Nonlocal conditions for the transition from damage to a localized failure in granular composites under quasistatic loading

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Abstract. A two-level structural-phenomenological model was developed for a granular composite with random strength/deformation properties. Materials of this class include, specifically, modern ceramics and composites obtained by power metallurgy methods. The objectives of the model development were: i) to research the major regularities and the mechanisms of strain-induced damages in heterogeneous materials at the strain-softening stage; ii) to formulate nonlocal conditions for transition to a localized failure in anisotropic media. The model allowed describing inelastic quasistatic deformation and failure of heterogeneous solids, accompanied by nucleation and evolution of defects, as a multistage process of damage accumulation, and macrofailure as a result from the loss of stability of the latter process. Changing the mechanisms and scale levels of predominant damage evolution was found and analyzed numerically. New criteria for transition to a localized failure under triaxial quasistatic proportional and nonproportional macrodeformation have been formulated.

1. Introduction
The research of inelastic deformation and failure of composites is associated with the necessity to develop mechanical models for the correct description of the behavior of damaged heterogeneous materials in elements of structures and facilities [1]. When constructing the models of damage accumulation for heterogeneous media, it is necessary to describe not only nucleation and evolution of individual damages, but also the multi-particle interactions in the defect ensemble [2]. These interactions determine the conditions of macrofailure and strength characteristics of the material under loading.

Loading conditions, mechanical properties and responses to changing external mechanical actions on polymers, composites, and rocks differ widely. Notwithstanding this fact, it is possible to set aside general mechanisms of damage accumulation process and unified conditions for transition to macrofailure of the above mentioned materials, when limiting defect-concentration values are reached at a local domain. The results of experiments [3–9] showed that microcrack accumulation appears to differ essentially in those materials, but limiting defect-concentration values are very close to each other (if uniformly distributed failure domains appear). Besides, in the works under review the inference is drawn about the universality of the concentration criterion for transition from equilibrium disperse fracture to nonequilibrium macrofailure.

The results of computational experiments on uniaxial deformation and compression of a model granular composite [10, 11] indicated that the realization of the equilibrium states of the material and
sequent changes in stages of damage accumulation process are determined not only by heterogeneity of structure, mutual arrangement of defects, and its concentration. The character of the energy redistribution between a solid and a loading-system is also responsible for that.

As it is shown by experimental researches, macrofailure of a composite is due to an increasing number of cumulative defects if the void fraction of reinforcement aggregates is small or dispersion of their mechanical properties is significant [12]. Otherwise, material tends to brittle failure [13, 14]. Besides, computational experiments [11] showed that the limiting void fraction of damages is found to be significantly dependent on the dispersion of strength/deformation properties of structural elements, presence of initial imperfections, stress-strain state, and the stiffness of the loading-system as well.

It should be noted that damage accumulation process occurs uniformly within the representative volume element of composite at the initial stage of loading only. At the stages before failure, the process is of clearly pronounced localized nature. Therefore, the application of averaged limiting defect-concentration values seems impossible when defining the macrofailure. Considering that these values are functions or functionals that depend on physico-mechanical properties of the material and loading process it testifies the necessity to refine the strength concept for heterogeneous solids based on the assumption that constants of critical defect concentration exist [3–9].

Besides, there is a demand to improve strength analysis procedures that consider the real loading conditions, evolution and character of the collective interaction in the system of defects defining the macrofailure point as a result of loss of stability of damage accumulation. Without understanding major regularities and mechanisms of defect accumulation, without evaluating its stability and determining the conditions of localization beginning, the macrofracture of composites will remain latent and poorly predictable phenomenon of internal structure evolution of the material.

The mechanism of transition to localized failure can be determined from a complex experimental research of the inelastic behavior of heterogeneous materials combined with an analysis of the defect ensemble evolution. The research requires special equipment and is currently performed for the simplest loading modes only (i.e., uniaxial monotonic tension and/or compression). In regard with it, it is profitable to carry out auxiliary computing experiments with representative volume elements of the model granular composite for various triaxial stress-strain states and modes of macrodeformation.

2. Boundary-value problem

Let us consider a heterogeneous body \( \Omega \) with isotropic scleronomic components geometry, relative position, and the symmetry type of which remain unchanged during deformation and damage accumulation processes; prior to applying the load, the body is in the natural undeformed state. Let us assume that the full adhesion conditions are fulfilled on the contact boundaries of structural elements, i.e.

\[
\left[ \sigma_{ij} (r) n_j (r) \right] = \left[ \sigma_{ij} (r) n_j (r) \right]^+ \quad \text{and} \quad \left[ u_i (r) \right] = \left[ u_i (r) \right]^+.
\]

The quasistatic step-by-step loading of the body \( \Omega \) is described by the closed system of differential equations in the incremental form, i.e.

\[
d\sigma_{ij} (r) = 0, \quad d\sigma_{ij} (r) = \frac{d u_{i,j} (r)}{2}, \quad d\sigma_{ij} (r) = K' (r) d\sigma_{kk} (r) \delta_{ij} + 2 G' (r) d\sigma_{ij} (r), \quad \forall r \in \Omega,
\]

\[
K' (r) = K (r) \left[ \frac{1}{1 - \xi} \left[ j^{(1)}_e (r), j^{(2)}_e (r) \right] \right], \quad G' (r) = G (r) \left[ 1 - \xi g \left[ j^{(1)}_e (r), j^{(2)}_e (r) \right] \right].
\]

Herein, \( d u_i (r) \), \( d \sigma (r) \) and \( d \epsilon (r) \) are the increments of displacements, stresses, and strains which are random functions of the space coordinate \( r \); \( K (r) \) and \( G (r) \) are the elastic bulk and shear moduli; \( \xi = 0 \) under unloading and after loading until the elastic limit, \( \xi = 1 \) under active loading.

Constitutive equations (2) contain the independent material functions

\[
g = \begin{cases} 0, & j^{(2)}_e (r) < j^{(2)}_{ccr}, \\ 1, & j^{(2)}_e (r) \geq j^{(2)}_{ccr} \end{cases}, \quad \kappa = \begin{cases} 0, & j^{(2)}_e (r) < j^{(2)}_{ccr} \lor j^{(2)}_e (r) \geq j^{(1)}_e (r) \land j^{(1)}_e (r) \leq 0, \\ 1, & j^{(2)}_e (r) \geq j^{(2)}_{ccr} \land j^{(1)}_e (r) > 0 \end{cases}.
\]

arguments of which are independent invariants of the structural strain tensor,
\[ f_{e}^{(1)}(r) = e_{kk}(r) \quad \text{and} \quad f_{e}^{(2)}(r) = \sqrt{e_{ij}(r)e_{ij}(r)}. \]

Herein, \( d\bar{\varepsilon}_{ij} = d\varepsilon_{ij} - 1/3 d\varepsilon_{kk} \delta_{ij}. \) If the inequalities (3) are satisfied, the material functions \( \kappa \) and \( g \) take its limit values 0 or 1, change the mechanical characteristics step-like, and allow accounting the states of the total or partial loss of strength capacity of a structural element. In regard with the type of the stress-strain state the inequalities describe (the) various mechanisms of the shear damage if the condition \( f_{e}^{(2)}(r) \geq f_{e}^{(2)}(r) \) is satisfied (herein, \( f_{e}^{(2)}(r) \) is the strength constant). The complete failure of the structural element occurs if \( f_{e}^{(1)}(r) > 0 \), while when \( f_{e}^{(1)}(r) \leq 0 \) the element can still resist hydrostatic compression only.

Let us assume a macrohomogeneous continuum with effective macroproperties corresponding to a real damaged heterogeneous solids. Let us assign a representative volume element \( \Omega_{RVE} \) in the continuum, state of which will be characterized by the tensors of macrostresses \( \sigma^{*} \) and macrostrains \( \varepsilon^{*} \),

\[
\sigma^{*}_{ij} = \frac{1}{\text{mes} \Omega_{RVE}} \int_{\Omega_{RVE}} \sigma_{ij}(r) d\Omega, \quad \varepsilon^{*}_{ij} = \frac{1}{\text{mes} \Omega_{RVE}} \int_{\Omega_{RVE}} \varepsilon_{ij}(r) d\Omega. \quad (4)
\]

The resistance of representative volume element to the external loading determines the relation

\[
d\sigma^{*}_{ij} = \mathbf{N}^{ijkl}_{ijkl}(\varepsilon^{*}, \chi^{(\alpha)})d\varepsilon^{*}_{kl}. \quad (5)
\]

between the increments of macrostresses \( d\sigma^{*} \) and macrostrains \( d\varepsilon^{*} \), where \( \mathbf{N}^{ijkl}_{ijkl} \) are the material functions reflecting the effective properties of the heterogeneous material; \( \chi^{(\alpha)} \) are the parameters that define the macrodeformation process. Postulating macroisotropy and absence of deformation anisotropy during the damage accumulation, and assuming that the structure of equations (2) is unchanged at the macrolevel, we will represent the constitutive equations for \( \Omega_{RVE} \) in an invariant form \[10\]

\[
dJ^{(1)}_{\sigma} = 3K^{*} [1 - \xi^{*} \left( J_{e}^{(1)}, J_{e}^{(2)}, \chi^{(\alpha)} \right)] dJ^{(1)}_{\varepsilon}, \quad dJ^{(2)}_{\sigma} = 2G^{*} [1 - \xi^{*} \left( J_{e}^{(1)}, J_{e}^{(2)}, \chi^{(\alpha)} \right)] dJ^{(2)}_{\varepsilon}. \quad (6)
\]

Herein, \( K^{*} \) and \( G^{*} \) are the effective elastic moduli; \( J_{e}^{(1)} \) and \( J_{e}^{(2)} \) are the independent invariants of macrostress \( \sigma^{*} \) and macrostrain \( \varepsilon^{*} \) tensors. Due to the postulated macroscopic heterogeneity of the material the representative volume elements chosen around an arbitrary pair of points have the same effective properties.

The major damage accumulation mechanisms under monotonic proportional and nonproportional loading of \( \Omega_{RVE} \) will be studied on the basis of the numerical solution of boundary-value problem (1), (2) by the finite element method. The components of the macrostrain \( \varepsilon^{*} \) tensor enclosed in boundary conditions that correspond to displacement-controlled mode

\[
\left[d\varepsilon^{*}_{ij} \right]_{\partial \Omega_{RVE}} = d\varepsilon^{*}_{ij}(r), \quad \forall r \in \partial \Omega_{RVE}
\]

will be changed; and strength conditions (3) will be verified on each loading step, being determined automatically according to the developed iteration procedure \[10\]. If the strength conditions are not satisfied then, the strain constants of structural elements change. Herein, \( d\varepsilon^{*}_{ij}(r) \) are the displacements specified in every point \( r \) of the surface \( \partial \Omega_{RVE} \).

3. Structural failure as a reason to strain-softening

Let us consider some simulation results of damage accumulation process in representative volume elements of model granular composites that occupy cubic domains and contain 6 000 uniform tetrahedral elastic-brittle structural elements with random strength constants (distributed by the Weibull law) and nonrandom elastic moduli \( G(r) = 4 \cdot 10^{4}\) MPa, and \( K(r) = 6.7 \cdot 10^{4}\) MPa.

Figure 1 gives a part of the calculation stress-strain diagram for the model granular composite in an invariant form under pure shape change (i.e., \( \varepsilon_{11}^{*} = \varepsilon_{22}^{*} = -0.5 \varepsilon_{33}^{*}, \varepsilon_{33}^{*} > 0 \)); the curve does not break at
the peak maximum under displacement-controlled mode. The presence of the descending branch in the diagram indicates strain-softening. Multiple jumps and the nonlinear character of the stress-strain curve are induced by structural damage accumulation process that begins on the ascending branch and stops at the stage of residual strength.

4. Structural failure mechanisms under monotonic proportional loading

Let $\tau(r)$ be the parameter of a random strain field, and $\lambda(r)$ be the random arbitrary unit indicator function that is defined by the determinate radius-vector $r$ and takes on the value 1 if $r \in \Omega_D$, and 0 if $r \in \Omega_{RVE} \setminus \Omega_D$ ($\Omega_D$ is a set of damaged grains). Statistical expectation of the multiplication of centered functions $\tau'(r) = \tau(r) - \langle \tau(r) \rangle$ and $\lambda'(r) = \lambda(r) - \nu_D$ (herein, $\nu_D$ is the void fraction of damages) determined in different points $r$ and $r + \Delta r$ are the correlation functions of the random strain field $K^{(2)}_\tau(|\Delta r|) = \langle \tau'(r)\tau'(r+\Delta r) \rangle$ and of the damaged structure $K^{(2)}_\lambda(|\Delta r|) = \langle \lambda'(r)\lambda'(r+\Delta r) \rangle$.

The authors [16, 17] showed that the developed two-level structural-phenomenological model in combination with the correlation analysis of damage evolution allow describing the mechanisms of inelastic deformation and failure of granular composites under quasistatic loading. They studied the changes in normalized (i.e., related to the dispersions $\langle \tau(r)\tau(r) \rangle$ and $\nu_D(1-\nu_D)$) correlation functions $\tilde{K}^{(2)}_\tau$ and $\tilde{K}^{(2)}_\lambda$ during damage accumulation for various modes of proportional macrodeformation in detail.

At the initial stage of pure shape change (i.e., $\epsilon_{11}^* = \epsilon_{22}^* = -0.5\epsilon_{33}^*$, $\epsilon_{33}^* > 0$) of granular composite damages are accumulated uniformly over the whole representative volume element (state 1, Fig. 1). The normalized correlation functions $\tilde{K}^{(2)}_\lambda$ corresponding with the deformation stage are local, close to exponential ones and damp completely over the distance $(2\times3)r_h$. Hence, $r_h$ is the average heterogeneity size. The subsequent increase in macrostrains gives rise to defect growth (equilibrium states 2 and 3, Fig. 1). When the strength limit is achieved, localized failure domains (i.e., clusters into
which defects begin to coalesce) expand in the composite significantly. The intensification of multi-particle collective interaction in a defect ensemble (the functions $\tilde{K}^{(2)}_\lambda$ in the states 2 and 3 damp over the distances $(4\pm5)r_h$ and $(5\pm7)r_h$ correspondingly) leads to the appearance of a periodic term in random fields $\lambda(r)$. A uniform cluster accumulation together with the intensive stress redistribution, and partial or total unloading of undamaged grains surrounding defects, are followed by macrostress decrease that points out the beginning of strain-softening. The transition to the strain-softening associated with the beginning of individual cluster coalescence leads to even greater intensification of interaction in the defect ensemble. At the final deformation stage all damaged domains gradually coalesce into a single branching macrodefect (state 4, Fig. 1), while the functions $\tilde{K}^{(2)}_\lambda$ damp over the distances $(7\pm8)r_h$.

Hence, the normalized correlation functions defined at deformation stages make it possible to determine the character of collective multi-particle interactions in the defect ensemble and naturally separate the stages of dispersible and localized failure. Besides, the correlation analysis of the damaged structure allows the authors [16] determining changes of the stages of equilibrium and nonequilibrium failure and proving (in the framework of the model description) the self-similarity of defect evolution at the strain-softening stage for the first time.

5. **Nonlocal criterion of transition to localized failure**

If the macrofailure is considered to be the critical state, where structural transition under loading results in a loss of continuity in the damaged solids or in reaching of connectivity in the defect ensemble, we can determine parameters widely used in the physics of critical phenomena which characterize collective multi-particle interactions and the mutual arrangement of failed grains. The universal regularities in behavior of stochastic systems that close to critical point (that can be the state of failure localization onset) are the appearance of the long-range interactions in the defect ensemble, which occurs in a sharp increase of the correlation integrals [18]

$$ R_\lambda/\varepsilon = \int J^{(2)}_\lambda (|\Delta \varepsilon|) d|\Delta \varepsilon| = \int \tilde{K}^{(2)}_\lambda (|\Delta \varepsilon|) d|\Delta \varepsilon|, $$

**Figure 2. Evolution of correlation integrals for various modes of proportional macrodeformation**
for the random fields $\lambda(\mathbf{r})$ and $\tau(\mathbf{r})$. Herein, $\tau(\mathbf{r})$ is a second invariant of the microstrain tensor.

To define the conditions of start of failure localization in model granular composite, we analyze the changes in the dimensionless values of the correlation integrals $R_\lambda/r_h$ and $R_\tau/r_h$ (Fig. 2 and 3) during the process of deformation under different proportional modes and 6 trajectories as of two-segment polygonal lines. The location of their characteristic points is presented in Table 1.

Curve 7 in Fig. 3 corresponds to (with) the mode of proportional macrodeformation $\varepsilon_{11} = \varepsilon_{22} = -\varepsilon_{33}$, $\varepsilon_{33} > 0$. As damages accumulate, $R_\lambda/r_h$ and $R_\tau/r_h$ gradually increase. In Fig. 2 and 3 the points $A_k$ denote the dimensionless correlation integrals corresponding with the strength limit and the failure localization onset. Owing to the nonuniform damage resistance of the granular composite [19] and to the dependence of the failure on the deformation process, the values of the second invariant of the macrostrain tensor $J^{(2)}_\varepsilon$, which correspond with the above-mentioned points, are essentially different. The coalescence of individual damages and clusters is accompanied by the enhancement of collective interactions in the defect ensemble (the macrostrains are more and more determined by the damaged grains) and by a sharp increase of $R_\lambda/r_h$ and $R_\tau/r_h$.

Let us emphasize that the maximum difference in the values $R_\lambda/r_h$ and $R_\tau/r_h$ corresponding with the strength limit (Fig. 2) and with the failure localization onset (Fig. 3) does not exceed 7% for various modes of triaxial proportional and nonproportional macrodeformation. This behavior confirms the hypothesis (first proposed by the authors of [10, 16, 17]) about the existence of critical value of the correlation integral $R_{\lambda,cr}$, which is independent of the stress-strain state and quasistatic macrodeformation. The critical value $R_{\lambda,cr}$ is a nonlocal constant of the material which accounts the heterogeneity and character of collective multi-particle interaction in the defect ensemble under loading.

Hence, the inequality

$$R_\lambda > R_{\lambda,cr}$$

is the nonlocal criterion of transition from the stage of disperse damage accumulation to a localized failure for the damaged model granular composite, independent of the quasistatic deformation modes. The relation found for the nonlocal parameter $R_{\lambda,cr}$ and the physico-mechanical constant of material
(i.e., the strength limit) allows formulating a new criteria for transition to a localized failure and/or to the strain-softening.

Let us define a critical value of the correlation integral $R_{\lambda_{cr}}^{(\alpha)}$ for each set of structural elements of heterogeneous anisotropic solids, where these elements lost their strength capacity to resist $\alpha$ external action (i.e., transversal or antiplain shear, etc.). Then the fulfillment of the following conditions

\[ R_{\lambda}^{(m)} < R_{\lambda_{cr}}^{(m)} \]

corresponds to the strain-hardening and/or with the stage where damages are accumulated uniformly over the whole representative volume element. But should the inequalities

\[ R_{\lambda}^{(m)} \geq R_{\lambda_{cr}}^{(k)} \land R_{\lambda}^{(m)} < R_{\lambda_{cr}}^{(m)} \]

hold true for each $k \neq m$, then the next equilibrium stress-strain state of the damaged material corresponds to the state when the failure localization starts or when the strain-softening stage according to the $k$ mechanism occurs. Such problems as determining mutual influence of different mechanisms of structural damage accumulation on the transition to failure localization and to strain-softening, and also simultaneity of these transitions according to all mechanisms for anisotropic media require further investigations.

Now we should like to dwell on practical importance of the developed nonlocal criteria (8) and (9). On one hand, the values of the correlation integrals $R_{\lambda}$ defined at different stages of damage accumulation process exclude defects of some certain kind from consideration. On the other hand, they establish a unique quantitative relation between the regularities of multy-particle interactions in the defect ensemble and mechanical behavior of a model granular composite under quasistatic loading. Therefore, regardless of loading conditions, the study on a certain representative volume element allows determining the deformation stage of a damaged material and predicting the proximity of its macrofailure with the boundary-value problem, being unsolved.

6. Conclusion

The developed two-level structural-phenomenological model of granular composites made it possible to describe a collective multi-particle interaction in a defect ensemble, scale levels of damage accumulation process, major failure mechanisms, and their changes in various modes of triaxial proportional and nonproportional macrodeformation. In the framework of the model description of damage accumulation process in granular composites the nonlocal conditions for transition to a localized failure and/or to strain-softening are formulated independent on the stress-strain state and quasistatic proportional loading modes.

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