Stochastic simulation of the micro-meso transition in the evolution process of defective structure in loaded high-strength material

A N Nasonov and V P Baranov
Department of Applied Mathematics and Computer Science, Tula State University, Tula, 92 Lenin Avenue, 300012, Russia
E-mail: anton.nasonov3@gmail.com, baranov_1955@mail.ru

Abstract. Based on synergetic principles and statistical approach, mathematical modeling of the micro-meso transition in microdefects accumulation process in loaded high-strength material has been performed. The stochastic model of submicrocracks system evolution in the material at micro level has been constructed. The computational experiment has been performed for the case of uniaxial plastic deformation of structural steel 30HGS. Calculated submicrocracks density curves for different degree of the system non-additivity, characterizing the material structure ordering degree, have been presented and analyzed.

A system of a large number of objects is complex if its behavior can change radically with an arbitrarily small external impact on it. A key feature of a complex system is that each object that composes it behaves randomly. Thus, complete picture of a complex system behavior is stochastic. The set of microdefects in a loaded high-strength material at initial stage of its deformation is a complex non-additive synergetic system. Non-additivity means that the system entropy is not equal to the sum of entropies of its parts. The evolution of such synergetic systems depends on processes that cannot be predicted with absolute accuracy. But they can be taken into account when modeling the system behavior, if we introduce “fluctuating forces” – fluctuations. Fluctuations play a special role in formation of complex synergetic system behavior. In a real system, in addition to external environment fluctuation action, which sets multiplicative noise, there are always internal fluctuations caused by processes occurring in the system itself. So, random fluctuations are the main reason of self-organization [1].

Let us consider a non-additive synergetic system in the form of statistical ensemble of particles, the evolution of behavior of which satisfies self-organization principles. In order to the particles system to be capable of presenting self-organized behaviour, according to the Ruelle-Takens theorem [2], the presence of at least three independent equal parameters is necessary. Collective behavior of the particles system is described by the order parameter, entropy is described by the conjugate field parameter, and external action is described by the control parameter. The analysis of experimental results of research of plastic deformation structural levels and fracture of high-strength steels under static loading [3] allows us to choose submicrocracks with sizes of 0.1–0.3 μm as such particles. The kinetics of steels delayed fracture was studied using stress relaxation curves. The procedure was developed [4–5] for determining the time dependence of submicroscopic defects density, based on
using of the machine relaxation curve initial part of the stress applied to the sample, assuming that at the early deformation stages at ordinary temperatures, submicroscopic discontinuities have a maximum concentration and the condition that the specific plastic deformation work to change the free energy density of the sample.

In the model of evolution of submicrocracks synergetic system at micro level in a loaded high-strength material during its deformation, the order parameter is the submicrocracks density in representative volume of the material, the conjugate field parameter is entropy, and the control parameter is an external stress.

Consider the nonlinear stochastic differential equation

$$\dot{p} = \frac{\partial F(p, \sigma)}{\partial p} + \omega p^a \xi,$$

where \( p = p(t) \) is the submicrocracks density in representative volume of the material, \( \text{cm}^{-3} \); \( \sigma = \sigma(t) \) is the external stress, MPa; \( F = F(p, \sigma) \) is the synergetic potential of the system, J; \( \xi = \xi(t) \) is the stochastic noise; \( \omega p^a, \ a \in [0,1] \) is the noise amplitude. The stochastic noise function \( \xi(t) \) represents medium fluctuation destructive effect, structural heterogeneity of the material and internal fluctuations caused by deformation and fracture processes. The noise amplitude under an assumption of self-similarity of phase space has a power-law form. The power \( a \) reflects fluctuations type in the system: if \( a = 0 \) the type is additive noise, if \( a = 1/2 \) the type is directed percolation fluctuations, if \( a = 1 \) the type is population dynamics fluctuations [2].

The sought bounded solutions of the equation (1) tend to attractors \( \tilde{p} \), which are defined by the stochastic differential equation

$$\frac{\partial F(\tilde{p}, \sigma)}{\partial p} + \omega p^a \xi = 0.$$

The solutions \( \tilde{p}_1(\tilde{\sigma}), \tilde{p}_2(\tilde{\sigma}), ..., \tilde{p}_n(\tilde{\sigma}) \), which satisfy the equation (2) at a given value \( \tilde{\sigma} \), are named critical points of synergetic system [6]. Let us state that the system control parameter \( \sigma \) changes much more slowly than the system order parameter \( p \). Then the trajectories \( p(t, \tilde{\sigma}) \) tend to one of their attractors \( \tilde{p}(\tilde{\sigma}) \).

The key issue in constructing the evolution model of the synergetic system is a determination of the system synergetic potential \( F(p, \sigma) \), whose change is due to the order parameter evolution in the field of external forces. In our case, the material free energy is the synergetic potential. Its change is associated with the kinetics of the submicrocracks density in the deformation process. To represent the free energy we use the famous equation [7]

$$F = E - TS,$$

where \( E = E(t) \) is the system internal energy, \( T \) is the absolute temperature, \( S = S(t) \) is the system entropy.

Let us consider the internal energy of the material:

$$E = \varepsilon \sigma p,$$

where \( \varepsilon \) is the energy of one submicrocrack formation, J.

It is well known that the Boltzmann entropy describes only the behavior of simple synergetic systems. Therefore it must be deformed for the statistical description of complex systems, i.e. we must use the generalized Boltzmann formula, depending on the deformation parameter. As deformed entropy, we use the Tsallis entropy [8]

$$S = \ln_q W_q,$$

where \( W_q \) is the statistical integral of the following form.
and \( k \) is the Boltzmann constant. The Tsallis entropy is expressed by using functions of the deformed logarithm and the deformed exponent of Tsallis, which are defined as follows [8]

\[
\ln_q(x) = \frac{x^{1-q} - 1}{1-q},
\]

\[
\exp_q(x) = \left[1 + (1-q)x\right]^{\frac{1}{1-q}},
\]

where \( q \in (0,1] \) is the deformation parameter expressing a non-additivity degree of the system. The non-additivity degree characterizes the material structure ordering degree. If \( q \neq 1 \) then the Tsallis entropy is a nonadditive quantity. If \( q \to 0 \) then the system non-additivity increases. Non-additive character of the Tsallis entropy is its important feature, which allows it to be used to describe the behavior of non-additive synergetic systems.

Now we transform the entropy expression (3) by using the formulas (4), (5) and we have

\[
\exp_q\left(\frac{\varepsilon\sigma p}{kT}\right) = \left[1 + (1-q)\left(\frac{\varepsilon\sigma p}{kT}\right)\right]^{\frac{1}{1-q}},
\]

\[
S = \ln_q \int \left[1 + \frac{1-q}{kT} \varepsilon\sigma(\tau) p(\tau)\right]^{\frac{1}{1-q}} d\tau = \frac{1}{1-q} \left[\int_0^1 \left[1 + \frac{1-q}{kT} \varepsilon\sigma(\tau) p(\tau)\right]^{\frac{1}{1-q}} d\tau\right]^{1-q} - 1.
\]

Thus, the free energy of the material takes the form

\[
F = \varepsilon\sigma p - \frac{T}{1-q} \left[\int_0^1 \left[1 + \frac{1-q}{kT} \varepsilon\sigma(\tau) p(\tau)\right]^{\frac{1}{1-q}} d\tau\right]^{1-q} + \frac{T}{1-q}.
\]  

(6)

In order to express a partial derivative \( \frac{\partial F}{\partial p} \), we differentiate the left and right sides of the expression (6) with respect to \( t \), considering that \( F = F(p), p = p(t) \), and the integral is differentiable with respect to the upper limit.

\[
\frac{\partial F}{\partial p} = \varepsilon\sigma \frac{\partial\hat{p}}{\partial p} - \frac{T}{\hat{p}} \left[1 + \frac{1-q}{kT} \varepsilon\sigma(t) p(t)\right]^{\frac{1}{1-q}} \left[\int_0^1 \left[1 + \frac{1-q}{kT} \varepsilon\sigma(\tau) p(\tau)\right]^{\frac{1}{1-q}} d\tau\right]^{1-q},
\]

\[
\frac{\partial F}{\partial p} = \varepsilon\sigma \frac{\partial\hat{p}}{\partial p} - \frac{T}{\hat{p}} \left[1 + \frac{1-q}{kT} \varepsilon\sigma(t) p(t)\right]^{\frac{1}{1-q}} \left[\int_0^1 \left[1 + \frac{1-q}{kT} \varepsilon\sigma(\tau) p(\tau)\right]^{\frac{1}{1-q}} d\tau\right]^{1-q}.
\]  

(7)

Put the expression (7) in the original equation (1):

\[
\hat{p} = -\varepsilon\sigma + \frac{T\rho}{\hat{p}} \left[1 + \frac{1-q}{kT} \varepsilon\sigma p\right]^{\frac{1}{1-q}} \left[\int_0^1 \left[1 + \frac{1-q}{kT} \varepsilon\sigma(\tau) p(\tau)\right]^{\frac{1}{1-q}} d\tau\right]^{1-q} + \omega p^2 \xi,
\]

\[
\hat{p} = -\varepsilon\sigma + \frac{T\rho}{\hat{p}} A_q(p,t) + \omega p^2 \xi,
\]  

(8)

where \( A_q(p,t) = \left[1 + \frac{1-q}{kT} \varepsilon\sigma p\right]^{\frac{1}{1-q}} \left[\int_0^1 \left[1 + \frac{1-q}{kT} \varepsilon\sigma(\tau) p(\tau)\right]^{\frac{1}{1-q}} d\tau\right]^{1-q} \).

Next, we transform the equation (8), omitting the linear stochastic term

\[
(\hat{p})^2 = -\varepsilon\sigma \hat{p} + T\rho A_q(p,t),
\]
\[(\dot{q})^2 + \varepsilon \sigma \dot{q} - T \rho A_q(p,t) = 0.\]  

(9)

Now we have the quadratic equation (9) with respect to \( \dot{q} \). We solve it by using the discriminant:

\[
a = 1, \quad b = \varepsilon \sigma \rho, \quad c = -T \rho A_q(p,t),
\]

\[
D = b^2 - 4ac = (\varepsilon \sigma \rho)^2 + 4T \rho A_q(p,t).
\]

Then we get the nonlinear differential equation with respect to \( p \):

\[
\dot{p} = \frac{1}{2} \left\{ (\varepsilon \sigma p)^2 + 4T \rho \left[ 1 + \frac{1 - q}{kT} \varepsilon \sigma p \right] \left[ \int_0^t \left( 1 + \frac{1 - q}{kT} \varepsilon \sigma(\tau) p(\tau) \right)^{\gamma(1-q)} \, d\tau \right] \right\}^{\gamma(1-q)}.
\]

The final equation for modeling the submicrocracks system evolution at micro level is the stochastic Langevin differential equation with multiplicative noise [9] with respect to the order parameter and it has the following form

\[
\dot{p} = -\frac{\varepsilon \sigma p}{2} + \frac{1}{2} \left( (\varepsilon \sigma p)^2 + 4T \rho \left[ 1 + \frac{1 - q}{kT} \varepsilon \sigma p \right] \left[ \int_0^t \left( 1 + \frac{1 - q}{kT} \varepsilon \sigma(\tau) p(\tau) \right)^{\gamma(1-q)} \, d\tau \right] \right) + \omega p^a \xi. \tag{10}
\]

And according to the equation (2), the bounded solutions of the equation (10) tend to the attractors \( \tilde{p} \), which are defined by the following equation

\[
\dot{\tilde{p}} = -\frac{T}{\varepsilon \sigma} \left( 1 + \frac{1 - q}{kT} \varepsilon \sigma p \right)^{\gamma(1-q)} \left[ \int_0^t \left( 1 + \frac{1 - q}{kT} \varepsilon \sigma(\tau) p(\tau) \right)^{\gamma(1-q)} \, d\tau \right] + \omega p^a \tilde{\xi}. \tag{11}
\]

The equation (11) is the nonlinear stochastic differential equation with multiplicative noise.

Computational experiment to simulate the micro-meso transition in the process of non-additive submicrocracks synergetic system evolution has been performed. The experiment was performed on the example of uniaxial plastic deformation of structural steel 30HGSА by using the initial part of the stress relaxation curve, which corresponds to the deformation process at micro level [10]. To obtain a numerical solution to the equation (11), we used the Milstein method [9], which is a numerical method for solving stochastic differential equations. The solution was found by using the following iterative scheme.

\[
\tilde{p}_{k+1} = \tilde{p}_k - \frac{T}{\varepsilon \sigma} A_q(\tilde{p}_k, t_k) \Delta t_k + \omega \tilde{p}_k^a \Delta \tilde{W}_k + \frac{1}{2} a \sigma^2 \tilde{p}_k^{2a-1} \left( \Delta \tilde{W}_k^2 - \Delta t_k \right),
\]

where

\[
A_q(\tilde{p}_k, t_k) = \left( 1 + \frac{1 - q}{kT} \varepsilon \sigma \tilde{p}_k \right)^{\gamma(1-q)} \left[ \int_0^t \left( 1 + \frac{1 - q}{kT} \varepsilon \sigma(\tau) \tilde{p}_k(\tau) \right)^{\gamma(1-q)} \, d\tau \right].
\]

\( \tilde{p}_k = \tilde{p}(t_k) \) is the approximate value of the sought function at given time \( t_k \), \( \Delta t_k \) is the iteration step, \( \Delta \tilde{W}_k = \tilde{W}(t_{k+1}) - \tilde{W}(t_k) \) is the increment of the Wiener process implementation, which is calculated at each iteration by using the generation of independent random numbers \( \varepsilon_k \), that follow the Gaussian distribution with a mathematical expectation equal to 0 and a dispersion equal to \( \Delta t_k \). So

\[
\Delta \tilde{W}_k = \varepsilon_k \sqrt{\Delta t_k}, \quad \text{where} \quad \varepsilon_k \sim N(0, \Delta t_k).
\]

The approximation error in the Milstein method is

\[
\forall t_k \in [t_0, t_n], \quad E[\tilde{p}(t_k) - \tilde{p}(t_k)] = O(\Delta t)
\]

and tends to zero at \( \Delta t \to 0 \).

In figure 1 the calculated dependences of submicrocracks density on the deformation time are presented for various degrees of the system non-additivity \( q \) with the following parameter values:
\( p(t_0) = 0 \text{ cm}^{-3}, \sigma = 0.8\sigma_0 = 1015 \text{ MPa}, \varepsilon = 10^{-18} \text{ J}, k = 1.38 \times 10^{-23} \text{ J/K}, T = 293 \text{ K}, \omega = 10^{-2}, a = 1/2, \Delta \varepsilon = 10^{-3} \text{ sec}. \) The parameter value \( a = 1/2 \) reflects the directed percolation fluctuations, since the submicrocracks system evolves to the formation of percolation clusters \([10]\). The deformation parameter is a constant in these calculations: \( q = \text{const} \). The fractal view of calculated curves is obtained due to the effect of continuous stochastic noise.

In figures 2, 3 the calculated dependences, for which the deformation parameter \( q \) is not a constant and tends to zero over time, are presented. This means that the submicrocracks synergetic system evolves from a more additive state to a more nonadditive one.

**Figure 1.** The submicrocracks density evolution for steel 30HGSA at \( q = \text{const} \):
(a) \( q = 0.8 \), (b) \( q = 0.4 \).

**Figure 2.** The submicrocracks density evolution for steel 30HGSA at \( q \neq \text{const} \):
(a) \( q \) changes from 0.9 to 0.8, (b) \( q \) changes from 0.9 to 0.7.
Figure 3. The submicrocracks density evolution for steel 30HGSA at \( q \neq \text{const} \):

(a) \( q \) changes from 0.4 to 0.3, (b) \( q \) changes from 0.4 to 0.2.

One can readily see in all plots that, regardless of the non-additivity degree of the submicrocracks synergetic system, the submicrocracks density reaches a stabilization level over time. Then after a short period of time, the density begins to decrease, which indicates a qualitative change in the submicrocracks system evolution at micro level – micro-meso transition. If the deformation parameter is a constant (\( q = \text{const} \)) throughout the entire process of the system evolution, then the following picture is observed (figure 1). For more non-additive systems (\( q \to 0 \)) with a low degree of the material structure ordering (high-strength steels) the system stabilization phase starts earlier, at lower values of the submicrocracks density and lasts less time. The micro-meso transition also begins earlier and the rate of decrease of the submicrocracks density, i.e. of the percolation clusters formation is higher. If the deformation parameter is not a constant (\( q \neq \text{const} \)) and tends to zero over time (\( q \to 0 \)), i.e. the system evolves from a more additive state to a more nonadditive one, then the conclusions made earlier remain true for such systems (figures. 2,3). Moreover, the greater the rate of decrease of \( q \), then the earlier the micro-meso transition begins and proceeds faster. The system stabilization phase is shorter and the transition to the percolation clusters formation often occurs spasmodically.

Thus, the constructed mathematical model of the non-additive submicrocracks synergetic system evolution at micro level and the obtained calculations allow us to simulate the micro-meso transition taking into account the influence of external and internal stochastic factors and explain mechanisms of influence of the non-additivity degree of the studied defects system on the course of the micro-meso transition in the defective structure evolution process of loaded high-strength material.

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