New strategy for identification parameters of a micromechanical model coupled with ductile damage

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Abstract
A low-cyclic fatigue micromechanical model proposed recently [1] for emphasizing the concept of damage induced anisotropy is used. The solution of these nonlinear constitutive relations is an important topic since it requires an important computational time. With a high nonlinearity due to damage, the identification of model parameters represents consequently an important subject. In fact, a combination of the genetic algorithm (for the global optimization) with pattern search algorithm (for the local optimization) is proposed. A comparative study is conducted under complex cyclic loadings showing the ability of the proposed approach in calibrating model parameters.

Keywords Low-cyclic fatigue, parameters identification, global minimum and local minimum optimization

1. Introduction

Despite the existence of increasingly powerful computers, the progress in the constitutive equations development is continuous and can be conducted via computational optimization process. Several types of modes like micromechanical approaches are proposed for describing mechanical complex phenomena. Non-linear responses under cyclic loading, for example, make the related resolutions very expensive in computing time and in memory capacity. Numerically, it has been recently reported that the algorithm of Burlisch–Stöer gives the best compromise between computational time and precision compared to other well-known algorithms.
For a given model, the identification of parameters is an important issue and should be as accurate as possible to describe efficiently the material behavior. In fact, the use of reliable optimization algorithms is to minimize the difference between the model prediction and experimental behavior. Different methods have been developed to resolve this type of problem. They can, in general, be divided into two major groups: the first one which converges quickly is for local optimization. However, its major disadvantage is the possibility of converging towards local minimums. The Pattern Search algorithm is part of this group. It does not require the gradient calculation of the objective function and accepts parallel computing on different computer processors. The second group is formed by the evolutionary method based on the evolution of individuals. The genetic algorithm is a part of this group which is related to the global minimum convergence. However, it is slow because it requires several evaluations of the objective function.
Therefore, this study highlights the concept of damage induced anisotropy via the used model. Numerical solutions of these nonlinear constitutive equations require normally an important computational time. Therefore, a new strategy of model parameters calibration is considered. In fact, a hybrid approach is used, in this paper, to exploit the benefits of these groups of algorithms. Hence, a combination of the genetic algorithm (GA) with pattern search algorithm (PSA) is proposed. The basic idea of this approach is to look for the global minimum with the GA, then move to the local

minimum search via the PSA to improve the obtained result. Since the identification of the model parameters is of particular interest in this paper, therefore, several applications are presented. They deal with cyclic plasticity with damage induced anisotropy behavior of polycrystals and its related phenomena under complex history of loading path conditions. To conduct the identification process, the two methods (GA&PSA) are complementary and have different applications. The GA optimizes globally the model parameters leaving the field to the local method, PSA, to determine the final values of these parameters. Then, in order to evaluate the performances of the proposed method, a comparative study is performed under complex cyclic loadings showing the ability of such strategy to identify the model parameters.

2. Employed Micromechanical Model

The used micromechanical model utilizes three operating levels which are: microscale (slip system), mesoscale (granular) and macroscale (overall). The theoretical formulation of the developed model is presented in detail in [1]. However, a short description of the main features of the model equations at the overall level is illustrated below.

$$\underline{\underline{\Sigma}} = \sum_{i=1}^{3} \sum_{i}^{*} p_i \otimes \underline{p}_i \tag{1}$$

$$\underline{\underline{Q}} = \sum_{i=1}^{3} p_i \otimes p_i \tag{2}$$

$$\underline{\underline{Q}}^{+} = \sum_{i=1}^{3} H(\Sigma_i^{*})\, p_i \otimes p_i \tag{3}$$

$$p_{ijkl}^{+} = Q_{ia}^{+} Q_{jb}^{+} Q_{ka}^{+} Q_{lb}^{+} \tag{4}$$

$$\underline{\underline{\underline{\underline{D}}}} = D^{T}\, \underline{\underline{\underline{\underline{p}}}}^{+} \tag{5}$$

$$\underline{\underline{\underline{\underline{R}}}}^{d} = \left(\underline{\underline{\underline{\underline{I}}}} - \underline{\underline{\underline{\underline{D}}}}^{T} \right) : \underline{\underline{\underline{\underline{R}}}}^{o} \tag{6}$$

$$\dot{\underline{\underline{\underline{\underline{R}}}}}^{d} = \left(\dot{D}^{T}\, \underline{\underline{\underline{\underline{p}}}}^{+} + \dot{D}^{T}\, \underline{\underline{\underline{\underline{p}}}}^{+} \right) : \underline{\underline{\underline{\underline{R}}}}^{o} \tag{7}$$

$$\dot{\underline{\underline{\Sigma}}} = \dot{\underline{\underline{\underline{\underline{R}}}}}^{d} : \underline{\underline{E}}_{e} + \underline{\underline{\underline{\underline{R}}}}^{d} : \dot{\underline{\underline{E}}}_{e} + \dot{\underline{\underline{M}}} \tag{8}$$

$$\dot{\underline{\underline{M}}} = -\frac{1}{2} \dot{D}^{T} \frac{\partial\, \underline{\underline{\underline{\underline{p}}}}^{+}}{\partial\, \underline{\underline{E}}_{e}} : \underline{\underline{\underline{\underline{R}}}}^{o} : \underline{\underline{E}}_{e} : \underline{\underline{E}}_{e} - \frac{1}{2} D^{T} \frac{\partial\, \dot{\underline{\underline{\underline{\underline{p}}}}}^{+}}{\partial\, \underline{\underline{E}}_{e}} : \underline{\underline{\underline{\underline{R}}}}^{o} : \underline{\underline{E}}_{e} : \underline{\underline{E}}_{e} - D^{T} \frac{\partial\, \underline{\underline{\underline{\underline{p}}}}^{+}}{\partial\, \underline{\underline{E}}_{e}} : \underline{\underline{\underline{\underline{R}}}}^{o} : \dot{\underline{\underline{E}}}_{e} : \underline{\underline{E}}_{e} \tag{9}$$

To determine the overall damage tensor $\underline{\underline{D}}$ (Eq. 5), the spectral decomposition concept of stress tensor is adopted (Eqs. 1-4). Σ_i^* is the i^{th} principal strain and p_i the i^{th} corresponding to the unit principal direction of eigenvalue and eigenvector of Σ^*. The symbol $\otimes$ represents the tensor product. The 4^{th} order positive spectral projection tensor $\underline{\underline{P}}^+$ given in (Eq. 4) is determined by equations (Eq. 2) and (Eq. 3). According to (Eq. 5), the damage is considered to be entirely active when all the eigenvalues are positive in the three principal directions; whereas, it becomes fully passive once the eigenvalues are negative, i.e., depending on the $\underline{\underline{P}}^+$ configuration. Hence, $\underline{\underline{P}}^+$ allows verifying naturally the complexity of the damage activation/deactivation phenomenon whatever the applied loading path. The overall rigidity tensor for a damaged material $\underline{\underline{R}}^d$ and its evolution $\dot{\underline{\underline{R}}}^d$ are defined respectively by equations (Eq. 6) and (Eq. 7), where $\underline{\underline{R}}^o$ is the classical 4^{th} order rigidity tensor for an initially isotropic material. As recently proposed [1], the overall stress tensor evolution coupled with damage activation/deactivation phenomenon is mathematically described by (Eq. 8). In (Eq. 9), the second term in the right-hand side depends explicitly on the eigenvectors variation during cyclic loading. Thus, when the loading is applied according to laboratory reference axes, the principal vectors coincide with the latter. In this case, these vectors are constant, i.e., their characteristics vary neither with respect to time, nor according to the deformation. Hence, the second and third terms in the right-hand side of (Eq. 9) vanishes. As a result, (Eq. 8) has the advantage to successfully treat a great number of loading types especially the multiaxial ones.

3. Algorithms of optimization

The identification process is to find numerically a set of model coefficients, which correlates the best possible predictions and experimental results. It is based on minimizing the difference between the recorded model response and the given experimental result. Such a difference can never be zero. However, the rule states that when the difference is smaller, the set of coefficients is better. In this work, identification (calibration) of the model parameters is to find a search space where these values should minimize the gap between experimental results and predictions. Solving this problem is realized by minimizing the following function:

$$F(P) = \sum_{n=1}^{N} F_n(P), \tag{10}$$

$$F_n(P) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \left(V_{\exp} - V_{sim}\right)^T D \left(V_{\exp} - V_{sim}\right) dt. \tag{11}$$

where, P: Model parameters, N: number of tests, $[t_0, t_1]$: time interval of the test n, V_{exp}-V_{sim}: difference between observed experiments and their simulations for the test n, D: weighting matrix of the test n.

The complexities of search space are the minimum function using radically different methods of resolutions. As a first approximation, the deterministic method is suitable for search in small

state-space; whereas for complex and large search state-space, this requires rather a method of stochastic search (genetic algorithm, pattern search ...).
The difficulties of these problems via conventional optimization methods give rapidly this family of algorithms able to handle large combinatorial problems with mixed variable. It is more interested for solving practical problems by a general classification of optimization problems and solved methods [2,3]. Briefly, genetic algorithms are adaptive heuristic search algorithm based on the evolutionary idea of natural selection and genetic. Moreover, they are a part of evolutionary computing, a rapidly growing area of artificial intelligence.
The strategy proposed in this work is to utilize a combination of the GA with the PSA. We will briefly describe these two algorithms.

3.1 Genetic Algorithm

This algorithm starts with the creation of the initial population of individuals and terminates with the convergence towards the best individuals of population giving therefore the optimized solution. The transition from one generation to another is accomplished by applying the following process: (i) mechanism of evaluation, (ii) selection and (iii) modification, up to obtaining a stopping criterion. The structure of this algorithm is given by the flowchart [4] (figure 1).

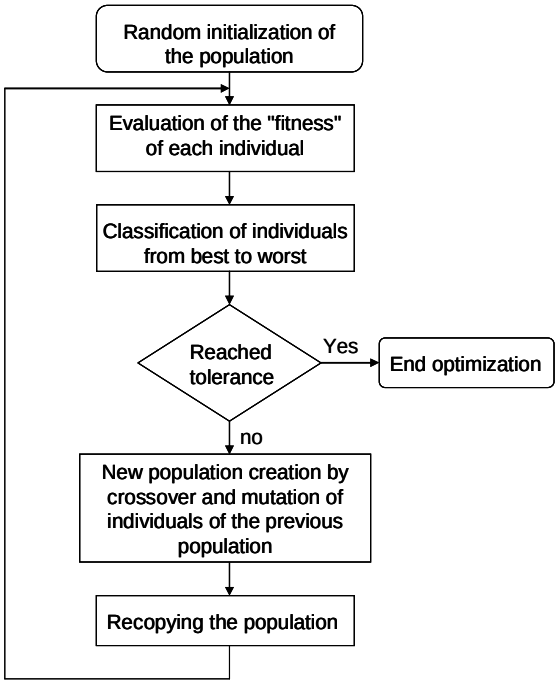

Figure 1 Structure of the genetic algorithm

Each individual of a given population is defined by a chain of genes that correspond to the different parameters to be identified. To avoid the difficulties that may arise in the binary coding and decoding of individual, a real coding GA is used [4]. The values of each parameter are bounded by

an interval [x_{min}, x_{max}] normally determined in this type of modeling according to mechanical bases. The main reason to establish these limits is to make the search process more efficient by reducing its space.

The initial population is produced by:

- Initial solutions (individuals) proposed based on the expert opinion and on experimental observations;
- Solutions chosen randomly in the search space.

This allows, in fact, to start the search from various solutions of the search space incorporating expert opinion.

Different numerical tests should be conducted and led to choice of stochastic operators as follows:

- Selection type elitism, which allows to highlight the best individuals in the population. These are the most developed individuals which will participate in the improvement. Such a technique has the advantage of faster convergence to the best individuals to the detriment of individuals which seem less appropriate and could provide elements for the creation of new individuals.
- Crossover scattered, which is cut individuals into several portions (2 or 3 portions) to obtain new individuals
- Adapt feasible mutation which randomly generates directions that are adaptive compared to the last generation successful or not. The feasible region is limited by the constraints. A pitch length is selected along each direction in such a manner that the bounds constraints are satisfied.

3.2. Pattern Search Algorithm

Pattern search is a direct search method. This method is employed for solving optimization problems that does not require any information about the gradient of the objective function. The pattern search begins at the initial point x_o. At the first iteration the mesh size is 1 and the GPS (Generalized Pattern Search) algorithm adds the pattern vectors to the initial point x_o to compute the following mesh points. The algorithm computes the objective function at the mesh points using the following approach:

$$xm_i = x_n + v_i \Delta_n \tag{12}$$

$$x_{n+1} = xm_j \,/\, f(xmj) = \min_i(f(xm_i)) \tag{13}$$

Where xm_i: the mesh points, x_n: the current point, v_i: the pattern vector and Δ_n: the current mesh size.

A pattern is a set of vectors $\{v_i\}$ that the PSA utilizes to define which points to search at each iteration. The set $\{v_i\}$ is determined by the number of independent variables in the objective function. For example, if there are three independent variables in the optimization problem, the default for a 2N positive basis consists of the following pattern vectors:

$$\begin{cases} v_1 = [1 \quad 0 \quad 0] \\ v_2 = [0 \quad 1 \quad 0] \\ v_3 = [0 \quad 0 \quad 1] \\ v_4 = [-1 \quad 0 \quad 0] \\ v_5 = [0 \quad -1 \quad 0] \\ v_6 = [0 \quad 0 \quad -1] \end{cases} \tag{14}$$

For a more description of this, see Kolda, Lewis, and Torczon [5].

To accelerate the convergence, we stop the iteration as soon as it finds a mesh point whose fitness value is smaller than that of the current point.
After a successful poll, the algorithm multiplies the current mesh size by 2. If none of the mesh points has a smaller objective function value at current point, so the poll is unsuccessful, the algorithm does not change the current point at the next iteration and multiplies the current mesh size by 0.5.
In our application the criteria for stopping the pattern search are the number of objective function evaluations.

4. Numerical applications

The evaluation of the proposed new strategy for identification is carried out through the description of the elastic-inelastic cyclic behavior of a polycrystal under uniaxial tension-compression (TC), biaxial tension-torsion with 90° out-of-phase angle (TT90). Our polycrystal is a random orientation distribution of 40 grains of a single-phase FCC. Initially, a database for both cyclic loading (TC and TT90) is numerically made up to final damaging of this grains distribution using the coefficients summed up in (Table 1)

Table 1 Coefficients used to create the database

Elastic-Inelastic parameters												
Model parameters	E (MPa)	ν	α	z	K	b^s	K_o (MPa)	Q^s (MPa)	$h_1=h_2=\ldots=h_5$	h_6	C^g (MPa)	a^g
coefficients	215000	0.32	1	20	50	13	240	256	1	2.29	95100	10

Damage parameters						
Model parameters	S^s	s_o	w^s	d_1	d_2	γ_0
coefficients	2	0.95	1	1	1.4	1.25

Such a database is considered as an experimental one. Thereafter, the identification process of model parameters is started by setting the damage parameters changing six key parameters related to the inelastic behavior (b^s, k_o, Q^s, h_6, C^g and a^g). Therefore, the identification process by the global minimum optimization concept is made through the genetic algorithm. After several tests on the population size, a population of 600 individuals is employed to optimize 6 coefficients of the model. Several iterations are made obtaining several families of model parameters followed by a local identification using the pattern search algorithm. The optimized model parameters are summed up

in (Table 2).

Table 2 Initial and optimized coefficients

Elastic-inelastic parameters												
Model parameters	E (MPa)	ν	α	z	K	b^s	k_o (MPa)	Q^s (MPa)	$h_1=h_2=\ldots=h_5$	h_6	C^g (MPa)	a^g
Initial	215000	0.32	1	20	50	24.5	340	100	1	1.7	75100	6
Optimized	215000	0.32	1	20	50	14.5	267.5	397.6	1	6.3	33830	8.71

Damage parameters						
Model parameters	S^s	s_o	w^s	d_1	d_2	γ_0
Initial	2	0.95	1	1	1.4	1.25
optimized	2	0.95	1	1	1.4	1.25

One of the main reasons which promotes this association is that both algorithms are parallelizable as shown in [2,3]. This allows gaining in computation time by exploiting computer multiprocessor. The experimental recorded fatigue lives are 38, and 14 cycles for TC and TT90, respectively. The model predicts these lives faithfully giving therefore 38, and 12 cycles in TC and TT90, respectively.

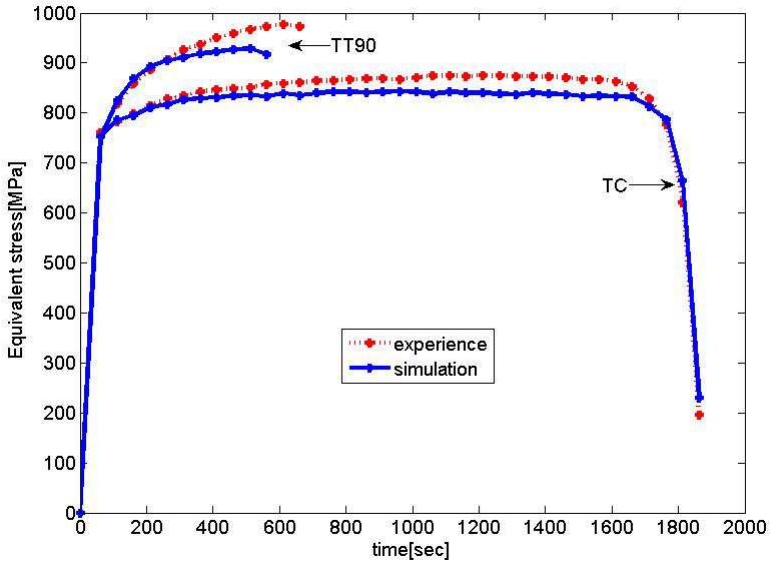

Figure 2 Evolution of the overall stress during TC and TT90 up to the final fracture

Figure 2 represents the typical evolutions of the maximum overall stress (pick stress value for each cycle) versus cyclic time using the same maximum von-Mises equivalent macro-strain for the two cyclic loading paths (TC and TT90). The predicted responses describe properly the experimental

results. Note that these predicted results are computed with the optimized model parameters summarized in table 2.

5. Conclusion

The objective of this work is to propose a new strategy to optimize the identification parameters of a micromechanical model coupled with damage [1]. Hence, a combination of genetic algorithm with pattern search algorithm is developed. The genetic algorithm optimizes globally the model parameters; whereas the pattern search algorithm, considered as a local method, has a role to determine the final values of these model coefficients. This model is tested under different cyclic loading complexities. It is recognized that this combination shows its ability to optimize the identification process. Consequently, the predicted responses describe faithfully the experimental results.

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References

[1] Abdul-Latif, A., and Mounounga T., B. S., (2009), Damage Deactivation Modeling under Multiaxial Cyclic Loadings for Polycrystals, International Journal of Damage Mechanics, 18, 177-198.
[2] Dréo J., Pétrowski A., Siarry P,.and Taillard E. (2003), Métaheuristiques pour l’Optimisation Difficile, Eyrolles, ISBN : 2-212-11368-4.
[3] Smith R.E., Perelson A.S., and Forrest S., (1993), Searching for diverse, cooperative populations with genetic algorithms, Evolutionary Computation, 1(2), pp.127–149.
[4] Christophe Bontemps, Principes Mathématiques et Utilisations des Algorithmes Génétiques, Extrait de cours, Novembre 1995.
[5] Kolda, Tamara G., Robert Michael Lewis, and Virginia Torczon. "A generating set direct search augmented Lagrangian algorithm for optimization with a combination of general and linear constraints." Technical Report SAND2006-5315, Sandia National Laboratories, August 2006.