrink the ROA.
8. Repeat steps 4–7, but find only two successful hits. This progressively shrinks the ROA until, after a large number of tries, N_{max}, no successful hits are made. L_{low} now represents the maximized value of

LMP_{100} and the random composition that gave rise to this maximized value is the optimized alloy composition.

The random number generator used generates uniform random deviates, r, so that 0.0 < r < 1.0. To generate uniform random deviates, Xi, so that Cil < Xi < Cih, the relation Xi = Cil + r(Cil − Cil) was used12–14. After some experimentation using different random number generator initializers (seeds) for each trial, Nmax was set = equal to 10 000. This value was sufficient to ensure convergence.

Alloy design

Results

A computer program, ALLOYOPT, was written to perform the optimization calculations for designing a superalloy, designated SMP14[15], with maximized creep strength. Inputs to this program are the compositional constraints for each constituent of the alloy, as well as the maximum allowable alloy density. The output is a value for the maximized Larson–Miller parameter $LMP_{100(max)}$, as well as the composition, in weight or atomic per cent, of the optimized alloy. *Table 1* shows the composition limits, C_{il} and C_{ih}, used in the calculation as well as the composition of the optimized alloy and the maximized value of LMP_{100}.

Creep tests were performed on single crystal test pieces of SMP14 at the temperatures and applied stresses shown in *Table 2*. *Figure 2* shows the Larson–Miller plots of the test results as well as those for a superalloy, MC2[16], with comparable creep properties. The results show that SMP14 has significantly higher creep strength than MC2. The point c in *Figure 2*, which represents the predicted maximized Larson–Miller parameter for SMP14, lies on the extrapolation of line a which represents the experimental Larson–Miller parameters of SMP14. This confirms the accuracy of the predicted Larson–Miller parameter. It is known that high chromium contents adversely influence the creep strength of superalloys, and the higher creep strength of SMP14 can be partially attributed to the lower chromium content. The optimization technique also shows that rhenium addition increases the creep strength. However, this addition sharply increases the materials cost of the alloy.

Future applications

The density of a superalloy can be functionally related to the composition[17], and this function can either be used as an objective function that needs to be minimized, or as a constraint where a maximum permissible value of the density is specified. Such alloys have been designed, but not experimentally verified.

The ability of a superalloy to withstand corrosion at high temperatures, the so-called hot corrosion rate, is probably dependent on the composition. The parabolic rate constants for certain types of corrosion have been related to the composition[18], and data like this could be used to design superalloys with superior corrosion resistance using constrained optimization techniques.

Table 1 Optimization constraints

Element	C_{il} (at.%)	C_{ih} (at.%)	SMP14 (at.%)	MC2 (at.%)[16]
Al	12.0	13.0	12.9	11.2
Co	8.0	9.0	8.61	5.14
Cr	5.0	7.0	5.80	9.31
Mo	0.5	0.8	0.65	1.26
Nb	0.7	1.1	0.89	–
Re	1.2	1.4	1.35	–
Ta	2.0	3.0	2.42	2.01
Ti	–	–	–	1.90
W	0.0	3.0	2.53	2.63
Ni	30.0	99.0	64.85	66.55
LMP_{100}(max)			31.815	

Table 2 Creep test data for SMP14

Stress (MPa)	Temperature (°C)	Rupture time (h)	Strain at rupture (%)
278	975	219	–
281	975	197	–
160	1050	189	9.9
160	1050	615	15.1
420	900	374	16.6
420	900	403	16.1
190	1050	123	20.3

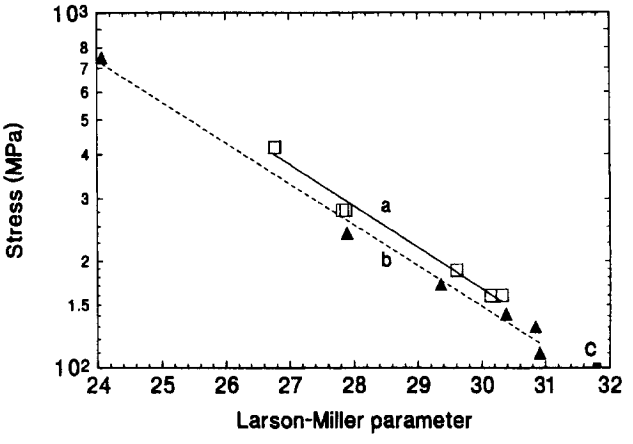

Figure 2 Plot of experimental Larson–Miller parameters versus stress for (a) SMP14, (b) MC2 and (c) optimized value

Conclusions

The results of the computations and the experimental work show that constrained optimization is a potentially useful technique for designing superalloys with superior creep strength. Other properties of these materials such as tensile strength, density, and hot corrosion rate can also be optimized if adequate objective and constraint functions can be formulated. Although present experience is limited to the design of superalloys and related materials, the techniques described can probably be applied to the design of other alloys and materials.

The Monte Carlo optimization technique described and tested is a relatively simple computational method that can be applied to materials-related non-linear constrained optimization problems. This is especially true when the non-linearity of the model functions cause difficulties in finding an analytical solution.

Acknowledgements

The author wishes to thank Dr N. R. Comins for helpful comments, P. Rossouw for the manufacture and heat treatment of the alloys, D. Hope and O. E. Schmid for determining some creep strengths and J. M. B. Benson for help with microstructural analysis.

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