NUMERICAL SIMULATION OF THE DISSIPATED AND STORED ENERGY IN METALS UNDER CYCLIC LOADING

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Abstract. This work is devoted to the numerical simulation of the energy storage and dissipation processes. The mathematical model of the considered processes is based on the further development of a statistical description of the mesodefect ensemble evolution. Defect evolution is described by a kinetic equation for structural tensor parameter which coincides with a strain caused by defects. The use of such approach let us to obtain the value of the stored end dissipated energies during cyclic loading.

1 INTRODUCTION

In order to describe the deformation process of metals under cyclic loading adequately we should take into account that a part of the mechanical work converts into the heat and the remainder stores in the material. The stored energy is the energy connected with the different types of the defects which accumulate in the material.

It was experimentally shown [1] that an endurance limit can be determined by using almost any thermodynamic characteristics of the process: inelastic deformation per one load cycle, irreversibly consumed energy per one load cycle, self-heating, temperature, energy dissipation rate, and energy storage rate. The analysis of the experimental studies carried out in USSR in 1970-1980 has let us to the conclusion that the obtained parameters are indirect and thus cannot be used as a basis for the development of the universal material failure criteria.

For example, it is experimentally shown [1] that the thermal energy dissipated during the cyclic deformation of specimens made from 40X, 2X10, 25, 45 steels (Russian marking) may have very different values [1].

In this work the stored energy is used as a fracture criterion and a failure of the material occurs when the stored energy reaches its critical value. For its adequate description in the deformation process, we should take into account structural defect evolution in the material. Evolution of the defect ensembles is modeled with the use of the internal field variable which has a meaning of the defect density and coincides with an additional deformation caused by
the defects.

2 MATHEMATICAL MODEL

In this work, the parameter associated with typical mesoscopic defects (mesoshears) is introduced [2] as the symmetrical second order tensor \( s \):

\[
s = \frac{1}{2} s(nb + bn),
\]

(1)

where \( n \) - is a unit normal to the shear plane, \( b \) - is a unit vector in the shear direction, \( s \) - is a shear intensity.

A macroscopic tensor, which characterizes a volume concentration and orientation of the defects, can be determined as averaging of \( s \):

\[
p = n \langle s \rangle.
\]

(2)

where \( n \) - is a number of the defects in the unit volume.

Tensor \( p \) can be considered as an additional strain, caused by the defects. This parameter can be considered as a thermo dynamic state variable in contradistinction to the plastic strain. Introduction of such parameter let us to propose a model of energy storage in metals under cyclic loading.

It is assumed that full strain rate \( \dot{\varepsilon} \) consists of elastic strain rate \( \dot{\varepsilon}^e \), plastic strain rate \( \dot{\varepsilon}^p \) and the strain rate due to the defects \( \dot{\varepsilon}_d \):

\[
\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^\text{pl} + \dot{\varepsilon}_d.
\]

(3)

Elastic strains are obeyed to the Hook’s law:

\[
\sigma_0 = K \varepsilon_0^e,
\]

(4)

\[
\sigma_d = 2G \varepsilon_d^e,
\]

(5)

where \( K \) – isotropic elastic modulus, \( G \) – elastic shear modulus, \( \sigma_0 \) - spherical stress tensor, \( \varepsilon_0^e \) - spherical elastic strain tensor, \( \sigma_d \) - stress deviator tensor, \( \varepsilon_d^e \) - elastic strain deviator tensor.

According to the thermodynamic laws, we can obtain the dissipation inequality in the following form:

\[
\sigma : \dot{\varepsilon}^p + (\sigma - \frac{\partial F}{\partial \sigma}) : \dot{p} - q \cdot \nabla T \geq 0,
\]

(6)

where \( F \) = \( e - TS \) - a free energy, \( e \) - an internal energy, \( T \) - temperature, \( S \) - entropy, \( q \) - heat flux vector.

In (6) values of \( \dot{\varepsilon}^p \), \( \dot{p} \) are the thermodynamic flows and \( \sigma \), \( (\sigma - \frac{\partial F}{\partial \sigma}) \) are the thermodynamic forces. According to the Onsager’s principle, quasilinear relations can be obtained from (6):
\[ \dot{\varepsilon}^\sigma = \Gamma_{\sigma} \sigma + \Gamma_{\rho \sigma} (\sigma - \frac{\partial F}{\partial \sigma}), \quad (7) \]
\[ \dot{p} = \Gamma_{\rho} (\sigma - \frac{\partial F}{\partial \sigma}) + \Gamma_{\rho \sigma} \sigma, \quad (8) \]

where \( \Gamma_{\sigma}, \Gamma_{\rho \sigma}, \Gamma_{\rho} \) - kinetic coefficients.

Constitutive equations (7)-(8) determine kinetics of plastic strain and strain caused by the defects.

With the use of a coaxiality hypothesis of \( \sigma \) and \( p \), for a thermodynamic force \( (\sigma - \frac{\partial F}{\partial \sigma}) \)

we can write the following expression:

\[ \sigma - \frac{\partial F}{\partial \sigma} = \left[ 1 - \frac{\sigma}{2G\sigma_c} + \frac{p}{p_c} \right] - \left[ f\left( \frac{|p|}{p_c} \right) \frac{p_c}{|p| + 1} \right], \quad (9) \]

where \( \sigma_c, p_c \) - scale factors, \( |p| \) - intensity of the \( p \) tensor, \( \delta = L_n^2/L_c^3 \) - structural scaling parameter, which is the ratio of the characteristic defect size \( L_n \) and correlation radius of the interaction between defects \( L_c \). It is assumed that \( f \) - is a power function of \( |p| \) for modeling of nonlinear hardening:

\[ f\left( \frac{|p|}{p_c} \right) = k \left( \frac{|p|}{p_c} \right)^a, \quad k = \text{const}, \quad (10) \]

where \( k \) is a scaling factor, \( a \) is an exponent.

Kinetic coefficients have the following form:

\[ \Gamma_{\sigma} = \frac{1}{\tau_{\sigma}} \frac{1}{1 + \exp \left( -\frac{|\sigma| - S_y}{a_1} \right)}, \quad (11) \]
\[ \Gamma_{\rho} = \frac{1}{\tau_{\rho}} \frac{1}{1 + \exp \left( -\frac{H(|\sigma|, |p|, \delta, p_c, S_y) - S_y}{a_2} \right)}, \quad (12) \]
\[ \Gamma_{\rho \sigma} = \frac{1}{\tau_{\rho \sigma}}, \quad (13) \]

where \( \tau_{\sigma}, \tau_{\rho}, \tau_{\rho \sigma} \) - characteristic relaxation times, \( |\sigma| \) - stress tensor intensity, \( S_y \) - yield stress, \( S_y, a_1, a_2 \) - material constants, the \( H(|\sigma|, |p|, \delta, p_c) \) function can be considered as the “degree of the system nonequilibrium”:

\[ H(|\sigma|, |p|, \delta, p_c) = |\sigma| - 2G\sigma_c \left[ \delta(f + 1)|p|p_c - |p||p_c| \right]. \quad (14) \]
So, the closed system of equations describing the cyclic deformation process consists of (3)-(5), (7)-(10) and kinetic coefficients (11)-(13).

Following [3], from the first thermodynamic law we can obtain the following expression:

$$\nabla \cdot \mathbf{q} + r + \dot{Q}_r + \dot{Q}_p = -\rho c \dot{T},$$

where $r$ - power heat source, $\dot{Q}_r = T \frac{\partial \sigma}{\partial T} : \dot{\varepsilon}^e$ - heat source connected with thermo elastic effect, $c = T \frac{\partial^2 F}{\partial T^2}$ - specific heat, $\dot{Q}_p$ - inelastic contribution to the heat generation.

The last term in left side of the (15) has the following form under isothermal conditions:

$$\dot{Q}_p = \sigma : (\dot{\varepsilon}^p + \dot{p}) - \frac{\partial F}{\partial\mathbf{p}} : \dot{\mathbf{p}} = \dot{W}^p - \dot{E}^s.$$

The first term in this relation is a plastic strain work rate ($\dot{W}^p$) and the second is a part of the mechanical work which stores in the material ($\dot{E}^s$). The critical value of last parameter is considered as a fracture criteria.

3 NUMERICAL RESULTS

There is simulated a cyclic loading of a steel specimen, geometry of which is shown on the figure 1. The sample has an initial central crack and its length is 17 mm.

![Figure 1: Geometry of the specimen. All sizes are in millimeters](image_url)

The numerical modeling was carried out in the finite-element package Simulia Abaqus 6.13 which was run under academic license. The above explained model was used for the material behavior description through the user subroutine UMAT. Arrays of material constants, strain, strain increments and the time step passed as the input data to the procedure. Increment of stress tensor components, increment of defect density tensor components and increment of a plastic strain are determined from the system of constitutive equations, which were represented as a finite difference scheme. Values of these components at the next time step are defined as the sum of values on the previous step and the appropriate increment.
The extended finite element method (XFEM) capability in Abaqus was used to model crack propagation. XFEM models a crack as an enriched feature by adding degrees of freedom in elements with special displacement functions. XFEM does not require the mesh to match the geometry of the discontinuities. It can be used to simulate initiation and propagation of a discrete crack along an arbitrary, solution – dependent path without the requirement of remeshing [4]. To specify a fracture criterion based on the critical stored energy there was used a UDMGINI subroutine.

There is considered a three-dimensional problem of cyclic loading during 49 cycles. Eight-node linear brick elements were used for the simulation. Figure 2 shows a loading diagram for the eleventh cycle (other cycles are similar) and figure 3 represents stresses corresponding to different time values of this cycle.

![Figure 2](image)

**Figure 2:** A pressure diagram for the 11th cycle of loading

![Figure 3](image)

**Figure 3:** Stress distributions in the crack tip corresponding to the 11th cycle for different time moments: A) t=5, B) t=5.07, C) t=5.25, D) t=5.43, E) t=5.5
Figure 4 A) demonstrates the initial crack of the specimen and figure 4 B) shows the crack at the end of the 49th cycle. The variable STATUSXFEM shows the state of the element. If it equals to one the element is completely cracked. So, after the 49th cycle, the specimen breaks down.

Figure 5: Stored energy distributions: A) 1st cycle, B) 15th cycle, C) 25th cycle, D) 33rd cycle, E) 43rd cycle, F) 49th cycle

Figures 5 and 6 provide information about the values of the stored energies and inelastic contribution to the heat generation at the different number of cycles. The crack starts to propagate when the value of the stored energy reaches $1.6 \times 10^6$J.
Figure 6: Inelastic heat: A) 1st cycle, B) 15th cycle, C) 25th cycle, D) 33rd cycle, E) 43rd cycle, F) 49th cycle

Figure 7 displays the evolution of the stored energy in the cracked element. It can be seen that there is a gradual growth of the stored energy almost through all deformation process (before crack initiation) and a sharp increase of it before the crack initiation.

![Figure 7: Stored energy evolution](image-url)
4 CONCLUSIONS

This paper is devoted to the simulation of energy dissipation and storage processes in metals under cyclic loading. There were formulated constitutive equations for elasto-plastic medium with mesodefects. These equations were adopted for the three-dimensional modeling in the finite-element package Simulia Abaqus 6.13 with the use of the subroutine UMAT. Fracture process simulation was carried out using XFEM capability in Abaqus and critical stored energy criterion was used for the crack propagation. It was shown that crack started to propagate when the stored energy reaches $1.6 \times 10^6 J$ and there was a complete sample failure after 49th cycle.

The simulation results let us to obtain the stresses fields in the crack tip, the values of the stored energies, inelastic contribution to the heat generation and the stored energy evolution. This information can be used for a crack branching prediction.

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