Material Behavior Simulation of 42CrMo4 Steel

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Abstract: It is becoming increasingly important to make possible constitutive modelling and simulation of material behaviour for the prediction of possible failures in material. This can allow to the optimization of design of highly loaded engineering components. In order to achieve that goal, material parameters should be accurately determined for the chosen material model. The major step in material parameters identification is material behaviour simulation. The procedure of material behaviour simulation is based on the results of the fatigue testing on the materials' samples. The paper presents the procedures required for the material behaviour simulation of 42CrMo4 steel, starting from the fatigue testing, through numerical procedures related to complex material model, which results in material parameters identification, to the validation of described procedures by comparison of the simulated and real materials response in cyclic loading conditions.

1 INTRODUCTION

The optimal engineering design consists of the knowledge on the loading applied on the components, together with the knowledge on material behaviour in different loading conditions. Although many researchers prefer to use simple material models to take into account the material fatigue and its influence on materials' life-time, the development of ever more complex material models makes possible description of material behaviour even in different phases of its' loading cycles. With the usage of complex material models, it is possible to take into account wide range of phenomena that occur in the materials' structure and influence the material behaviour through its' life cycles. These complex material models are usually highly non-linear and they consist of large number of unknown material parameters, which have to be identified on the basis of fatigue testing results.

The main goal in material parameters identification is to use stress-strain data, recorded through loading cycles of materials' specimen life and on the basis of developed procedures define optimal set of parameters which describe the material behaviour as accurately as possible. The validation of both the procedures of parameter identification and the identified parameters' set is possible by the simulation of material behaviour in different loading conditions and its' comparison to the real material behaviour, acquired through fatigue testing results.

The material behaviour analysis in the low-cycle fatigue conditions is performed on the specimens produced out of the 42CrMo4 steel, which tend to experience both kinematic and isotropic softening behaviour. These phenomena can be described well by the Chaboche's material model (Chaboche, 2008, Lamaitre and Chaboche, 1990). Although it proved to be very efficient in the description of material behaviour in different operating conditions of the components, the simple parameters' identification processes proved to be very unreliable and time-consuming, because of the material model's nonlinearity and large amount of data that have to be taken into account. Therefore, the development of evolutionary algorithms, specifically genetic algorithm, is chosen to overcome these difficulties. It is known to be well-used in similar problems (Furukawa and Yagawa, 1997).

Genetic algorithm for the material parameters identification is proven to be insensitive to the possible errors in measured data, it has large probability to achieve global optima and to converge to the accurate results in very short time. It also works well with the large number of data and with the highly non-linear systems (Franulovic et al., 2009, Mahmoudi et al., 2011). In order to make possible for the genetic algorithm to work optimal in any given conditions, it's operators should be

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developed, together with the proper objective function.

2 MATERIAL PARAMETERS IDENTIFICATION

The parameter identification system consists of set of defined procedures which enable accurate description of material characteristics possible. These procedures are divided into two main parts. The first part consists of prescribed tasks that include material model definition, fatigue testing and numerical procedures definition. The second part includes controls that have to be performed in different phases of derived tasks in order to ensure an accurate solution of the parameter identification process. These controls relate to tests accuracy, irregularities in data sets, stress-strain hystereses comparison, evolution of parameters, but also to numerical procedures convergence. Although these procedures can be applied to a wide range of material models, they are mainly developed for advanced ones because all the tasks that have to be performed to identify their material parameters take much time to gain satisfactory results.

2.1 Material Model

Considered material model is a rate-independent version of the model, suitable to describe material behaviour in low-cycle fatigue regime, proposed by Chaboche (Chaboche, 2008), as a three-decompositioned Armstrong- Fredericks model for the back-stress tensor X_{ij}:

$$\mathrm{d}X_{\mathrm{ij}} = (2/3)C\mathrm{d}\varepsilon_{\mathrm{ij}}^{\mathrm{p}} - \gamma X_{\mathrm{ij}}\mathrm{d}p\,, \qquad (1)$$

$$\mathrm{d}X_{\mathrm{ij}} = \sum_{\mathrm{i}=1}^{n} \mathrm{d}X_{\mathrm{ij}}^{(\mathrm{n})}\,,\ n = 3. \qquad (2)$$

Values C and γ are material parameters, $\mathrm{d}\varepsilon_{\mathrm{ij}}$ is increment of plastic strain and $\mathrm{d}p$ is increment of accumulated plastic strain. The model is also appropriate to simulate the Bauschinger effect with kinematic and isotropic hardening/softening of the material. Isotropic hardening takes into account the cyclic evolution of the yield region in the strain-controlled conditions. It is expressed by:

$$\mathrm{d}R = b(R_{\infty} - R)\mathrm{d}\lambda\,, \qquad (3)$$

where R represents isotropic hardening, R_{∞} is the boundary of the isotropic hardening, b is the isotropic hardening rate and $\mathrm{d}\lambda$ is plastic multiplicator.

The constitutive equations are based on linear isotropic elasticity, while multiaxial plasticity criteria is described by well-known von Mises yield criterion (Chaboche, 2008, Lemaitre, 1996) with associated flow rule. This material model for kinematic and isotropic hardening description of material behaviour is consequently defined by the set of nonlinear equations with 11 unknown material parameters included, which have to be identified to make possible simulation of material behaviour. While one parameter is usually assumed, the rest 10 depend on the results of stress-strain relationship in real material behaviour, recorded through fatigue testing procedure.

2.2 Fatigue Testing

The fatigue testing was performed in the strain-controlled conditions, according to standard testing procedure (E606 – 92, 1992). The testing specimen were produced out of steel 42CrMo4 in tempered state. During testing, detailed stress-strain response was recorded through cycles, until the fracture of specimen in two parts. The materials response served later for the material behaviour simulation.

The measuring system was set in following conditions: strain rate of 1,5% s^{-1} was held constant for the duration of each test. The tests were performed at the temperature of 20 °C. The strain amplitude for symmetric cyclic testing were maintained at 0,9%, 1,2% and 1,8% respectively. The results showed that material experiences isotropic and kinematic softening with emphasized Bauschinger effect phenomenon (Bari and Hasan, 2000, Bari and Hassan, 2002). Prior to these fatigue testing, the monotonic tests were performed by using the same specimens made of the same materials. In these tests, the load was applied and increased until the specimen fracture to record the stress-strain response of the material.

2.3 Numerical Procedures

In order to identify material parameters of highly nonlinear material models and thus make possible material behaviour simulation, genetic algorithm is planned to be used. The procedure of genetic algorithm for parameter identification in its basic form could be relatively simple, but in that form is not suitable for the particular problem. Namely, in this case the large amount of experimentally obtained data influence the possibility of convergence to accurate results. In order to overcome this problem, specific genetic operators should be developed and finite element analysis should be used to make possible simulation of material behaviour and consequently calibration of material parameters. The numerical procedure for the parameter identification is shown in Figure 1.

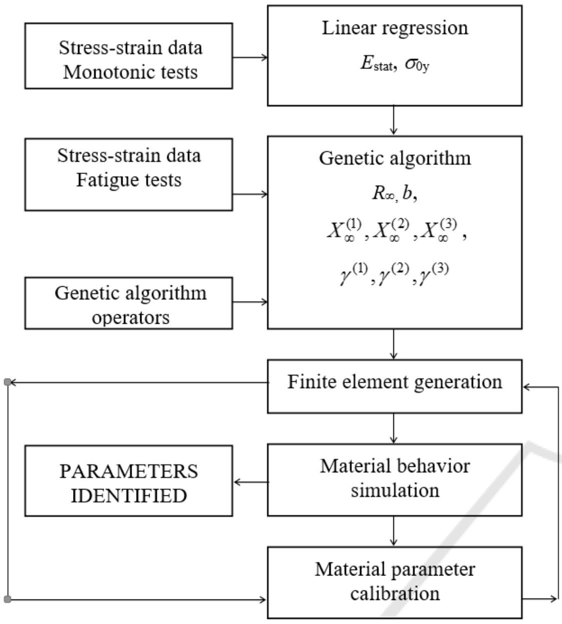

Figure 1: Parameter identification system.

Material parameters E_{stat} (Modulus of elasticity) and σ_{0y} (Yield stress) are obtained from the monotonic stress-strain curve by linear regression, while kinematic hardening/softening parameters $X_\infty^{(1)}, X_\infty^{(2)}, X_\infty^{(3)}, \gamma^{(1)}, \gamma^{(2)}, \gamma^{(3)}$ and isotropic hardening / softening parameters R_∞ and b are part of the algorithm's numerical procedures, which include simulation of material behaviour.

The accuracy of the results can be ensured through several controls (Franulovic et. al., 2009), such as: experimental tests accuracy control, accuracy of preliminary parameters identification through the phases (kinematic hardening and isotropic hardening behaviour) and comparison of simulated and real material behaviour during parameters calibration procedure.

The high non-linearity of the system is included in the hardening parameters' set identification, so the genetic algorithm for hardening parameters identification holds the greatest responsibility for this system to give satisfactory material behaviour simulation.

2.4 Genetic Algorithm

In order to apply the genetic algorithm for parameter identification, inverse analysis is applied (Tarantola, 2005, Hernandez et al., 2012). Inverse analysis consists of defining search methods of unknown material parameters by observing material sample's response to a probing signal. Proposed procedure consists of three main parts (Figure 2). The system characterization means that material parameters which can fully characterize the system should be defined. The second part is forward modelling. In this part mechanical principles and physical laws required to enable the prediction of the system behaviour have to be defined. The third part is backward or inverse modelling. In this part the actual measurement results, the stress - strain data obtained from fatigue tests affect the values of model parameters in order to characterize the system as accurately as possible.

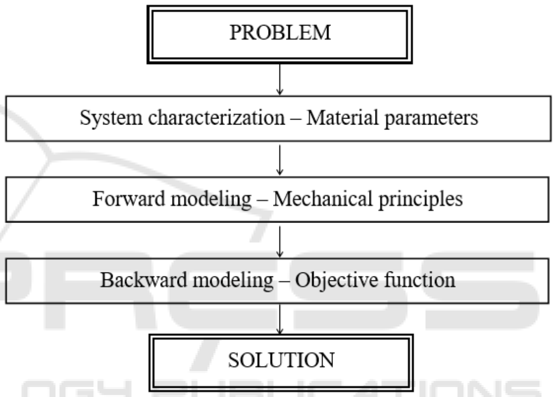

Figure 2: Inverse analysis for parameter identification.

The system characterization for the presented problem is based on the chosen material model definition and includes hardening material parameters. Forward modelling, based on mechanical principles of material behaviour, is defined in two domains. The first one

$$\sigma = \hat{\sigma}(\varepsilon; a_i) \tag{4}$$

$$a_i = [\, X_\infty^{(1)}, X_\infty^{(2)}, X_\infty^{(3)}, \gamma^{(1)}, \gamma^{(2)}, \gamma^{(3)} \,] \in \mathrm{A} \tag{5}$$

is generated for the identification of kinematic hardening parameters a_i, based on Eqs (1,2), by following relation:

$$\begin{aligned} \frac{\Delta\sigma}{2} &= (R_\infty + k) + X_\infty^{(1)} \tanh\left(\gamma^1 \frac{\Delta\varepsilon^p}{2}\right) \\ &+ X_\infty^{(2)} \tanh\left(\gamma^2 \frac{\Delta\varepsilon^p}{2}\right) \\ &+ X_\infty^{(3)} \tanh\left(\gamma^3 \frac{\Delta\varepsilon^p}{2}\right) \end{aligned} \tag{6}$$

The second one

$$\sigma_{\max}^{N} = \hat{\sigma}_{\max}^{N}(\varepsilon, N; b) \tag{7}$$

$$b \in \mathrm{B} \tag{8}$$

is for isotropic hardening parameter determination b, following relation:

$$b = \frac{\ln\left[1 - \left(\sigma_{\max}^{\mathrm{N}} - \sigma_{\max}^{1}\right) / \left(\sigma_{\max}^{\mathrm{S}} - \sigma_{\max}^{1}\right)\right]}{-2\Delta\varepsilon^{\mathrm{p}} N} \tag{9}$$

where $\sigma_{\max}$ is maximal stress in specific loading cycle (1-first cycle, S-stable cycle, N- Nth cycle).

Parameter R_∞ is calculated as the difference between initial yield stress and yield stress in stable cycle and therefore isn't part of the genetic algorithm calculation procedure.

Domains A and B are predefined for each procedure in order to improve genetic algorithms' calculation performance. The objective functions in backward modelling for each procedure are based on least squares method with w_{ij} as the weighting factor (Fedele et al., 2005.). Procedure for domain A is performed on all data of j tests with different measuring protocols that are executed for one material.

$$f_A = \sum_{j=1}^{m} \sum_{i=1}^{m_j} w_{ij} \left[\sigma_i^{j*} - \hat{\sigma}\left(\varepsilon_i^{j*}; a\right)\right]^2 ; w_{ij} = \left(\frac{1}{\sigma_i^{j*}}\right)^2 \tag{10}$$

Procedure for domain B is performed for each test separately and then average values of the parameters are determined for each material.

$$f_B = \sum_{i=1}^{m} w_i \left[\sigma_{\max\ i}^{*N} - \hat{\sigma}_{\max}^{N}\left(\varepsilon_i^{*}, N_i^{*}; b\right)\right]^2 ; w_i = \left(\frac{1}{\sigma_{\max\ i}^{*N}}\right)^2 \tag{11}$$

The asterisk refers to experimental data (stresses and strains).

In order to accomplish as fast and as accurate solution as possible, the genetic algorithm creates a population of solutions and applies genetic operators, such as scaling, selection, mutation and crossover to evolve the solutions in order to find the best ones. They influence the initial population through phases in order to converge to the final population (Figure 3).

The best individuals have low fitness value and the possibility of their selection is high, but genetic algorithm procedure is developed to take into account also the genetic material of the individuals with lower fitness value, but with the lower expectancy of selection.

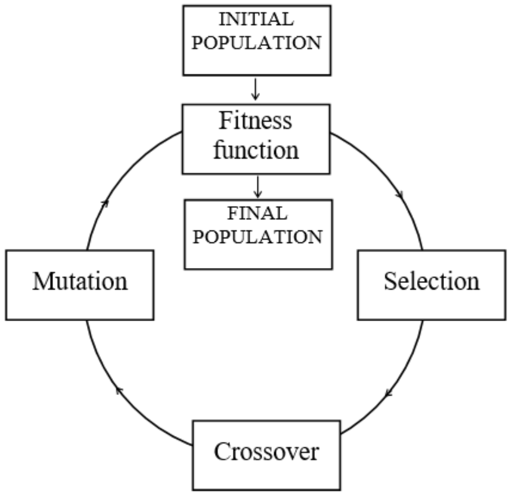

Figure 3: Genetic algorithm operators.

The 4-tournament selection mechanism is chosen to select individuals which are going to be a part of the mating pool. For the crossover the intermediate recombination is used in this case (Pohlheim, 1999). In order to achieve low fitness value in short time, both domain procedures have specific crossover technique, which means different dispersion and solution controls, as shown in Figure 4.

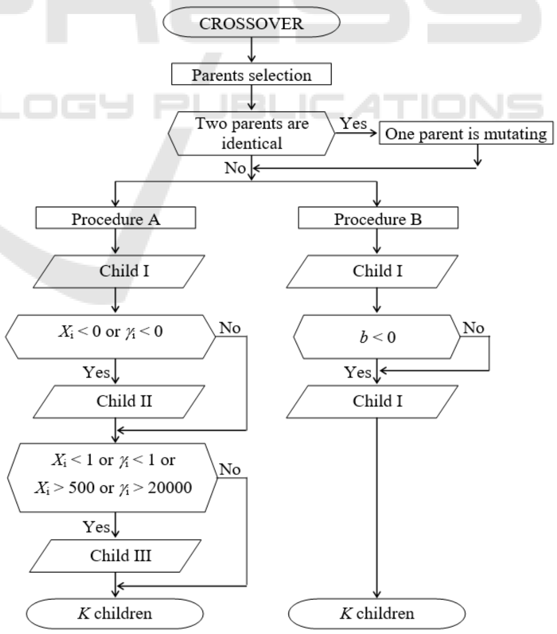

Figure 4: Crossover operator procedure.

In each generation, the parent who contributes its variable to the child is chosen randomly with equal probability. There is, however, possibility to select two identical parents. If that is the case, one parent is mutating with the 25% ratio. The child's value can be calculated through one, two or three stages, depending upon performed genetic algorithm's control points. Mutation procedures of the proposed genetic algorithm in both domains have the same mutation routine. Within this procedure each variable is changing, while the mutation ratio is decreasing through generations. The mutation procedure is shown in Figure 5.

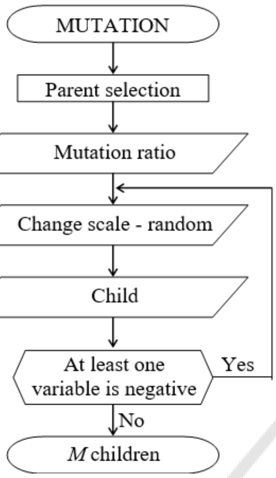

Figure 5: Mutation operator procedure.

3 MATERIAL BEHAVIOR SIMULATION

The validation of material behaviour simulation and thus accuracy of obtained material parameters is performed as comparison of numerical models' and real materials' response under cyclic loading, as shown in Figures 6 and 7. The maximum, minimum and mean stresses through cycles for both simulated and real material's response have the same tendency through materials life (Figure 6).

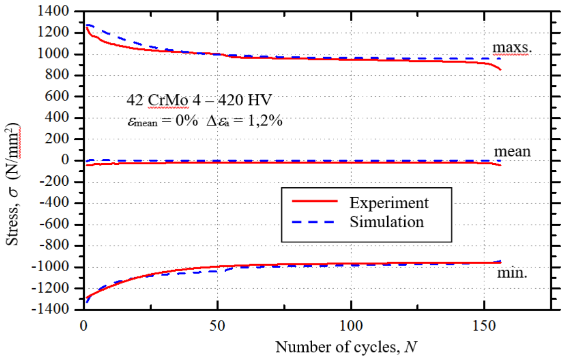

Figure 6: Stress – Number of cycles curves.

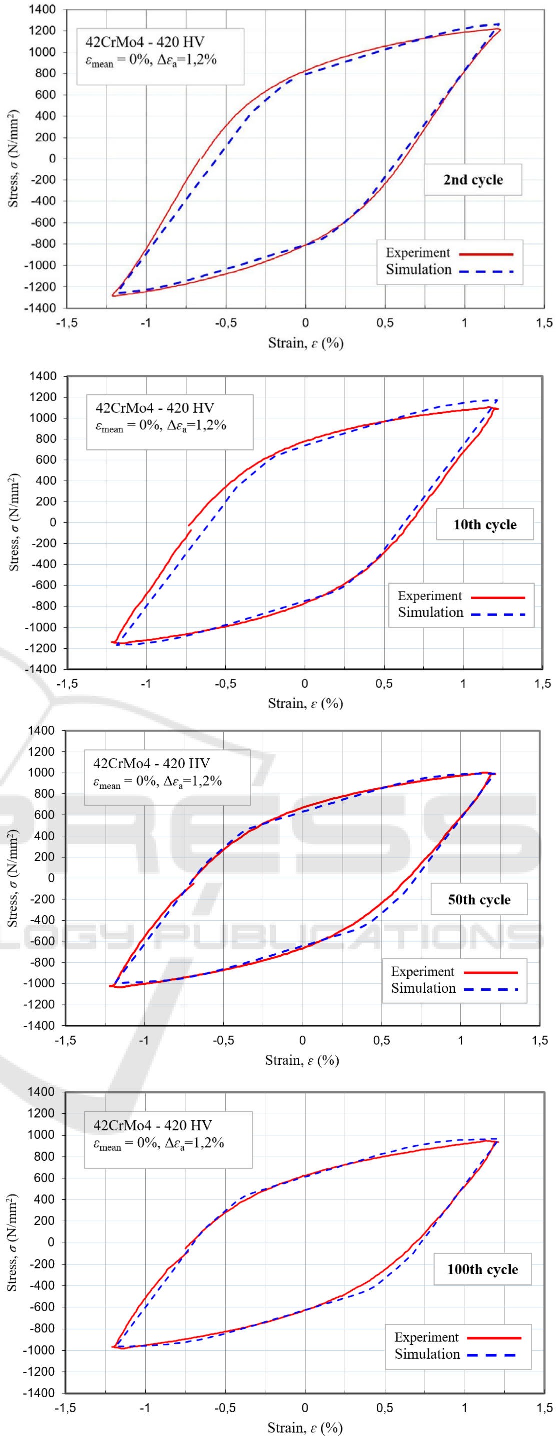

Figure 7: Stress – Strain relationships for 2nd, 10th, 50th and 100th loading cycle.

In the presented example of the stress-strain relationship (Figure 7), the second, tenth, fiftieth and the hundredth cycles are simulated and compared to the real material behaviour. The simulation of the material behaviour shows very good results in comparison to the real material behaviour and thus validate the proposed material parameters identification procedure.

4 CONCLUSIONS

The design and optimization of mechanical structures depend largely on accurate modelling of material behaviour. If large number of phenomena that occur in the material in hard operating conditions need to be described, advanced material models are necessary to be used. Since these models are quite complex, their parameter identification process is also challenging. The genetic algorithm proved to be a good choice for this task. In order for it to be effective, its' operators have to be specifically developed for the task. The simulation of material behaviour, together with the usage of developed optimization procedures are crucial to validate the process and also acquire set of results which are as accurate as possible. The presented procedure for material parameter identification, which is validated by the simulation of material behaviour and its' comparison to the real material behaviour of 42CrMo4 steel, can be further used for the description of material behaviour of other metallic, but also different innovative materials. The research on the material behaviour of new materials can enhance mechanical engineering design of components and bring new findings in this area.

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