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# SIMULATION OF ROCK DEFORMATION BEHAVIOR

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A task of simulating the deformation behavior of geomaterials under compression with account of over-extreme branch has been addressed. The physical nature of rock properties variability as initially inhomogeneous material is explained by superposition of deformation and structural transformations of evolutionary type within open nonequilibrium systems. Due to this the description of deformation and failure of rock is related to hierarchy of instabilities within the system being far from thermodynamic equilibrium. It is generally recognized, that the energy function of the current stress-strain state is a superposition of potential component and disturbance, which includes the imperfection parameter accounting for defects not only existing in the initial state, but also appearing under load. The equation of state has been obtained by minimizing the energy function by the order parameter. The imperfection parameter is expressed through the strength deterioration, which is viewed as the internal parameter of state. The evolution of strength deterioration has been studied with the help of Fokker – Planck equation, which steady form corresponds to rock statical stressing. Here the diffusion coefficient is assumed to be constant, while the function reflecting internal sliding and loosening of the geomaterials is assumed as an antigradient of elementary integration catastrophe. Thus the equation of state is supplemented with a correlation establishing relationship between parameters of imperfection and strength deterioration. While deformation process is identified with the change of dissipative media, coupled with irreversible structural fluctuations. Theoretical studies are proven with experimental data obtained by subjecting certain rock specimens to compression.

***Key words:*** deformation, failure, stress, rocks, instability, parameters of imperfection and strength deterioration.

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**Introduction.** Following [2] we believe that the simulation of real physical and mechanical system of dynamic type shall begin with introduction of the state coordinates $\eta_1, \eta_2, ..., \eta_k$, also called the order parameters. Then additional set of parameters $T_1, T_2, ..., T_k$, simulating response to changed parameters $\eta_k$ and representing external exposures, is added thereto. Besides there shall be parameters $\beta_1, \beta_2, ..., \beta_k$, accounting for defects existing in initial state of the system and appearing after its loading.

The rocks are initially inhomogeneous materials, which in a steady state, stable with respect to small disturbances, can be interpreted as dissipative structures [3, 4]. In accordance with the known [8, 9] classification of spatial-temporal structures, the rocks at great depths may be considered as autostructures, i.e. the localized spatial formations, stably existing in non-equilibrium dissipative media and not dependent on changes in the initial or boundary conditions. That is exactly why the process of rock deformation and failure can be viewed as a hierarchy of instabilities, attributable to self-organization existing with the system being far from thermodynamic equilibrium. These considerations suggest the usefulness of employing synergistic concepts [15] to describe equilibrium and stability of rocks.

As the input data the passport dependencies [16] of maximal shear stress $T$ and the relative volumetric change $\theta$ on the maximum shift $\Gamma$ have been taken, which were derived on the basis of the well-known uniaxial compression experiments [13] (Fig.1).

The elastic segment of the deformations curve $T = T(\Gamma)$ $(T \le T_e;\ \Gamma \le \Gamma_e)$ elongates into the region of strength, which further $T \ge T_0$, $\Gamma \ge \Gamma_0$ passes into zone of strength degradation. After critical shift $\Gamma_c$ is reached, the rock gets destructed. It has been proven experimentally [12-14] that near the failure point $(T = T_0)$ the volumetric change is close to zero (the material is incompressible). Near this point the sign of volume deformation is changed. The latter means activation of dilatancy component of deformation.

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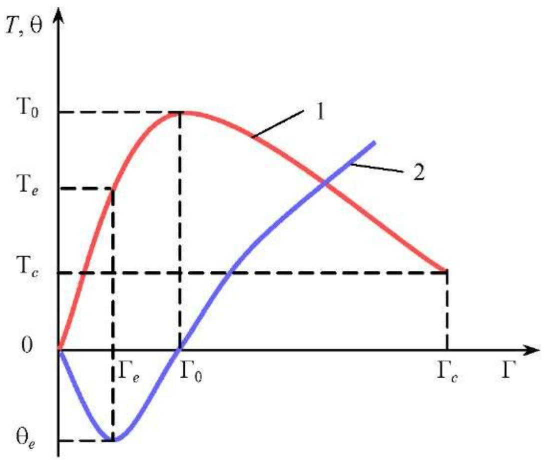


Fig.1. Graphical Representation of Passport Dependencies 1 – T = T(G); 2 – θ = θ(Γ)

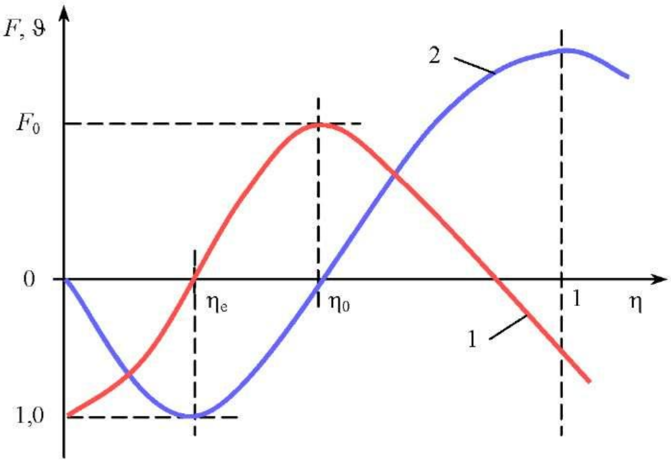


Fig.2. Rock Deformation Regularities Diagram: 1 – $F = F(\eta)$; 2 – $\vartheta = \vartheta(\eta)$

In order to describe the rock deformation regularities we introduced the coordinates normalization [5, 7].

$$F = \frac{T}{T_e} - 1;\ \eta = \frac{\Gamma}{\Gamma_c};\ \vartheta = \frac{\theta}{\theta_e}, \tag{1}$$

where $\theta_e$ is volume deformation corresponding to the elastic limit.

Based on dependencies (1) the schematic passport diagrams were built (fig.2).

**Equation of state.** Let current strain-stress state be represented by energy function [17] having the following form

$$V = V(F, \eta, \beta), \tag{2}$$

where $\beta$ is a parameter accounting for defects both existing in initial state and appearing under stress.

In the process of deformation the rocks go through several stages, which change in critical points. Thus when $\eta = \eta_e$ the process enters the plasticity stage and dissipative structure is formed, which at $\eta = \eta_0$ (over-extreme region) advances to another dissipative structure. Basically synergetic effects occur in the material under compression [8]. As in the compression experiment the rock is slowly exposed to external load, the said effects can be regarded as self-organization through control parameters $\beta$.

Let have function (2) be represented by superposition of potential $V_p(F, \eta)$, accounting for reversible processes and disturbances $S(\eta, \beta)$. Then

$$V = V(F, \eta, \beta) = V_p(F, \eta) + S(\eta, \beta).$$

The potential component of the energy function can be written down as a Taylor series expansion near equilibrium state

$$V = V_0 + V_1(\eta - \eta_e) + \frac{1}{2}V_2(\eta - \eta_e)^2 + \frac{1}{3!}V_3(\eta - \eta_e)^3 + \dots .$$

Function $V_p$ is chosen in such a manner, that $\eta = \eta_e$ corresponds to the state of equilibrium and consequently the following equation is true

$$\frac{dV_p}{d\eta} = V_1 + V_2(\eta - \eta_e) + \frac{1}{2}V_3(\eta - \eta_e)^2 + \dots = 0.$$

Thus the following condition $V_0 = V_1 = 0$ is arrived at. Assuming that change in the perfect system is related to increasing normalized stress $F \to F_0$, the potential function simulating it by shifting the origin of coordinates can be written down (Fig.2) in the form as follows

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$$V_p = \frac{1}{2}(F_0 - F)\eta^2 + \frac{1}{3}\eta^3 + \ldots$$

Let's use Morse decomposition to reflect disturbance [1]

$$S(\eta,\beta) = \beta_0\eta + \frac{1}{2}\beta_2\eta^2 + \frac{1}{3}\beta_3\eta^3 + \ldots \quad (3)$$

Relationship (3) following corresponding non-linear replacement may take a canonic form of catastrophe [2]. But such transformation leads to complex non-linear relationship between normalized strain $F$ and $\beta$ parameter. It can be shown that material sensitivity to imperfections is completely determined by the first component of decomposition (3), which allows to exclude all disturbances except for the linear one.

With account of the aforesaid, for function $V(F,\eta,\beta)$ the following equation is true

$$V(F,\eta,\beta) = \beta\eta + \frac{1}{2}(F_0 - F)\eta^2 + \frac{1}{3}\eta^3,$$

where $F_0 = F|_{\eta=\eta_0}$ (Fig.2).

Equilibrium state is reflected with the equation as follows

$$F = \frac{\beta}{\eta} + \eta + F_0, \quad (4)$$

where $\beta = \beta_1$ $(\beta < 0)$, $\eta \in (0.1)$.

Equation (4) from the standpoint of catastrophe theory can be viewed as a two-dimensional manifold, included in $\boldsymbol{R}^3$ space with coordinate axes $\eta, F, \beta$. The state of equilibrium will be found for each $\beta = \mathrm{const}$. The stability properties of critical points can be easily determined: all points to the left from $\eta = \eta_0$, $\eta \in (0,\eta_0)$ are locally stable critical points, while all points $\eta \in (\eta_0, 1)$ appear to be unstable critical points.

Thus an equation of state is derived (4), establishing relationship between the normalized maximal shear stress $F$ and shear strain$\eta$. Equation (4) includes a control parameter $\beta$, named by [2] the imperfection parameter.

**Evolution equation.** Paper [10] introduces a new concept of material strength deterioration in the process of deformation and its measure – the strength deterioration parameter. This measure $\omega$ is regarded as an internal parameter of state, which evolution is determined by a corresponding kinetic equation $\dot{\omega} = f(\omega)$, where $\dot{\omega} = d\omega/dt$; $t$ is time. It seems practicable to interrelate parameters $\beta$ and $\omega$, assuming that parameter $\omega$ represents the current structural state of the material.

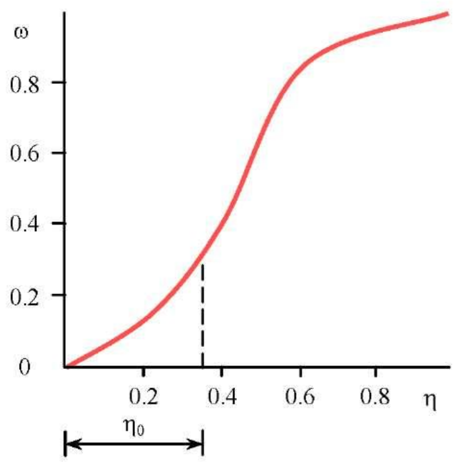


Fig.3. Graphical Representation of Strength Deterioration under Deformation

In order to analyze the physical nature of strength deterioration let's recall experiments carried out for different geomaterials in the Institute of Rock Physics and Mechanics under the National Academy of Sciences of the Kyrgyz Republic. During axial compression tests acoustic emission of specimen resulting from fracturing was registered. Figure 3 is a graphical representation of microcracking process. Here the horizontal axis shows the normalized deformation $\eta$, and the vertical axis represents the ratio of the current number of cracks in the specimen ($N$) to their maximum number ($N_{\max}$), corresponding to the moment of destruction. By identifying the strength deterioration parameter $\omega$ with $N/N_{\max}$ and analyzing its evolution, a conclusion can be made that the deformation process may be viewed as a multi-stage diffuse irreversible phase transition [11]. The graph $\omega \sim \eta$ depicts features typical

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for diffuse phase transition. It is obvious that the transition of material to the over-extreme region goes together with a change in the type of stability caused by strong structural fluctuations. That's why the presence of inflection point on the curve $\omega \sim \eta$ corresponding to the material failure point $(\eta = \eta_0)$ is entirely predictable.

It shall be noted that in the region of elastic deformations the increase of parameter $\omega$ is minor. Upon transition to plastic state $\omega$ intensive growth starts. This can be explained by the nature of residual strain of the materials that are initially heterogeneous, such as the rocks as was mentioned above. Here in addition to purely shear processes the deformation is largely contributed to by loosening, accompanied with a loss of cohesiveness and occurrence of separation surfaces [6].

Besides the localized areas where material particles get crushed are expected to appear in the strength region. Thereby within the resultant structure a brand new and more complex structure appears, transited to upon changes in the type of stability. In a new state, when strain declines with intensified deformations, the strength deterioration appears to be very rapid, and upon occurence of the main crack $\omega \to 1$.

Within the frames of nonequilibrium statistical mechanics in order to describe the rock strength deterioration a Fokker – Planck equation [1] can be used in the following form:

$$\frac{\partial \omega}{\partial t} + \frac{\partial}{\partial \eta}\left[ R(\eta) - \frac{1}{2}\lambda \frac{\partial \omega}{\partial \eta} \right] = 0. \quad (5)$$

Here $R = R(\eta)$ is the function reflecting internal sliding and loosening within the material ('drift' factor); $\lambda$ diffusion factor assumed to be constant for the rocks.

From a mechanical position the equation (5) can be regarded as an equality of change in the probability density of parameter $\omega = \omega(\eta)$ to the divergence of probability flow taken with minus sign.

Static loading of the rocks corresponds to a steady state. At the same time from (10) under certain conditions [15] we obtain

$$\lambda \frac{d\omega}{d\eta} = 2R(\eta)\omega. \quad (6)$$

Solution to equation (6), subject to [15], shall be found as follows

$$\omega(\eta) = A\exp\left( -\frac{2\Phi(\eta)}{\lambda} \right), \quad (7)$$

where integral

$$\Phi(\eta) = -\int_0^{\eta} R(\eta)d\eta \quad (8)$$

has the meaning of potential, and normalizing multiplier $A$ is determined on the basis of condition

$$\int_{-\infty}^{\infty} \omega(\eta)d\eta = 1.$$

The potential introduction explains the use of the methods of catastrophe theory for simulating the rock deformation processes with inclusion of the over-extreme branch. In such a case the process association with the gradient dynamic system [2] becomes obvious. With account of a strong non-linear dependency $\omega = \omega(\eta)$ (Fig.3), potential function $\Phi(\eta)$ and antigradient $R(\eta)$ of such function may be represented in the form of an elementary integration catastrophe. Then

$$\Phi(\eta) = \frac{a\eta^2}{2} + \frac{b\eta^4}{4}; \quad (9)$$

$$R(\eta) = -a\eta - b\eta^3,$$

where $a$, $b$ are constants to be defined.

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Now it is clear that the function of strength deterioration parameter based on (7)-(9) shall be derived from the following expression

$$\omega = A\exp\left[\frac{1}{\lambda}\left(-a\eta^2 - \frac{1}{2}b\eta^4\right)\right]. \tag{10}$$

Evolution of the strength deterioration parameter over time is reflected by the below equation

$$\frac{d\ln\omega}{dt} = -\frac{2}{\lambda}\left(a\eta + b\eta^3\right)\frac{d\eta}{dt}.$$

By inserting the result obtained in (10) into the normalizing condition and calculating the corresponding integral, we get

$$A\left(\frac{m}{2}\right)^{1/2}\sqrt{\exp\lambda}K_{1/4}(\lambda) = 1, \tag{11}$$

where $m = a/b$; $\lambda = a^2/4\lambda b = m^2 b/4\lambda$; $K_{1/4}(\lambda)$ is a modified Hankel function.

Now let's proceed to determining the parameters $A, a, b, \lambda$. For this purpose we assume that geomaterials transit into dissipative state due to the achievement of the elastic limit of $T = T_e$ (see Fig.1), and the change of the dissipative state (phase transformation) occurs at the limit of strength $T = T_0$. Let's consider that this statement is explaining the inflection point in the curve $\omega = \omega(\eta)$ (Fig.3).

Then with account of the aforesaid, $\left.\frac{d^2\omega}{d\eta^2}\right|_{\eta=\eta_0} = 0$, we arrive at

$$\frac{2b}{\lambda}\left(m\eta_0 + \eta_0^3\right)^2 - m_0 - 3\eta_0^2 = 0. \tag{12}$$

Relying on the obvious fact, in accordance with which $\omega|_{\eta=1} = 1$, we get

$$\ln\frac{1}{A} = -\frac{2b}{\lambda}\left(2m^2 + 1\right). \tag{13}$$

Thus, it has been established that three parameters of geo-environment ($A, a$ and $b/\lambda$) have a relationship expressed by equations (11)-(13).

Let's now focus on determining relationship between parameters of strength deterioration and imperfection.

Let's assume that at certain value of strength deterioration parameter $\omega = \omega_e$ imperfection parameter becomes equal to $\beta = \beta_e$, while $\omega_e$, $\beta_e$ correspond to the elastic limit of the rock. Assuming that when $\omega$ is changed by a small value $d\omega$ parameter $\beta$ responds by the value reduction proportional to $\beta$, so then

$$d\beta = -\beta K(\omega - \omega_e)d\omega, \tag{14}$$

where $K(\omega - \omega_e)$ is a kernel which decreases with increase in $\omega - \omega_e$.

Solution to differential equation (14) can be presented in the below form

$$\beta(\omega) = \beta(\omega_e)Q(\omega, \omega_e), \tag{15}$$

while

$$Q(\omega, \omega_e) = \exp\left[-\int_{\omega_e}^{\omega} K(\omega - \omega_e)d\omega\right]. \tag{16}$$

Let's take kernel of operator (14) equal to

$$K(\omega - \omega_e) = \frac{1-n}{(\omega - \omega_e)^n}, \tag{17}$$

where n is dimensionless constant.

Inserting (17) into (16), after calculation of the integral we may put down $Q(\omega,\omega_e) =$ $= \exp[-(\omega-\omega_e)^{1-n}]$. Now solution (15) to equation (14) becomes as follows

$$\beta(\omega) = \beta(\omega_e)\exp[-(\omega-\omega_e)^{1-n}], \tag{18}$$

while $\beta(\omega_e) = -\beta_e(F_0 + \eta_e)$.

Thus the model is built, which includes the equation of state (4), supplemented with condition (18), establishing relationship between parameters of imperfection and strength deterioration, with definition of four material constants *m*, *b*/2λ, *A*, *n*. This model can be used to describe deformation behavior of geomaterials up until their failure.

Without going into detail of the numerical procedure for solving the system of equations (11), (12), (13), (18), in the below table we present the values of material constants calculated for some rocks.

**Parameters of constants obtained upon solving the system of equations**

| Rock | *m* | *b*/2λ | *A* | *n* | Figure 4 |
|---|---|---|---|---|---|
| Sandstone not prone to outburst | 0.098 | 225.3 | 1.046 | – 2.64 | *a* |
| Sandstone prone to outburst | 0.131 | 99.792 | 5.525 | – 2.81 | *b* |
| Koelgin marble | 0.139 | 96.349 | 1.132 | – 3.089 | *c* |
| Biotite granite | 0.113 | 159.36 | 1.082 | – 2.17 | *d* |

**Comparison between Theoretical and Test Data** Results of experimental and theoretical studies are presented on graphs (Fig.4). Here points show experimental values of imperfection parameter β as dependent on deformation η, derived from comparing Stress – Deformation diagrams [13] and from

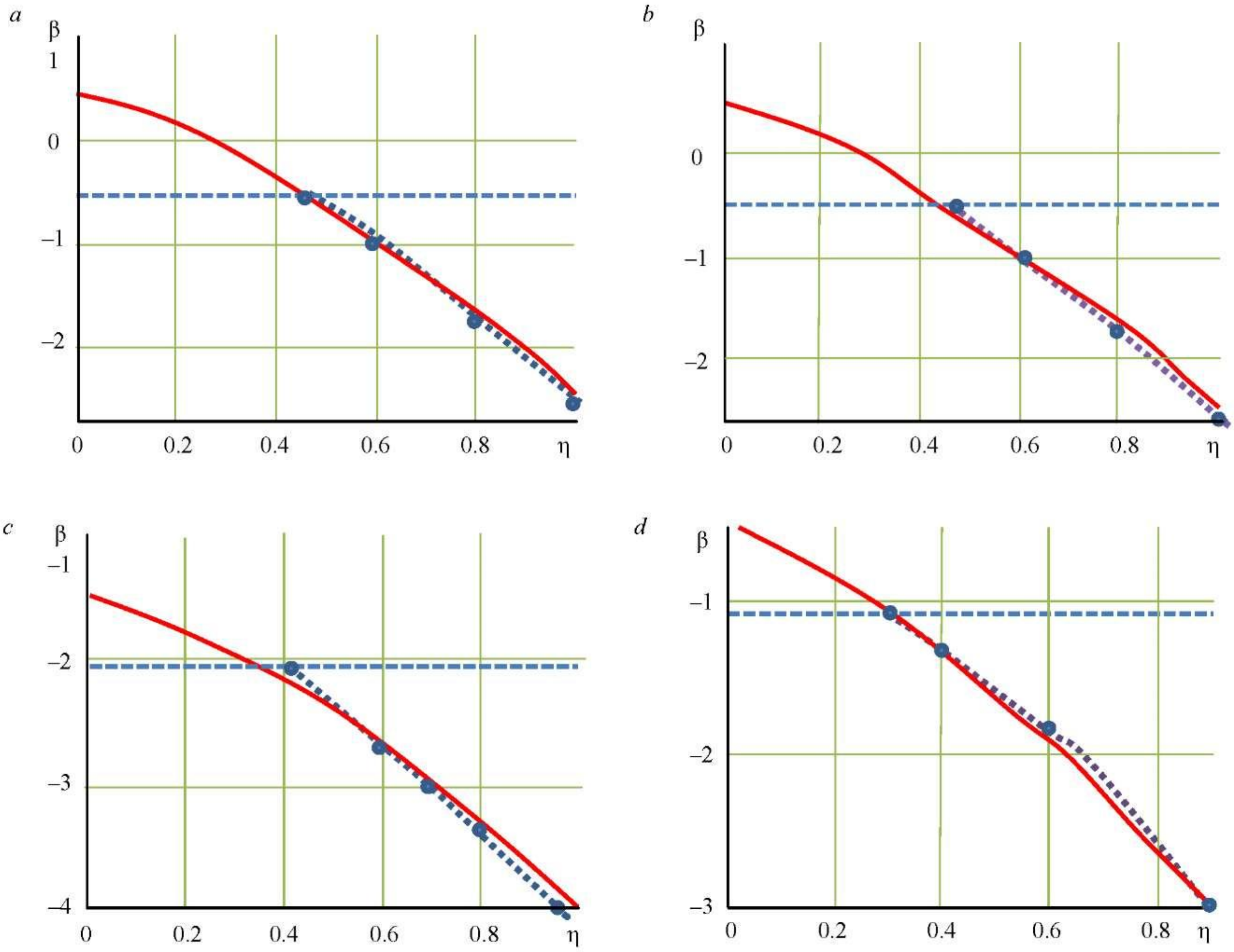


Fig.4. Comparison between experimental and theoretical data

equation of state (4). The solid lines correspond to the theoretical values of β, determined using the formula (18).

**Conclusion.** The proposed model, including the equation of state (4) and expression for imperfection parameter (18), subject to generalization for spatial case can be deemed appropriate for formulating and solving tasks involving analysis of stress-strain state of rocks within the mining and drilling fields. Strong prospects of synergy methods applying for building physically relevant non-linear constitutive relations are fully justified. This applies to the description of media, the deformation behavior of which is characterized by hierarchically irreversible change in dissipative structures [5, 18-20].

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