11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
E. Oñate, J. Oliver and A. Huerta (Eds)

NUMERICAL SIMULATION OF THE ENERGY STORAGE RATE IN METALS UNDER QUASISTATIC LOADING

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Key Words: *Plastic Deformation, Stored Energy, Mesoscopic Defects.*

Abstract. This work is devoted to the numerical simulation of the energy balance in metals under quasistatic loading. This process is described with the use of the statistical model developed in the Institute of Continuous Media Mechanics UB RAS. The defects ensemble evolution in the material is modeled using the internal field variable representing a defect density and coinciding with the additional deformation caused by the defects emergence and growth. The model takes into account the evolution of all tensor components, which describe the volume concentration and defect orientation and lets us to model the energy balance in the material under its plastic deformation.

1 INTRODUCTION

It is well known that the plastic deformation of metals is accompanied by the evolution of defects at different structural levels. It leads to convertion of the mechanical energy expended on the shape change of the specimen into thermal and stored parts. The thermal energy is generated by the defects motion and annihilation. The stored energy can be associated with energy accumulated in elastic defect fields. The simulation of this process can give us information about current state of material structure evolution and, as a consequence, allows us to forecast the service life of the sample.

The experimental and theoretical study of the energy balance during deformation has a long history. The importance of this problem was originally shown by J. H. Lambert in 1779 in his work concerning the energy similarity of mechanical and thermal failure processes of solids. A substantial contribution to this matter was made by V.S. Ivanova [1], who proposed the structure-energy theory of metal fracture. A detailed analysis of thermodynamic effects produced by cyclic deformation and failure in metals was carried out by V.T. Troshchenko and V.V. Fedorov [2, 3]. In 1937 Taylor and Quinney [4] made a first attempt to measure experimentally the value of the stored energy. They assumed that the rate of plastic work converted into heating is a constant, but further development showed its dependence upon strain and strain rate.

To improve the existing energy based model incorporated into standard final element codes we have to develop the equation describing the energy balance in materials under plastic deformation. One of the possible ways for modeling of the energy balance in metals under deformation and failure is incorporation into the classical mechanical model additional thermodynamic structural sensitive variables. The structural sensitive variable is determined in this paper based on the previous results of solution of statistical problem of typical mesodefect evolution. This variable can be considered as defect induced deformation. This deformation caused by no dissipative defect evolution process allows us to derive the relatively simple constitutive equation with can be generalize for 3D case and incorporated in Abaqus. The efficiency of the model is illustrated by calculation of stored energy evolution under quasistatic loading in two different metals (Armco iron and 316L steel). The numerical solution of the problem allows us also to propose the link between the stored energy rate and strain hardening rate in metals under quasistatic loading.

2 MATHEMATICAL MODEL

Mesoscopic defects (microshears) can be described as the symmetrical tensor having the following form [5]:

$$\mathbf{s} = \frac{1}{2} s(\mathbf{nb} + \mathbf{bn}), \tag{1}$$

where $\mathbf{n}$ - a unit normal vector to the shear plane, $\mathbf{b}$ - a unit vector in the shear direction, s - a shear intensity.

A macroscopic tensor, which characterizes a volume concentration and orientation of the defects, can be determined by the **s** averaging:

$$\mathbf{p} = n < \mathbf{s} >, \tag{2}$$

where n - a number of the defects in the unit volume. This parameter can be considered as a strain caused by the defects.

So, for the full strain rate $\dot{\boldsymbol{\varepsilon}}$ we can assume the following relation:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \dot{\boldsymbol{\varepsilon}}^{\mathbf{pl}} + \dot{\mathbf{p}}, \tag{4}$$

where $\dot{\boldsymbol{\varepsilon}}^{\mathbf{e}}$ - elastic strain rate, $\dot{\boldsymbol{\varepsilon}}^{\mathbf{p}}$ - plastic strain rate, $\dot{\mathbf{p}}$ - strain rate due to the defects.

Elastic strains are connected to the stresses according to the Hook's law:

$$\dot{\sigma}_0 = K \dot{\varepsilon}^e_0, \tag{5}$$

$$\dot{\boldsymbol{\sigma}}_d = 2G \dot{\boldsymbol{\varepsilon}}^e_d, \tag{6}$$

where K – isotropic elastic modulus, G – elastic shear modulus, σ_0 - spherical stress tensor, $\varepsilon^e{}_0$ - spherical elastic strain tensor, $\boldsymbol{\sigma}_{\mathbf{d}}$ - stress deviator tensor, $\boldsymbol{\varepsilon}^{\mathbf{e}}_{\mathbf{d}}$ - elastic strain deviator tensor.

The second thermodynamic law gives us the dissipation inequality in the following form:

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p + (\boldsymbol{\sigma} - \frac{\partial F}{\partial \mathbf{p}}) : \dot{\mathbf{p}} - \mathbf{q} \cdot \frac{\nabla T}{T} \geq 0, \tag{8}$$

where $F = e - TS$ - a free energy, e - an internal energy, T - temperature, S - entropy, $\mathbf{q}$ - heat flux vector.

According to the Onsager's principle, we can obtain from (8) quasilinear relations between thermodynamic flaws ($\dot{\boldsymbol{\varepsilon}}^p, \dot{\mathbf{p}}$) and forces ($\boldsymbol{\sigma}$, $(\boldsymbol{\sigma} - \frac{\partial F}{\partial \mathbf{p}})$) :

$$\dot{\boldsymbol{\varepsilon}}^p = \Gamma_\sigma \boldsymbol{\sigma} + \Gamma_{p\sigma} (\boldsymbol{\sigma} - \frac{\partial F}{\partial \mathbf{p}}), \tag{9}$$

$$\dot{\mathbf{p}} = \Gamma_p (\boldsymbol{\sigma} - \frac{\partial F}{\partial \mathbf{p}}) + \Gamma_{p\sigma} \boldsymbol{\sigma}, \tag{10}$$

where Γ_σ, $\Gamma_{p\sigma}$, Γ_p - kinetic coefficients.

With the use of a coaxiality hypothesis of $\boldsymbol{\sigma}$ and $\mathbf{p}$, for a thermodynamic force $(\boldsymbol{\sigma} - \frac{\partial F}{\partial \mathbf{p}})$ we can write the following expression:

$$\boldsymbol{\sigma} - \frac{\partial F}{\partial \mathbf{p}} = \left[\frac{1}{\delta} \left(\frac{\boldsymbol{\sigma}}{2G\sigma_c} + \frac{\mathbf{p}}{p_c} \right) - \left(f\left(\frac{|p|}{p_c} \right) \frac{p_c}{|p|} + 1 \right) \frac{\mathbf{p}}{p_c} \right], \tag{11}$$

where σ_c, p_c - scale factors, $|p|$ - intensity of the $\mathbf{p}$ tensor, $\delta = L^3_n / L^3_c$ - 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:

$$f\left(\frac{|p|}{p_c} \right) = k \left(\frac{|p|}{p_c} \right)^a, \; k = const, \tag{12}$$

where k is a scaling factor, a is an exponent.

Kinetic coefficients can be represented in the form:

$$\Gamma_\sigma = \frac{1}{\tau_\sigma} \frac{1}{1 + Exp\left(-\frac{|\sigma| - S_c}{a_1} \right)}, \tag{13}$$

$$\Gamma_p = \frac{1}{\tau_p} \frac{1}{1 + Exp\left(-\frac{H(|\sigma|, |p|, \delta, p_c, \sigma_c) - S_y}{a_2} \right)}, \tag{14}$$

$$\Gamma_{p\sigma} = \frac{1}{\tau_{p\sigma}}, \tag{15}$$

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

$$H(|\sigma|,|p|,\delta,p_c)=|\sigma|-2G\sigma_c\left[\delta(f+1)|p|p_c-|p|p_c\right]. \tag{16}$$

So, the closed system of equations describing the cyclic deformation process consists of (4)-(6), (9)-(12) and kinetic coefficients (13)-(15).

The first thermodynamic law can be written as:

$$\nabla\cdot\mathbf{q}+r+\dot{Q}_e+\dot{Q}_p=-\rho c\dot{T}, \tag{17}$$

where $\dot{Q}_e=T\dfrac{\partial\tilde{\sigma}}{\partial T}:\dot{\tilde{\varepsilon}}^e$ - heat source connected with the thermo elastic effect, $c=T\dfrac{\partial^2 F}{\partial T^2}$ - specific heat, $\dot{Q}_p=\boldsymbol{\sigma}:\left(\dot{\boldsymbol{\varepsilon}}^p+\dot{\mathbf{p}}\right)-\dfrac{\partial F}{\partial\mathbf{p}}:\dot{\mathbf{p}}$ - inelastic contribution to the heat generation in isothermal case.

The plastic strain work rate can be introduced as:

$$\dot{W}^p=\boldsymbol{\sigma}:\left(\dot{\boldsymbol{\varepsilon}}^p+\dot{\mathbf{p}}\right). \tag{18}$$

So, the dissipation energy rate β can be written as [6]

$$\beta=\frac{\dot{Q}^p}{\dot{W}^p}=1-\frac{\dfrac{\partial F}{\partial\mathbf{p}}:\dot{\mathbf{p}}}{\boldsymbol{\sigma}:(\dot{\boldsymbol{\varepsilon}}^p+\dot{\mathbf{p}})}. \tag{19}$$

The $1-\beta$ parameter is the energy storage rate and the investigation subject of this work.

3 NUMERICAL RESULTS

There were modeled a quasistatic loading of a steel specimen under strain rate $\dot{\varepsilon}=4.3\cdot10^{-3}c^{-1}$ and armco iron specimen under strain rate $\dot{\varepsilon}=2\cdot10^{-3}c^{-1}$. Numerical simulation of the considered process was carried out in the finite element package Simulia Abaqus 6.13 which was run under academic license. All using modulus have licenses. Fig. 1 shows the finite-element mesh of the specimen. Eight-node linear brick elements were used for the simulation. The above explained model was applied for the material behavior description using the subroutine UMAT. Arrays of material constants, strain, strain increments and the time step passed as input data to the procedure. Increments of the stress tensor components and increments of the defect density tensor components are determined from the system of constitutive equations. Values of these components at the next time step are defined as the sum of the values on the previous step and the appropriate increment.

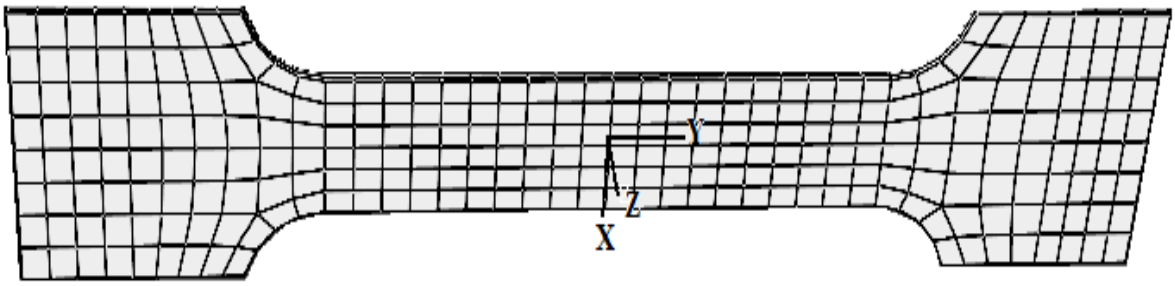

Figure 1: Finite-element mesh of the specimen

Figure 2 presents experimental and numerical stress-strain curves for AISI 304-L steel tension. Theoretical results have good agreement with the experimental data.

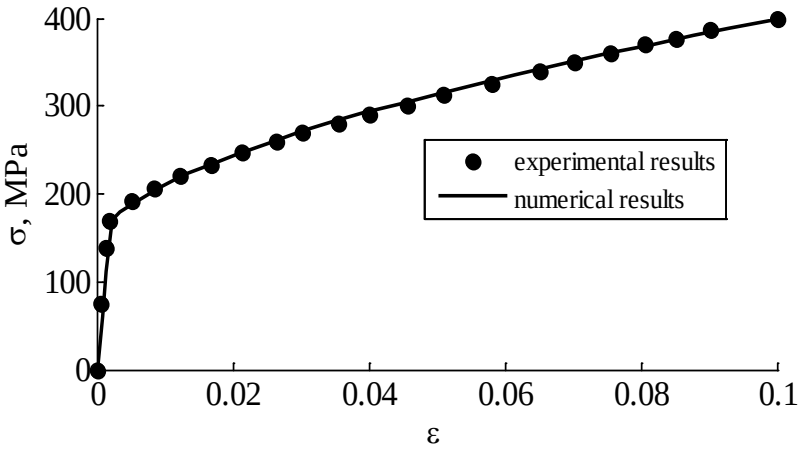

Figure 2: Stress-strain curve for AISI 304-L steel

The three-dimensional results of the considered process simulation are presented in figures 3 (steel specimen) and 4 (armco iron specimen). Almost uniform distribution of the (1-β) parameter in the gauge part is observed in both cases.

Figure 3: Simulation results of the energy storage rate for a steel

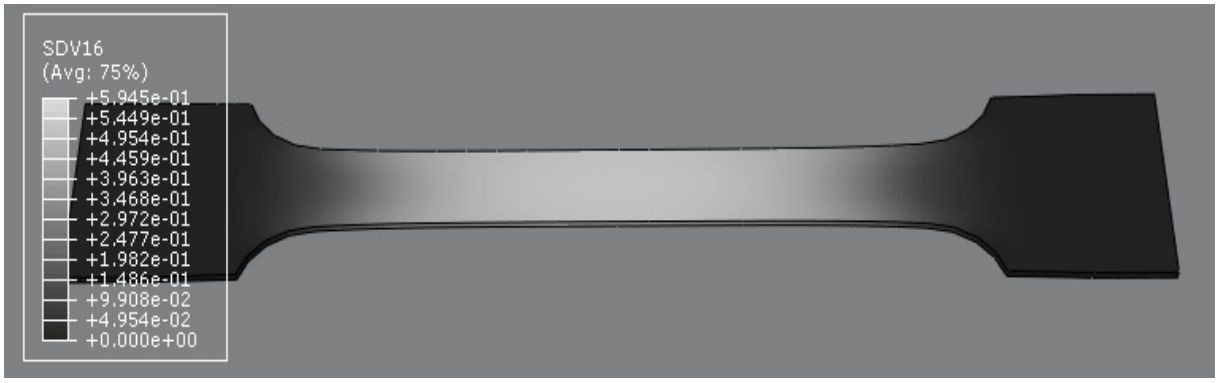

Figure 4: Simulation results of the energy storage rate for an armco iron

The modeling results of the energy storage rate evolution for the steel specimen are shown in figure 5. This dependence has a maximum which agrees with the experimental data [7]. According to the structural investigations, on the initial stage of a plastic deformation there is observed a preparation of the material structure associated with the initiation of new structural defects. This leads to a growth of the energy storage rate. When a strain reaches some level, the dominant processes are growth, movement and annihilation of structural defects that leads to a growth of a dissipated energy portion.

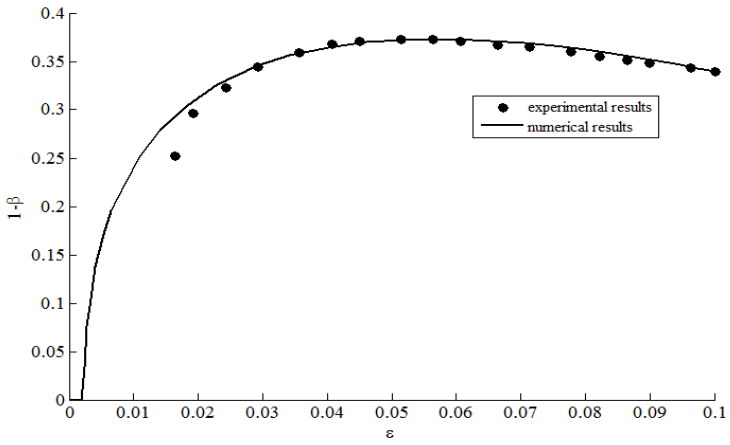

Figure 5: Value of the 1-β parameter (steel) versus strain. Numerical and experimental results

Figure 6 (a) illustrates the connection between the experimental dependence of the energy storage rate and strain hardening rate $d\sigma / d\varepsilon$. It can be seen that after energy storage rate reaches its maximum value, the strain hardening rate reaches a constant value (it is observed a transition from parabolic to linear hardening). This is confirmed by the numerical simulation results (fig. 6 (b)).

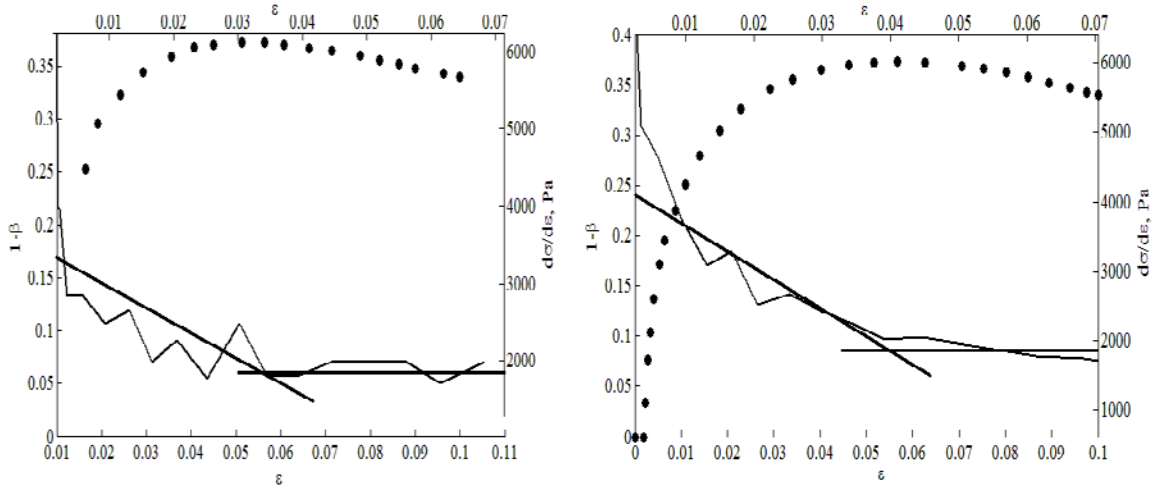

Figure 6: Experimental dependences of the energy storage rate (points) and strain hardening rate (solid line) versus strain (experimental data (a), simulation results (b))

Fig. 7 demonstrates the simulation results of the $1-\beta$ parameter for an armco iron specimen. The modeling results coincide to the experimental on the homogeneous stage of the plastic deformation.

The numerical results exhibit increasing branch of the energy storage rate and coincide to the experimental results after some deformation value. This fact can be explained by the initial conditions for the structural sensitive parameters of the model defined in the simulation process. The initial condition corresponds to the annealed materials with zero defect induced deformation. At the beginning of deformation process this material exhibits increasing rate of stored energy ratio corresponding to the increasing of the defect density [8]. In contrast to this, the experimental result corresponds to initially deformed material which has created effective defect structure for the dissipation of deformation energy.

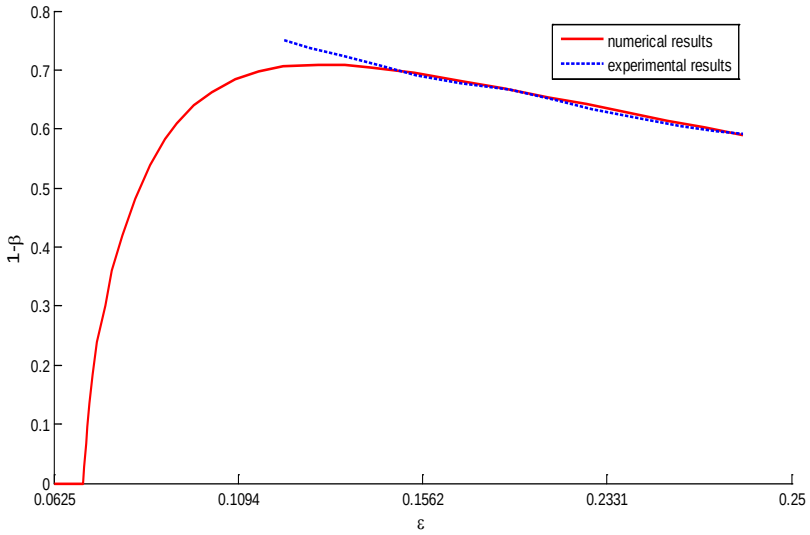

Figure 7: Value of the 1-β parameter (Armco iron) versus strain. Numerical and experimental results

4 CONCLUSIONS

This work is devoted to the numerical simulation of the storage energy process in metals under plastic deformation. Based on the above explained model there were considered numerical tensile quasistatic experiments of 316L steel and Armco iron specimens. This model let us to describe the stress-strain state of the material and to evaluate the values of stored energy rate $(1-\beta)$. On the initial stage of the plastic deformation the storage energy rate increases reaching its maximum value, that is equivalent to the defect density increase in the material. On the final stage of the plastic deformation the energy storage rate decreases. This can be connected with a predominance of dissipative processes. The obtaining results are in a quantitative agreement with the experimental.

The obtaining data analysis allows to connect energy storage process with a strain hardening. The initial stage of parabolic hardening corresponds to the energy storage rate growth which is accompained by the increase of the structural parameter. From the physical poin of view, this coreesponds to an increase of the dislocation density in grain boundaries and within them as well as intensive energy storage in the material. A decresing part of the curve is connected with dissipated processes predominance in the material structure. This is described within the model as the predominance of the plastic deformation over structural deformation.

ACKNOLEGMENTS

This work was supported by RFBR grant 12-01-33072 and 14-01-00122.

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